



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:33 PM JST

PDB ID : 8XNS / pdb_00008xns
EMDB ID : EMD-38513
Title : Respiratory complex Peripheral Arm of CI, close form B, focus-refined map of type IB, 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:

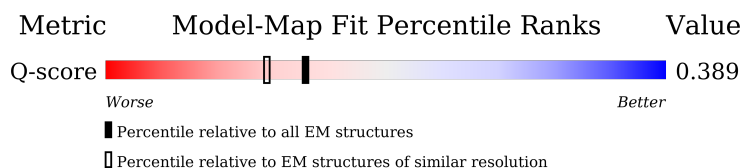
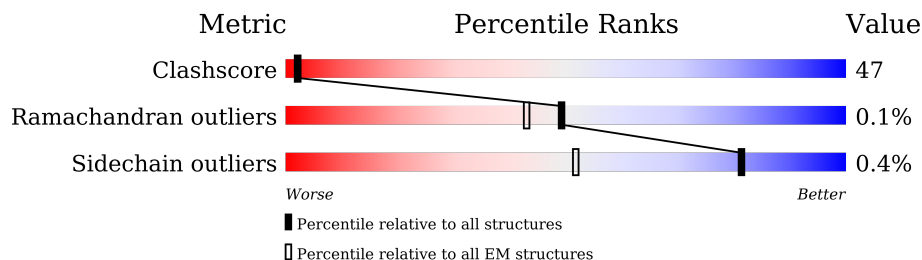
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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.



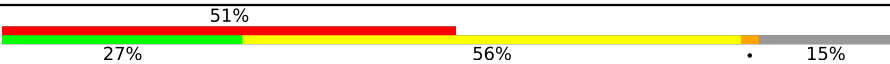
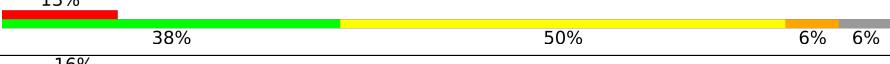
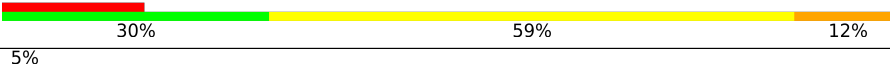
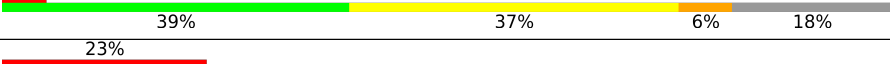
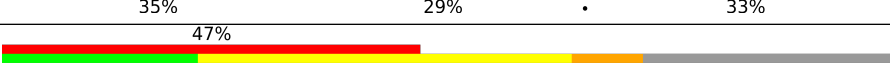
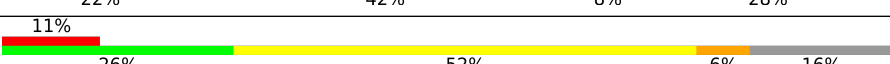
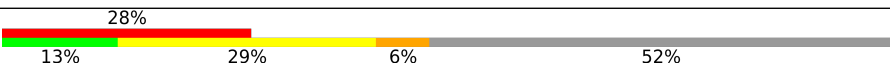
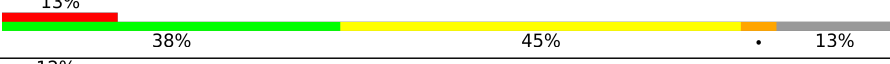
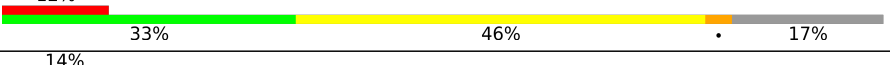
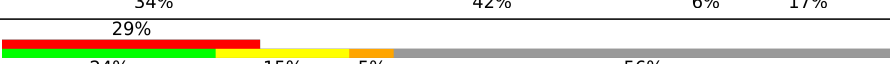
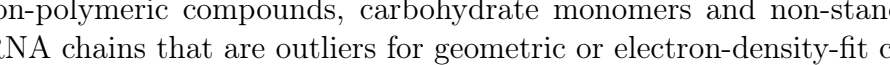
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	
2	B	224	
3	C	263	
4	D	463	

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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	301	-	-	X	-
24	SF4	I	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	UQ9	B	302	-	-	X	-
27	FES	E	301	-	-	X	-
27	FES	G	803	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 34029 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	66	Total	C	N	O	S	0	0
			540	351	96	90	3		

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

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

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

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

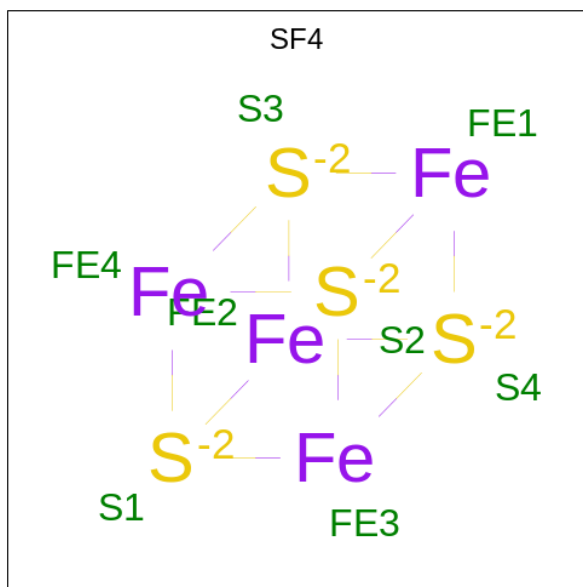
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	50	Total	C	N	O	S	0	0
			413	263	77	72	1		

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

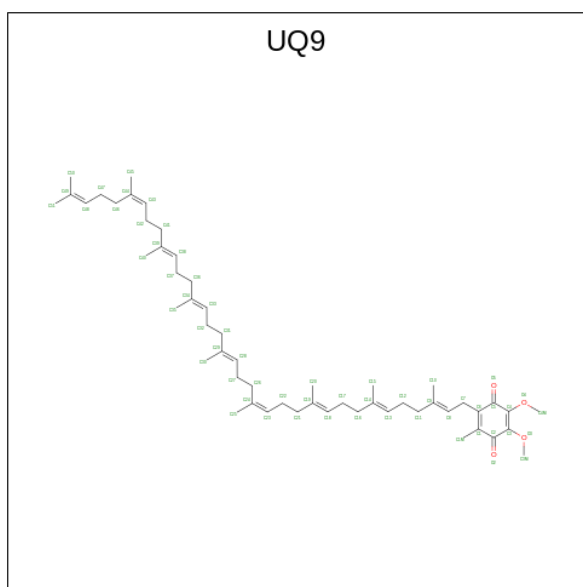
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	26	Total	C	N	O	0	0
			226	147	38	41		

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



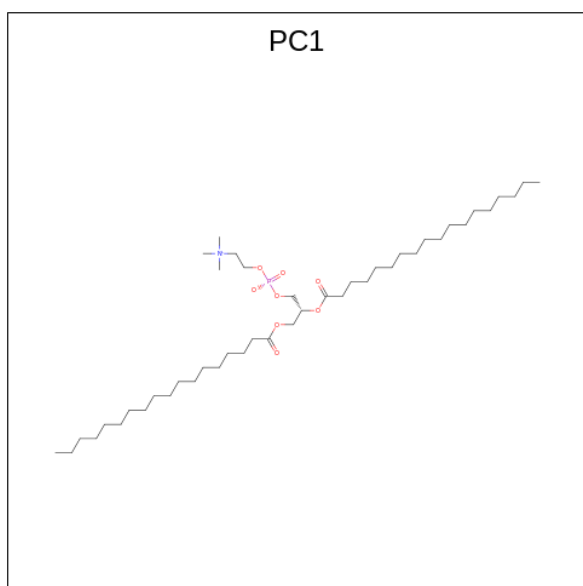
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



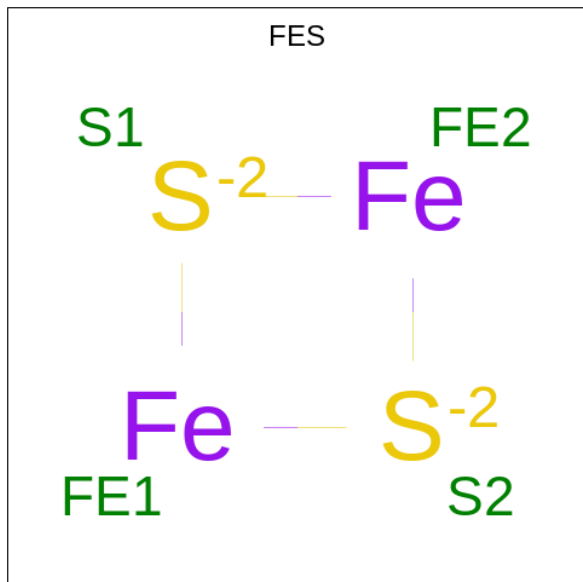
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			24	20	4	
25	H	1	Total	C	O	0
			35	31	4	

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



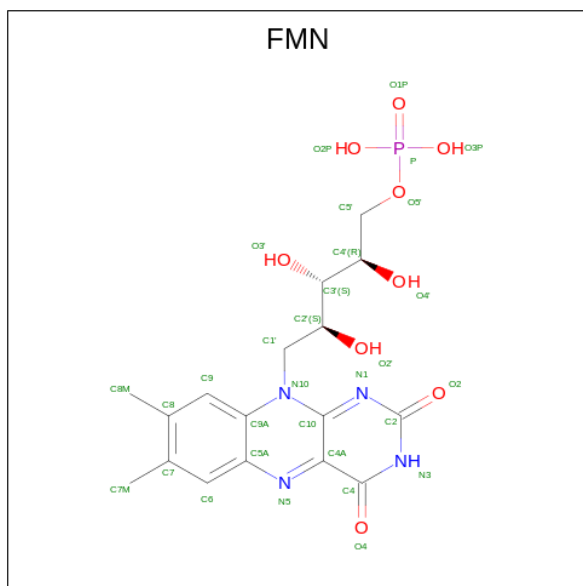
Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 27 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



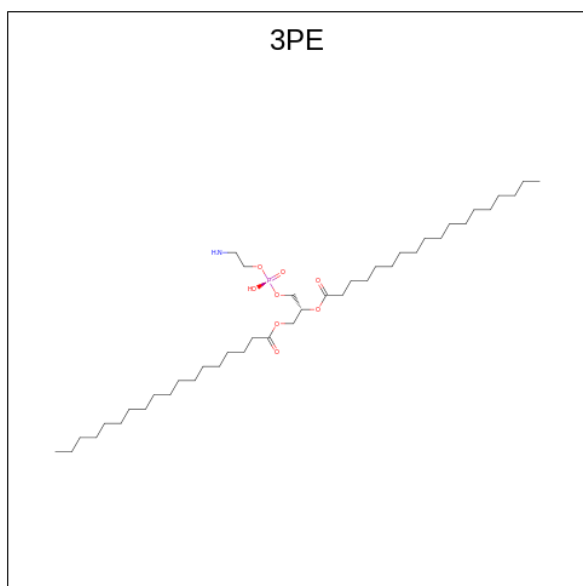
Mol	Chain	Residues	Atoms			AltConf
27	E	1	Total	Fe	S	0
			4	2	2	
27	G	1	Total	Fe	S	0
			4	2	2	

- 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).



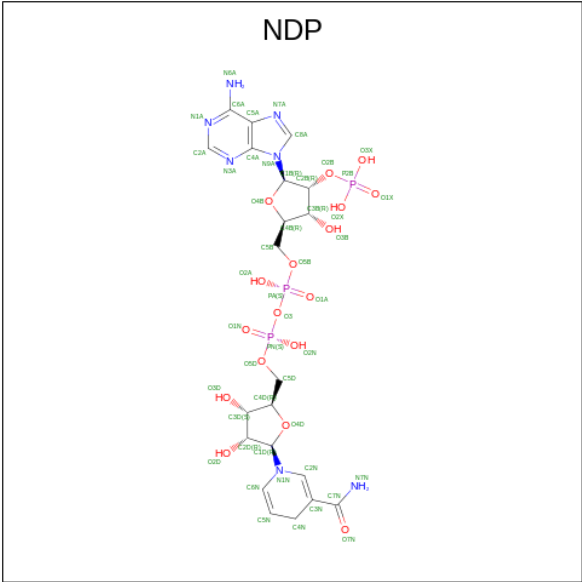
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 29 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
29	Z	1	Total	C	N	O	P	0
			46	36	1	8	1	

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

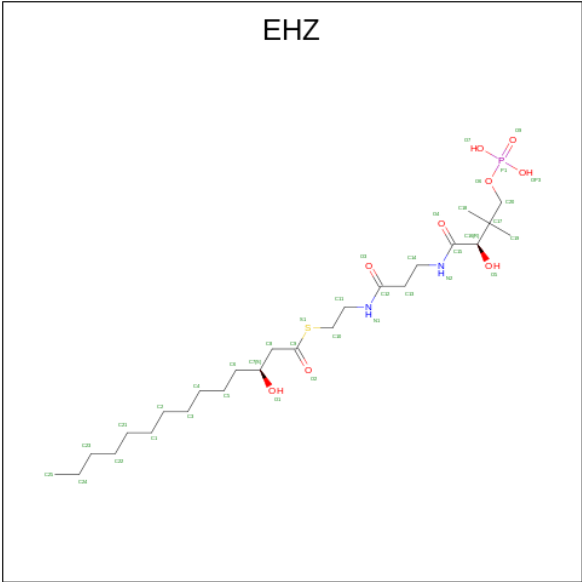


Mol	Chain	Residues	Atoms					AltConf
30	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

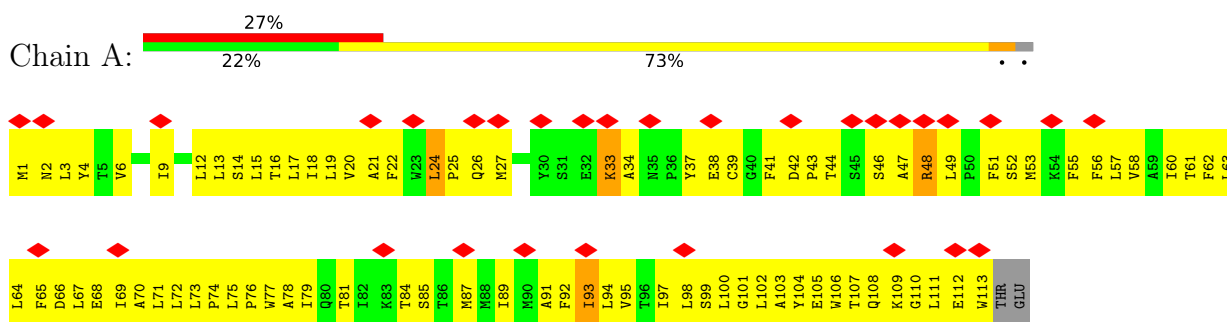


Mol	Chain	Residues	Atoms					AltConf	
32	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

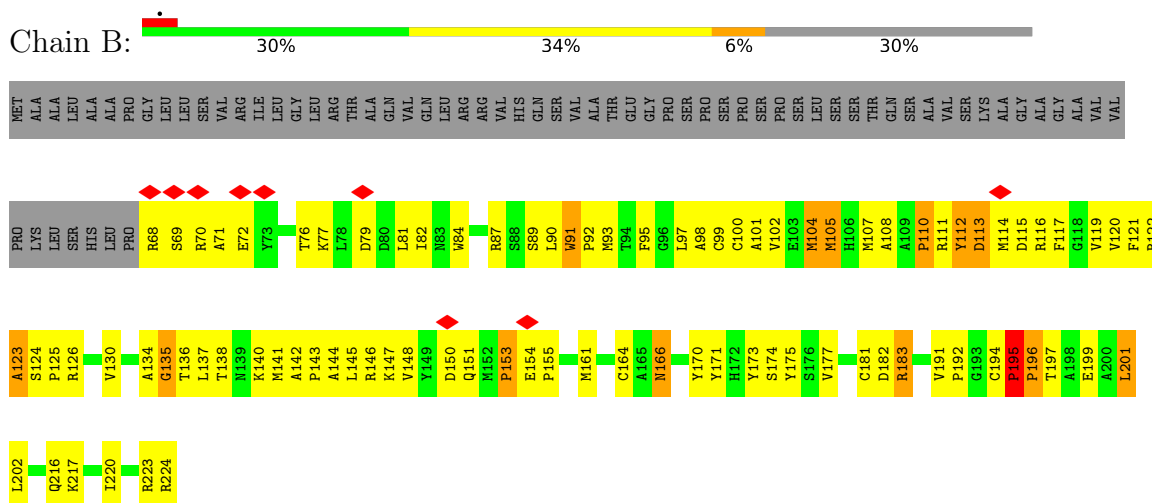
3 Residue-property plots

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.

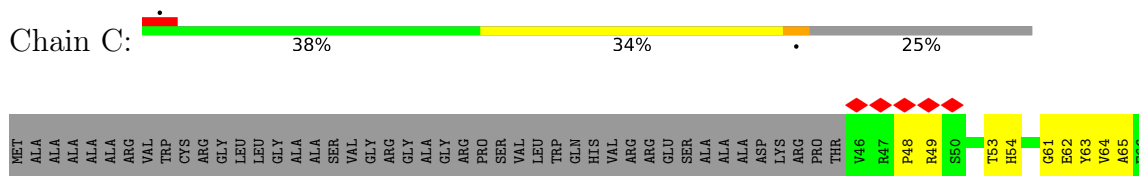
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

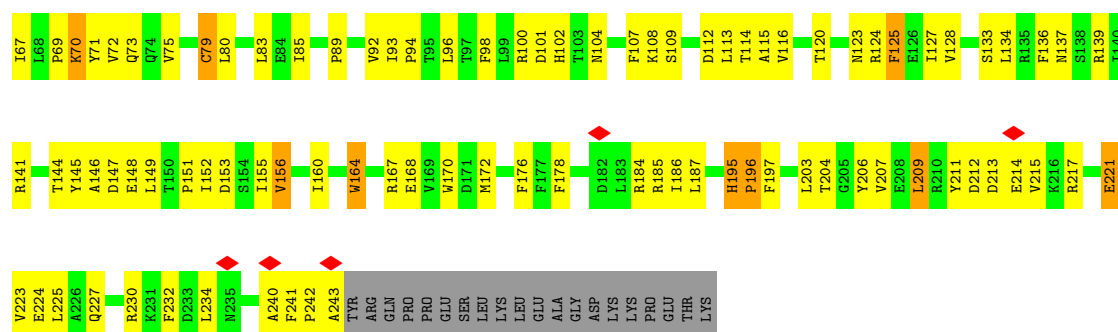


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

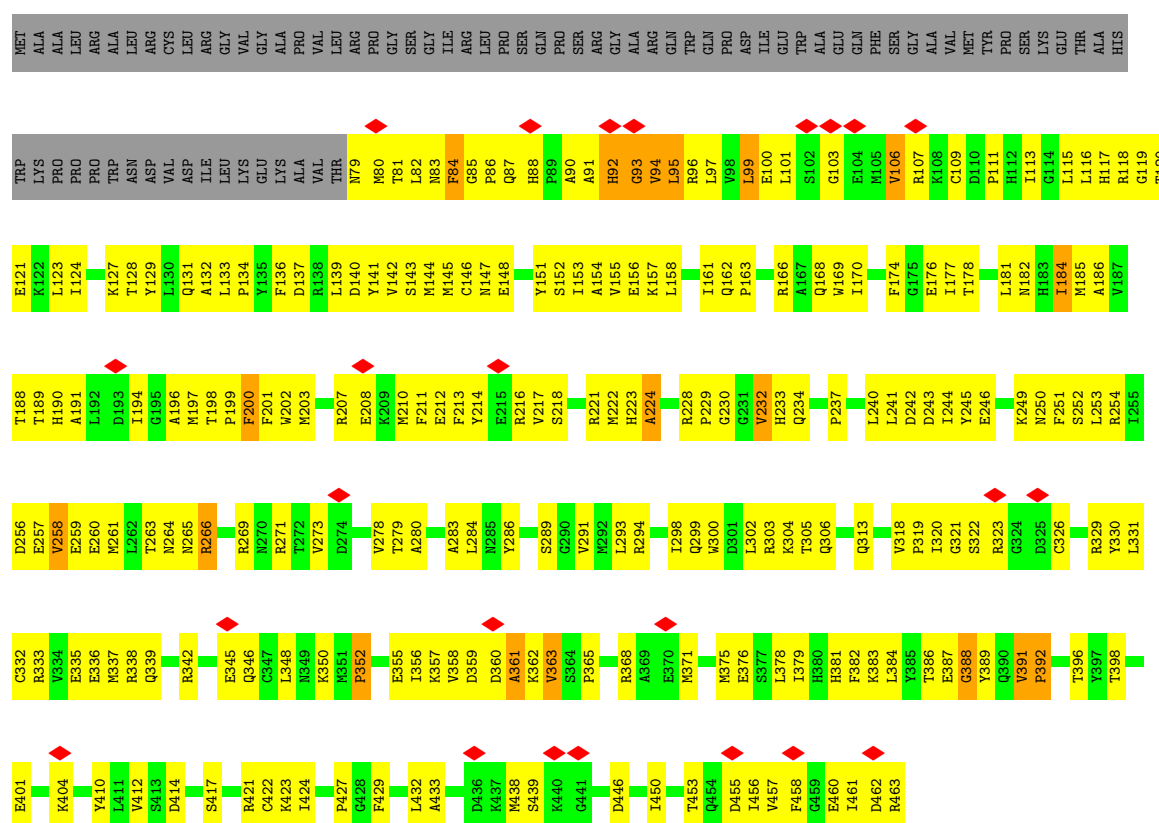


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

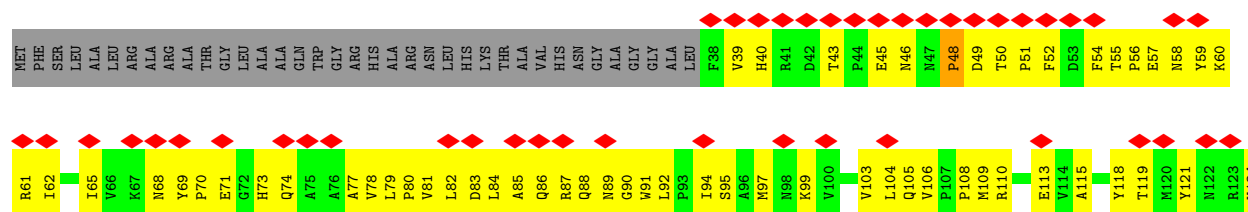


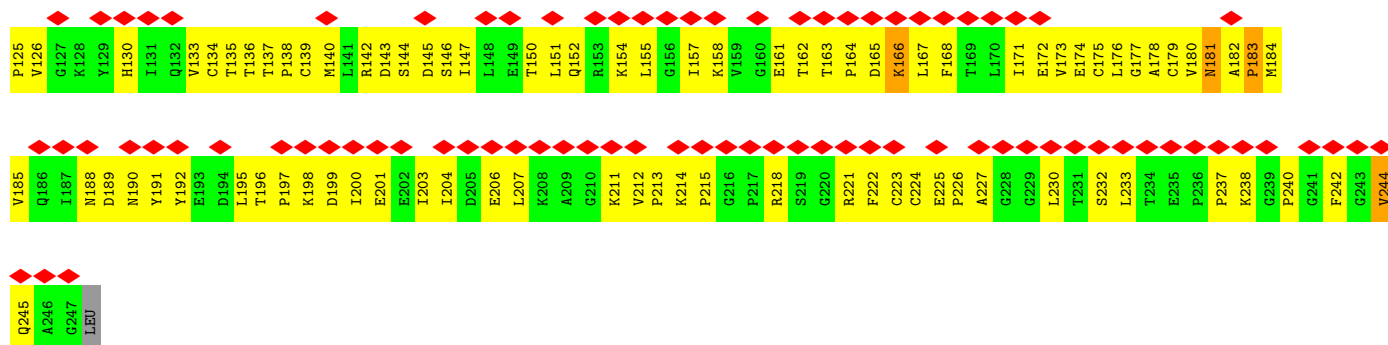


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

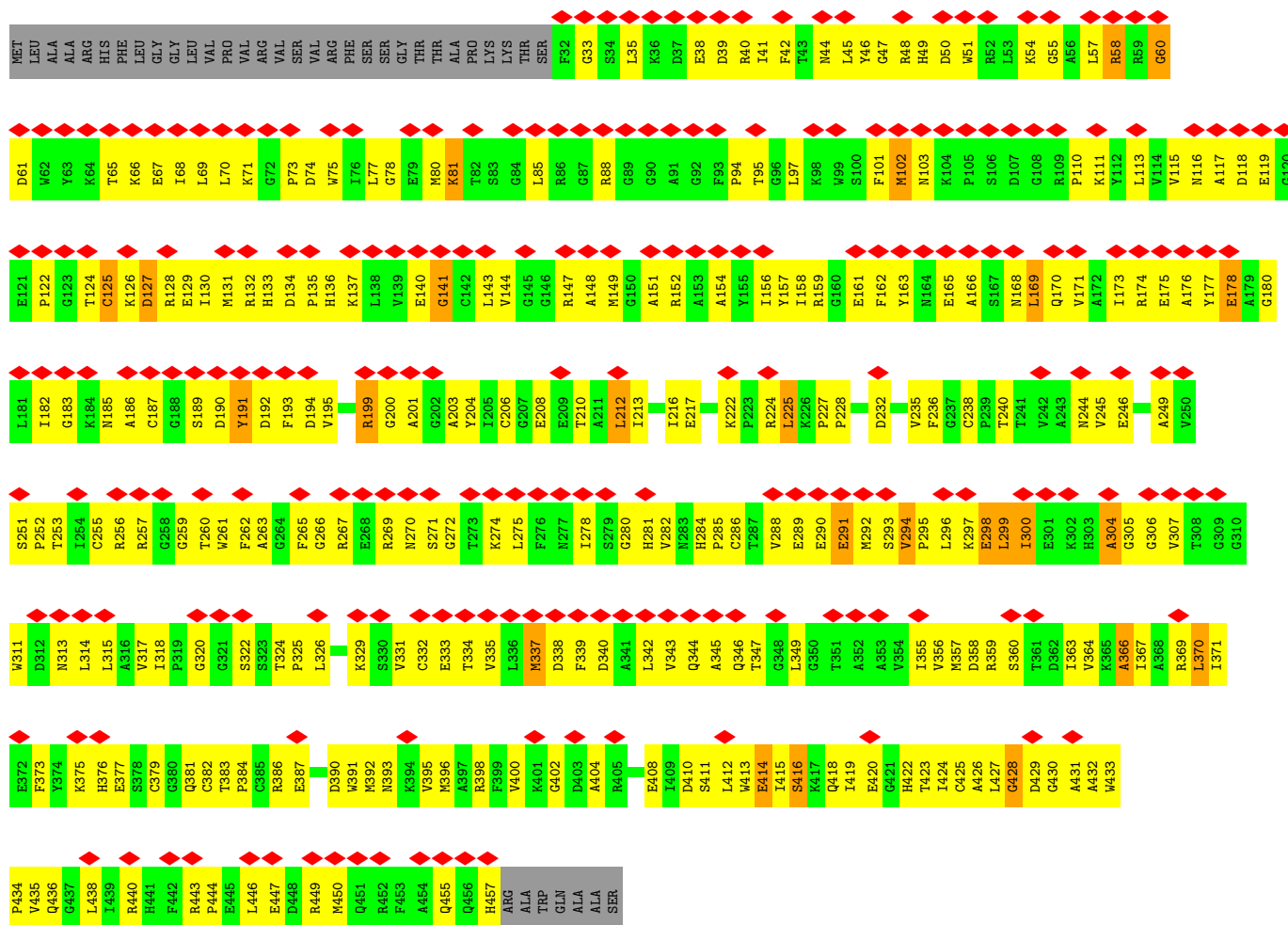


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



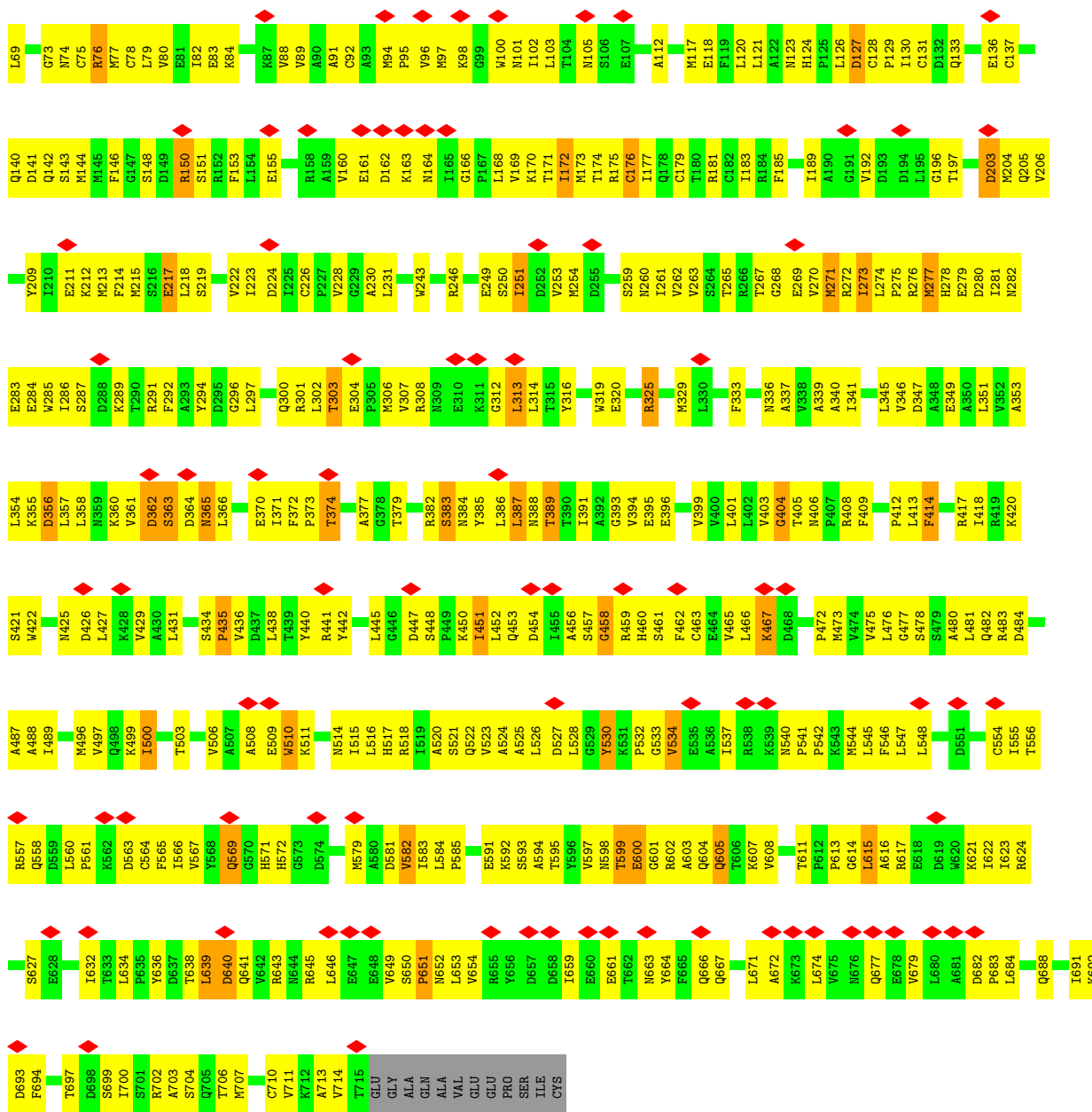


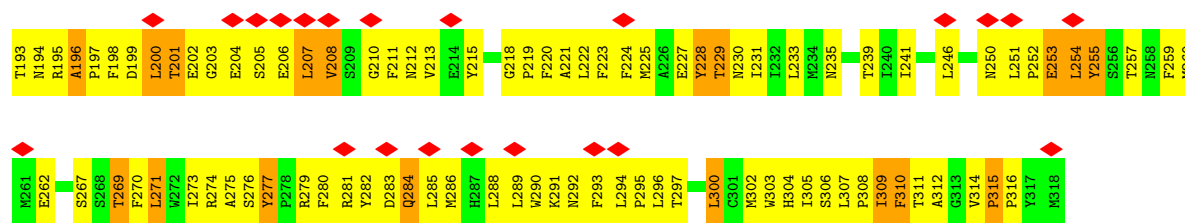
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



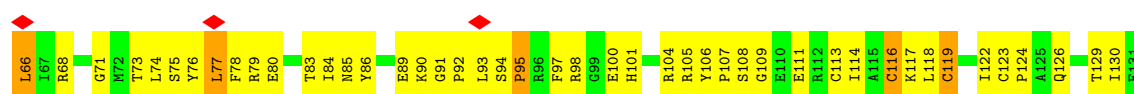
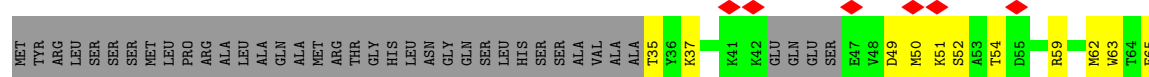
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



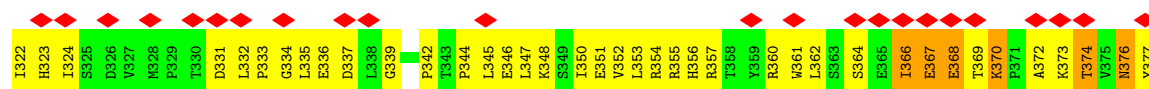
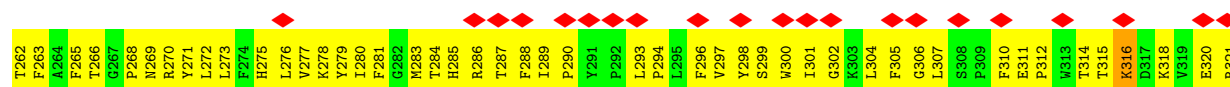
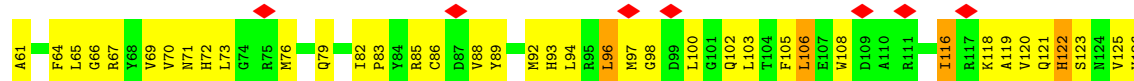
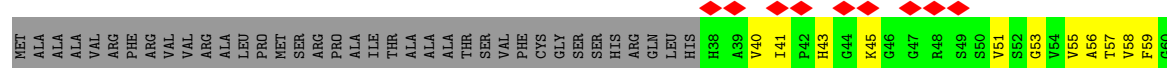




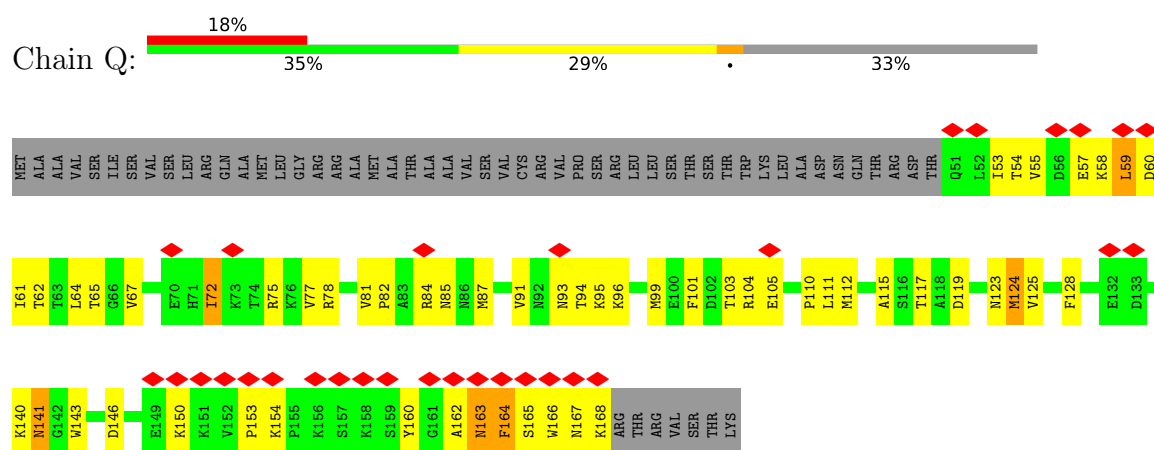
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



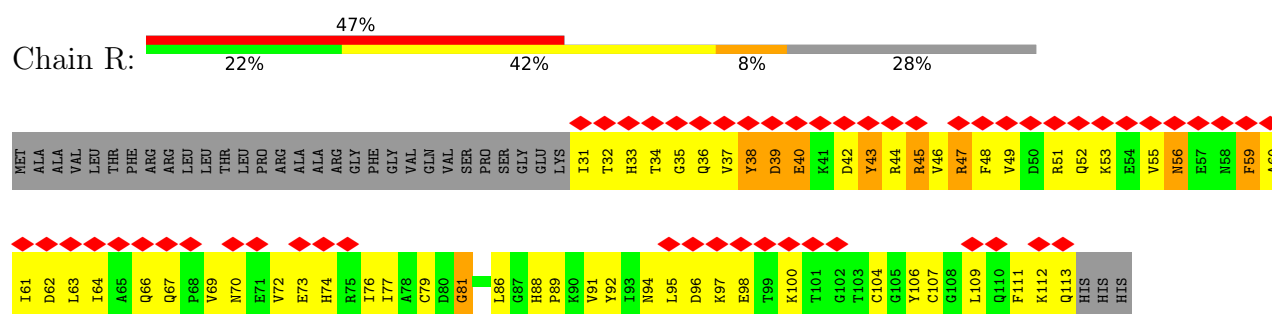
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



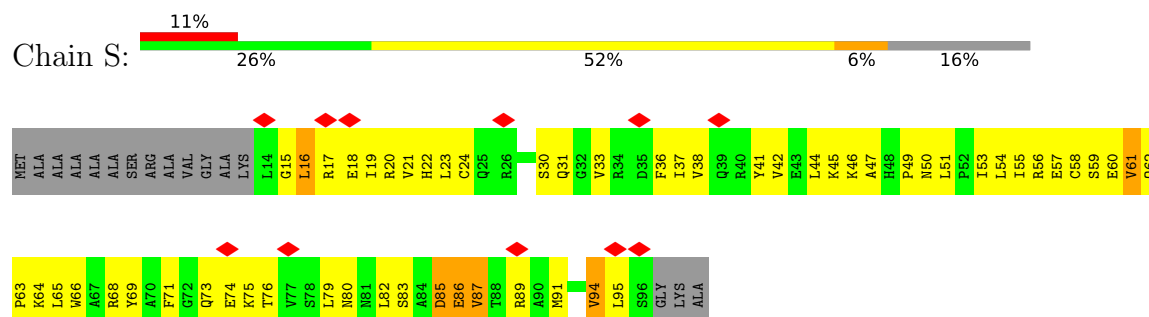
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



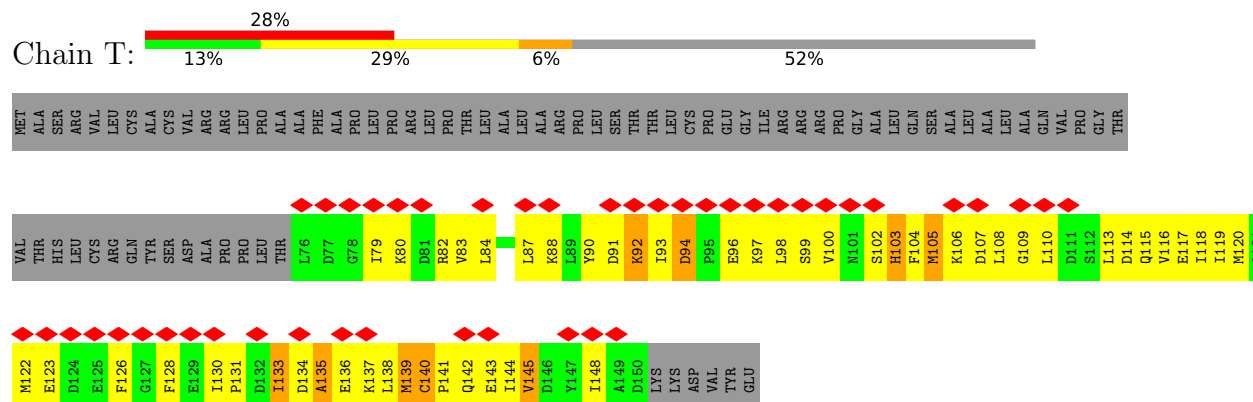
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



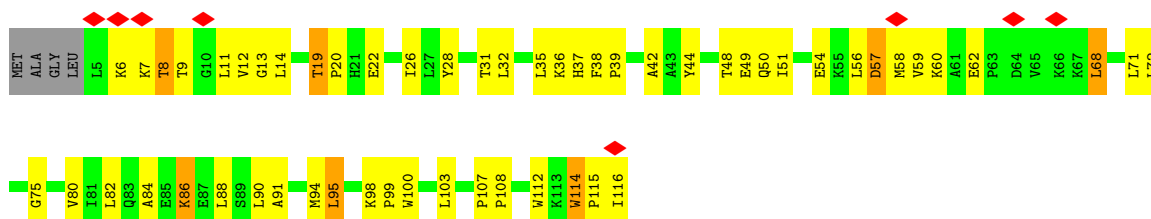
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



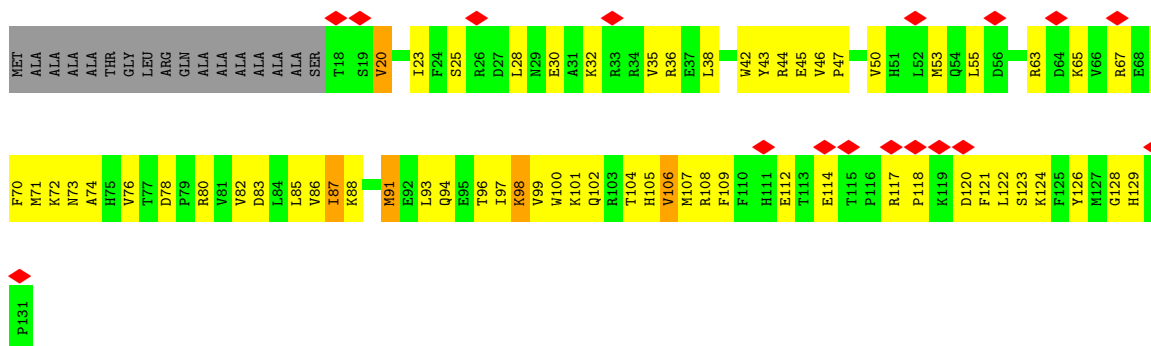
- Molecule 14: Acyl carrier protein, mitochondrial



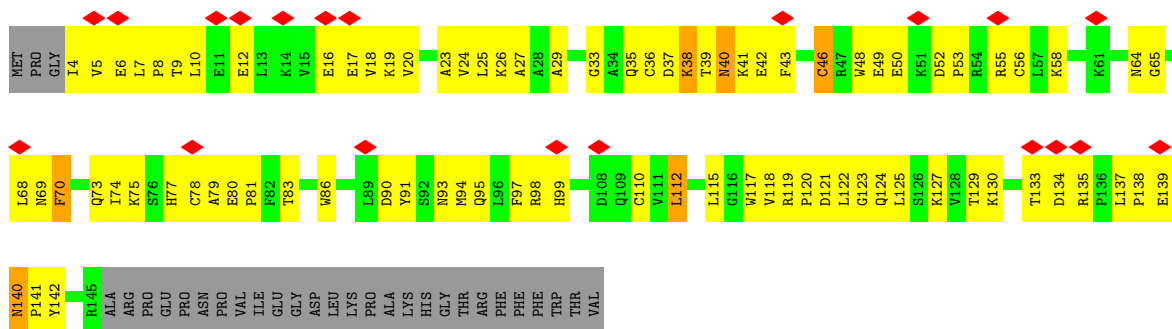
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



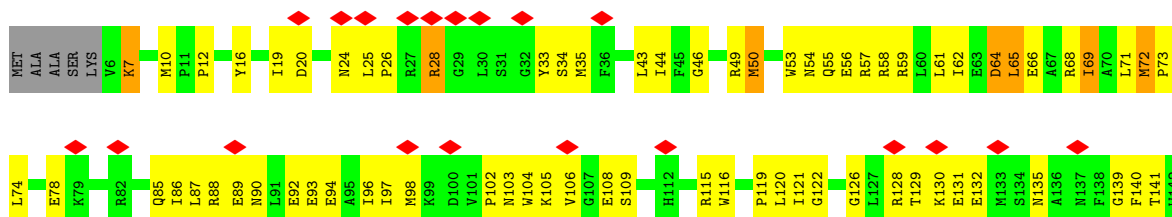
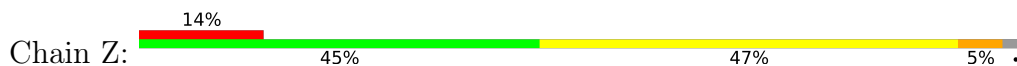
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



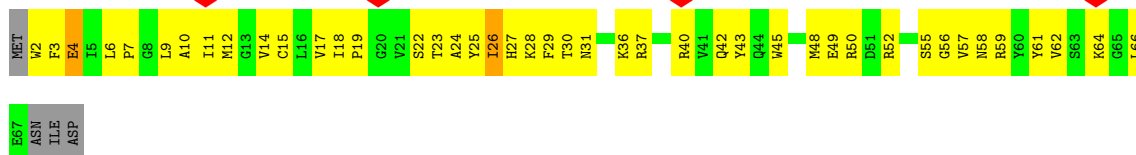
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



Y143
T144

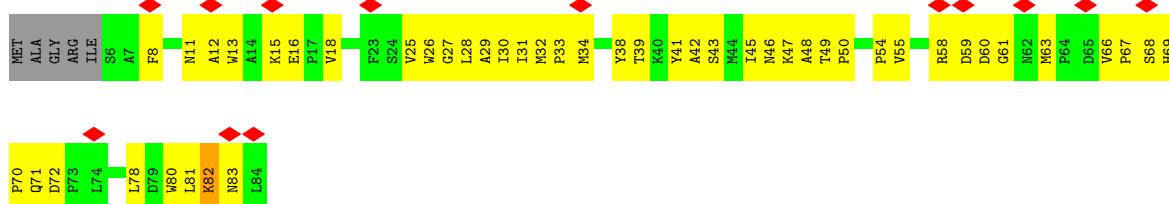
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a: 6% 33% 59% 6%

E67
ASN
ILE
ASP

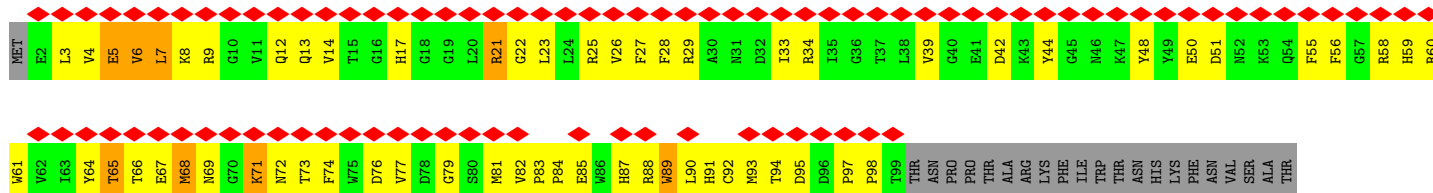
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 15% 38% 55% 6%

P70
Q71
D72
P73
L74
L78
D79
W80
L81
K82
N83
L84

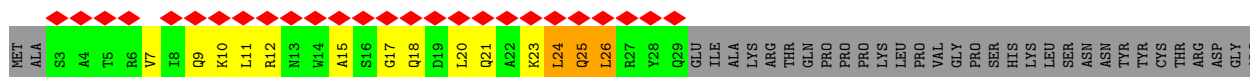
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 34% 68% 42% 6% 17%

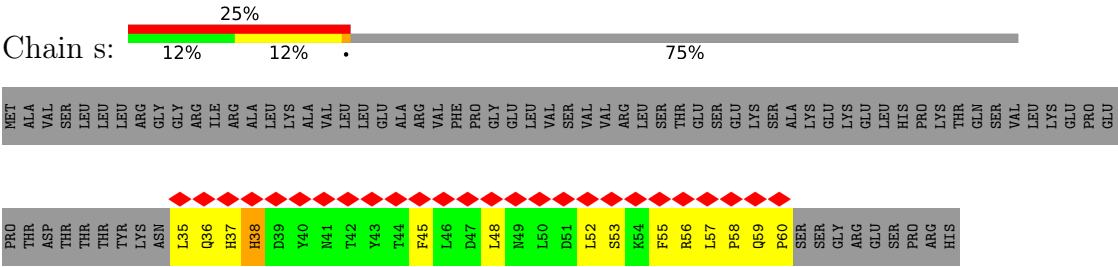
M61
V62
I63
V64
T65
T66
E67
M68
M69
G70
K71
N72
T73
F74
W75
D76
V77
D78
G79
S80
N81
W82
P83
P84
E85
W86
H87
R88
K89
L90
H91
C92
N93
T94
D95
D96
P97
P98
T99
THR
ASN
PRO
PRO
THR
ALA
ARG
LYS
PHE
ILE
TRP
THR
ASN
HIS
LYS
PHE
ASN
VAL
SER
ALA
THRPRO
GLU
Q123
Y124
V125
P126
Y127
S128
T129
T130
K131
K132
K133
P140
S141
T142
P143
Y144
LYS

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

Chain r: 29% 24% 15% 5% 56%

ARG
GLU
VAL
VAL
PRO
PRO
SER
ILE
MET
SER
SER
GLN
LYS
ALA
LEU
VAL
SER
GLY
LYS
ALA
GLU
SER
SER
ALA
ALA
MET
ALA
THR
E91
K92
K93
A94
P97
R103
W104
E105
L106
S107
K108
D109
Q110
L113

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22206	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	4.461	Depositor
Minimum map value	-1.075	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, FES, SF4, NDP, 3PE, FMN, UQ9, 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	0.97	0/941	1.23	7/1285 (0.5%)
2	B	1.00	1/1289 (0.1%)	1.41	15/1744 (0.9%)
3	C	0.90	1/1687 (0.1%)	1.30	13/2297 (0.6%)
4	D	0.94	5/3162 (0.2%)	1.32	24/4276 (0.6%)
5	E	0.75	0/1675	1.16	9/2282 (0.4%)
6	F	0.87	2/3363 (0.1%)	1.43	48/4543 (1.1%)
7	G	0.89	6/5374 (0.1%)	1.58	102/7281 (1.4%)
8	H	0.93	1/2615 (0.0%)	1.54	56/3574 (1.6%)
9	I	0.89	0/1427	1.49	18/1927 (0.9%)
10	P	0.77	1/2804 (0.0%)	1.22	27/3802 (0.7%)
11	Q	0.87	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	0.87	3/671 (0.4%)	1.34	11/903 (1.2%)
13	S	0.85	0/678	1.45	10/915 (1.1%)
14	T	0.92	0/613	1.51	9/826 (1.1%)
15	V	0.87	0/937	1.46	14/1270 (1.1%)
16	W	0.84	1/993 (0.1%)	1.15	8/1335 (0.6%)
17	X	0.78	0/1191	1.34	18/1605 (1.1%)
18	Z	0.78	0/1183	1.22	13/1597 (0.8%)
19	a	0.88	0/553	1.21	4/745 (0.5%)
20	b	0.74	0/643	0.95	1/884 (0.1%)
21	q	0.88	1/1037 (0.1%)	1.34	15/1408 (1.1%)
22	r	0.87	1/421 (0.2%)	1.38	8/566 (1.4%)
23	s	0.43	0/233	0.75	1/317 (0.3%)
All	All	0.87	24/34470 (0.1%)	1.38	443/46706 (0.9%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	106	VAL	C-N	-8.74	1.22	1.34
12	R	39	ASP	CA-C	7.94	1.64	1.53
11	Q	53	ILE	C-O	7.85	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	40	GLU	N-CA	7.75	1.56	1.46
7	G	203	ASP	CA-C	6.78	1.62	1.52
7	G	600	GLU	CA-C	6.53	1.61	1.52
4	D	106	VAL	C-N	-6.51	1.24	1.33
2	B	110	PRO	C-O	-6.35	1.16	1.24
7	G	127	ASP	CA-C	6.28	1.62	1.52
4	D	266	ARG	C-O	-6.23	1.16	1.24
7	G	76	ARG	CA-C	6.12	1.61	1.53
7	G	361	VAL	CA-C	5.88	1.60	1.52
22	r	25	GLN	CA-C	5.82	1.60	1.52
6	F	225	LEU	C-O	5.71	1.31	1.23
12	R	59	PHE	CA-C	-5.70	1.45	1.52
4	D	392	PRO	C-O	-5.58	1.20	1.24
6	F	414	GLU	C-O	-5.57	1.17	1.24
4	D	107	ARG	C-N	5.50	1.40	1.33
7	G	683	PRO	N-CD	-5.44	1.40	1.47
21	q	126	PRO	N-CD	5.36	1.55	1.47
10	P	235	THR	CA-C	5.31	1.59	1.53
4	D	266	ARG	CA-C	-5.24	1.45	1.52
8	H	310	PHE	CA-C	5.04	1.59	1.52
3	C	61	GLY	C-N	-5.02	1.27	1.33

All (443) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	174	THR	N-CA-C	-16.86	89.00	114.64
6	F	125	CYS	N-CA-C	-15.60	93.51	113.17
8	H	208	VAL	N-CA-C	-13.66	100.83	111.62
7	G	251	ILE	N-CA-C	13.37	126.89	108.17
7	G	77	MET	N-CA-C	-13.06	97.32	113.38
7	G	500	ILE	N-CA-C	-12.54	98.74	110.53
10	P	106	LEU	N-CA-C	12.18	128.68	109.07
6	F	171	VAL	N-CA-C	-11.90	99.35	110.53
6	F	449	ARG	N-CA-C	-11.67	98.64	111.36
7	G	204	MET	N-CA-C	-11.59	91.52	109.25
11	Q	60	ASP	N-CA-C	-11.32	90.34	109.24
7	G	599	THR	N-CA-C	11.26	126.12	112.38
16	W	87	ILE	N-CA-C	-11.09	99.78	110.42
15	V	57	ASP	N-CA-C	-11.01	99.29	111.07
8	H	259	PHE	N-CA-C	-10.96	99.41	111.36
9	I	164	VAL	N-CA-C	-10.60	100.19	113.22
9	I	77	LEU	N-CA-C	-10.48	99.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	139	MET	N-CA-C	-10.42	97.43	113.89
8	H	284	GLN	N-CA-C	-10.36	99.98	111.07
7	G	280	ASP	N-CA-C	10.31	122.51	111.28
2	B	195	PRO	N-CA-C	-10.29	98.14	110.70
4	D	337	MET	N-CA-C	-10.24	100.12	111.07
10	P	366	ILE	N-CA-C	10.21	121.03	110.62
19	a	4	GLU	N-CA-C	10.16	124.77	112.38
7	G	414	PHE	N-CA-C	-10.12	101.43	113.88
9	I	161	ALA	N-CA-C	10.08	122.27	111.28
14	T	135	ALA	N-CA-C	-10.07	100.30	111.28
7	G	325	ARG	N-CA-C	-9.85	100.23	110.97
6	F	178	GLU	N-CA-C	-9.85	99.30	111.11
9	I	166	ALA	N-CA-C	-9.84	100.82	113.12
6	F	103	ASN	N-CA-C	-9.79	101.02	113.16
6	F	141	GLY	N-CA-C	-9.77	101.17	112.50
6	F	144	VAL	N-CA-C	-9.75	101.37	110.53
7	G	654	VAL	N-CA-C	9.71	123.23	111.09
7	G	337	ALA	N-CA-C	-9.59	100.78	114.12
6	F	418	GLN	N-CA-C	-9.57	100.81	111.14
8	H	52	ALA	N-CA-C	-9.54	100.86	111.07
17	X	70	PHE	N-CA-C	-9.52	99.68	111.11
4	D	95	LEU	N-CA-C	9.47	122.74	110.53
4	D	427	PRO	N-CA-C	-9.47	95.64	110.50
17	X	112	LEU	N-CA-C	-9.45	100.94	111.14
12	R	38	TYR	N-CA-C	-9.45	96.36	110.24
8	H	200	LEU	N-CA-C	-9.44	101.00	111.28
10	P	367	GLU	N-CA-C	9.30	122.61	111.82
14	T	133	ILE	N-CA-C	9.29	119.83	110.82
7	G	692	LYS	N-CA-C	-9.28	100.54	112.23
7	G	694	PHE	N-CA-C	9.26	121.37	111.28
18	Z	69	ILE	N-CA-C	-9.21	100.68	110.36
10	P	369	THR	N-CA-CB	9.20	123.42	110.17
7	G	640	ASP	N-CA-C	-9.20	101.33	111.36
7	G	389	THR	N-CA-C	-9.15	96.23	109.96
5	E	85	ALA	N-CA-C	-9.10	101.44	111.36
19	a	57	VAL	N-CA-C	-9.01	105.16	113.71
7	G	133	GLN	N-CA-CB	8.82	121.56	110.45
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
16	W	20	VAL	N-CA-C	8.70	120.80	108.36
7	G	365	ASN	N-CA-C	-8.69	102.24	112.92
9	I	154	TYR	N-CA-CB	-8.66	99.24	111.62
8	H	207	LEU	N-CA-C	-8.62	92.44	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	96	LEU	N-CA-C	8.61	121.61	111.71
13	S	86	GLU	N-CA-C	-8.53	102.06	111.36
3	C	70	LYS	N-CA-C	8.51	121.62	111.33
13	S	18	GLU	N-CA-C	8.51	123.27	109.40
10	P	373	LYS	N-CA-C	8.50	121.91	110.35
16	W	100	TRP	N-CA-C	-8.43	99.90	112.04
17	X	99	HIS	N-CA-C	-8.41	102.19	111.36
3	C	108	LYS	N-CA-C	8.41	120.07	111.07
8	H	141	SER	N-CA-C	-8.32	102.17	111.07
7	G	558	GLN	N-CA-C	-8.30	102.19	111.07
7	G	452	LEU	N-CA-C	-8.29	102.24	111.28
11	Q	54	THR	N-CA-C	8.29	123.22	109.46
8	H	196	ALA	N-CA-C	8.23	128.00	109.81
8	H	311	THR	N-CA-C	-8.22	102.56	112.59
3	C	196	PRO	N-CA-C	8.17	124.89	113.53
6	F	298	GLU	N-CA-C	8.16	120.18	111.28
7	G	691	ILE	N-CA-C	8.15	123.62	111.89
16	W	96	THR	N-CA-C	-8.15	102.34	111.14
7	G	534	VAL	N-CA-C	-8.13	104.67	111.91
6	F	191	TYR	N-CA-C	8.12	121.68	110.24
2	B	110	PRO	N-CA-C	8.10	124.59	113.65
15	V	86	LYS	N-CA-C	-8.09	102.41	111.14
7	G	484	ASP	N-CA-C	8.07	120.99	111.71
13	S	76	THR	N-CA-C	8.07	122.06	108.90
7	G	500	ILE	N-CA-CB	8.03	120.85	110.57
16	W	98	LYS	N-CA-C	-8.02	101.53	113.72
9	I	201	ILE	N-CA-C	-8.01	102.63	110.72
8	H	271	LEU	N-CA-C	-7.99	102.51	111.14
17	X	43	PHE	N-CA-C	-7.99	102.52	111.07
17	X	46	CYS	N-CA-C	-7.98	102.66	111.36
21	q	67	GLU	CB-CA-C	-7.96	99.57	112.06
7	G	651	PRO	CB-CA-C	-7.94	98.45	111.56
10	P	206	ILE	N-CA-C	7.92	120.91	108.87
15	V	6	LYS	N-CA-C	-7.91	100.09	110.53
8	H	311	THR	N-CA-CB	7.90	123.56	110.92
9	I	160	GLU	N-CA-C	7.84	124.22	111.37
7	G	270	VAL	N-CA-CB	-7.83	100.68	110.31
10	P	235	THR	CB-CA-C	-7.83	100.02	112.07
9	I	74	LEU	N-CA-C	-7.80	102.77	111.28
7	G	389	THR	N-CA-CB	7.79	121.45	109.85
17	X	58	LYS	N-CA-C	-7.78	102.75	111.07
8	H	201	THR	N-CA-C	-7.74	99.82	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	47	ARG	N-CA-C	7.70	120.64	111.33
21	q	44	TYR	N-CA-C	-7.69	98.89	110.28
4	D	361	ALA	N-CA-C	-7.68	103.02	112.38
8	H	253	GLU	N-CA-C	7.67	121.90	112.54
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
21	q	89	TRP	N-CA-C	-7.63	102.90	111.14
2	B	153	PRO	CB-CA-C	-7.62	98.98	111.56
7	G	56	VAL	N-CA-C	-7.62	103.03	110.72
7	G	569	GLN	N-CA-C	7.59	121.97	108.24
6	F	171	VAL	N-CA-CB	7.58	120.27	110.57
12	R	74	HIS	N-CA-C	7.54	121.12	110.50
7	G	277	MET	N-CA-C	7.51	120.63	109.59
9	I	119	CYS	N-CA-C	-7.51	103.17	111.36
9	I	158	CYS	N-CA-C	-7.48	103.12	111.28
7	G	467	LYS	N-CA-C	-7.48	102.28	111.33
4	D	99	LEU	N-CA-C	7.43	121.04	109.07
7	G	510	TRP	N-CA-CB	7.42	120.91	109.85
6	F	430	GLY	N-CA-C	7.39	121.60	112.73
8	H	67	SER	N-CA-C	-7.38	101.00	110.53
7	G	303	THR	N-CA-C	7.38	122.99	113.18
15	V	57	ASP	N-CA-CB	7.37	120.69	110.01
12	R	39	ASP	N-CA-C	7.36	121.27	110.59
4	D	350	LYS	CB-CA-C	-7.36	101.04	111.85
13	S	94	VAL	N-CA-C	7.33	117.46	110.42
2	B	183	ARG	N-CA-C	-7.32	104.60	113.97
7	G	661	GLU	N-CA-C	7.30	118.93	110.97
8	H	309	ILE	N-CA-C	7.29	117.38	110.30
7	G	384	ASN	N-CA-C	-7.29	103.37	111.82
3	C	195	HIS	CB-CA-C	7.27	117.37	110.17
1	A	93	ILE	N-CA-C	-7.26	102.74	110.36
7	G	374	THR	CB-CA-C	-7.26	99.81	111.28
10	P	370	LYS	N-CA-C	7.24	119.31	109.24
8	H	50	ALA	N-CA-C	7.21	118.79	111.07
8	H	139	THR	N-CA-CB	7.18	120.43	110.01
14	T	105	MET	N-CA-C	7.18	119.19	111.36
4	D	92	HIS	N-CA-C	-7.17	102.83	113.72
15	V	68	LEU	N-CA-C	-7.13	103.51	111.28
8	H	254	LEU	N-CA-C	-7.12	103.56	111.82
6	F	81	LYS	N-CA-C	-7.11	103.61	111.36
7	G	497	VAL	N-CA-C	-7.11	103.37	110.62
7	G	461	SER	N-CA-C	7.10	119.92	111.33
7	G	217	GLU	N-CA-C	-7.08	101.70	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	73	PRO	N-CA-C	-7.06	103.93	113.40
7	G	465	VAL	N-CA-CB	7.06	118.35	110.51
7	G	150	ARG	N-CA-C	7.06	119.66	109.14
7	G	148	SER	N-CA-C	7.06	120.90	109.40
6	F	78	GLY	N-CA-C	-7.05	104.27	112.73
15	V	95	LEU	N-CA-C	-7.04	103.61	111.28
6	F	455	GLN	N-CA-C	7.04	118.60	111.07
10	P	235	THR	CA-C-O	7.03	128.21	121.67
11	Q	162	ALA	N-CA-C	7.02	118.94	111.28
6	F	169	LEU	N-CA-C	7.00	118.91	111.28
7	G	294	TYR	N-CA-C	-6.98	104.58	113.23
12	R	45	ARG	N-CA-C	-6.97	104.65	113.01
6	F	428	GLY	N-CA-C	-6.94	103.89	112.77
8	H	292	ASN	N-CA-C	6.94	118.92	111.36
18	Z	34	SER	N-CA-C	-6.94	103.65	111.07
2	B	166	ASN	N-CA-C	-6.93	103.42	110.97
6	F	418	GLN	N-CA-CB	6.93	120.11	110.07
16	W	87	ILE	N-CA-CB	6.92	118.65	110.55
7	G	582	VAL	N-CA-C	6.92	118.45	108.48
5	E	152	GLN	N-CA-C	-6.91	103.67	111.07
18	Z	28	ARG	N-CA-C	6.91	119.79	108.52
8	H	300	LEU	N-CA-C	-6.91	104.11	112.54
6	F	103	ASN	N-CA-CB	6.89	120.99	110.44
14	T	145	VAL	N-CA-C	-6.89	103.76	110.72
8	H	176	LEU	CA-C-N	-6.88	113.57	120.31
8	H	176	LEU	C-N-CA	-6.88	113.57	120.31
1	A	9	ILE	N-CA-C	-6.88	102.45	111.05
6	F	148	ALA	N-CA-C	-6.87	103.88	111.36
6	F	246	GLU	N-CA-C	-6.87	103.80	111.28
7	G	362	ASP	N-CA-C	6.86	125.40	110.80
7	G	300	GLN	N-CA-CB	6.85	122.43	112.08
7	G	268	GLY	N-CA-C	6.81	124.77	115.30
7	G	133	GLN	N-CA-C	-6.78	101.25	110.68
8	H	305	ILE	N-CA-C	-6.77	103.44	113.39
6	F	244	ASN	N-CA-C	-6.77	100.96	110.50
12	R	56	ASN	N-CA-C	6.77	119.93	108.90
15	V	114	TRP	N-CA-CB	6.74	120.34	110.30
7	G	434	SER	N-CA-C	-6.73	101.01	110.29
8	H	8	THR	N-CA-C	-6.71	101.22	110.35
3	C	79	CYS	N-CA-C	-6.69	101.66	110.43
15	V	8	THR	N-CA-C	6.69	119.03	108.79
9	I	208	ASP	N-CA-C	6.69	121.60	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	125	PHE	N-CA-CB	-6.67	100.56	110.17
16	W	105	HIS	N-CA-C	-6.67	104.96	113.23
10	P	116	ILE	N-CA-C	-6.66	104.00	110.72
7	G	601	GLY	N-CA-C	6.63	124.86	115.30
1	A	24	LEU	CA-C-N	-6.62	113.89	120.98
1	A	24	LEU	C-N-CA	-6.62	113.89	120.98
3	C	69	PRO	N-CA-C	-6.62	104.32	113.53
7	G	640	ASP	N-CA-CB	6.62	119.96	110.16
7	G	287	SER	N-CA-C	6.60	119.24	110.53
17	X	129	THR	N-CA-C	6.59	120.79	110.17
2	B	123	ALA	N-CA-C	6.59	118.25	111.14
4	D	93	GLY	N-CA-C	6.59	122.53	114.69
8	H	182	ALA	N-CA-C	-6.58	104.03	111.07
15	V	86	LYS	N-CA-CB	6.58	119.61	110.07
8	H	177	PRO	N-CA-C	-6.56	101.59	111.57
4	D	184	ILE	N-CA-C	-6.56	103.92	110.62
8	H	93	HIS	CB-CA-C	6.55	117.74	108.76
11	Q	141	ASN	N-CA-CB	6.55	120.75	110.46
18	Z	65	LEU	N-CA-C	-6.55	104.22	111.36
7	G	435	PRO	N-CA-C	-6.54	100.23	110.50
17	X	98	ARG	N-CA-C	6.53	120.50	112.54
7	G	250	SER	N-CA-C	6.48	116.82	108.34
8	H	267	SER	N-CA-C	-6.46	104.32	111.36
13	S	16	LEU	N-CA-C	-6.46	98.37	108.90
9	I	66	LEU	N-CA-C	-6.46	104.32	111.36
4	D	388	GLY	N-CA-C	6.45	119.54	110.38
7	G	605	GLN	N-CA-C	6.45	119.04	108.52
22	r	24	LEU	N-CA-C	6.45	119.59	110.50
3	C	125	PHE	N-CA-C	6.44	119.58	110.50
8	H	255	TYR	N-CA-CB	6.43	119.34	110.01
15	V	49	GLU	N-CA-C	-6.43	104.27	111.28
7	G	95	PRO	N-CA-C	-6.42	101.10	110.80
12	R	81	GLY	N-CA-C	-6.41	106.87	115.21
8	H	271	LEU	N-CA-CB	6.39	119.34	110.07
6	F	370	LEU	N-CA-C	-6.39	104.40	111.36
7	G	273	ILE	N-CA-C	-6.38	98.32	107.77
11	Q	59	LEU	N-CA-C	-6.38	100.73	110.30
21	q	28	PHE	N-CA-C	6.37	117.89	111.07
6	F	178	GLU	N-CA-CB	6.37	119.43	109.94
15	V	91	ALA	N-CA-C	-6.36	104.34	111.28
9	I	205	ILE	N-CA-C	-6.34	104.31	110.72
7	G	176	CYS	N-CA-C	6.34	119.67	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	71	LEU	N-CA-C	6.32	118.17	111.28
17	X	99	HIS	N-CA-CB	6.29	119.46	110.16
6	F	144	VAL	N-CA-CB	6.28	118.61	110.57
7	G	383	SER	N-CA-C	-6.26	106.86	114.75
8	H	52	ALA	N-CA-CB	6.25	119.08	110.01
11	Q	141	ASN	N-CA-C	-6.25	105.66	113.28
2	B	113	ASP	N-CA-CB	6.24	119.50	109.28
7	G	356	ASP	N-CA-CB	6.23	119.28	110.12
22	r	26	LEU	N-CA-CB	-6.22	101.08	110.35
21	q	69	ASN	N-CA-CB	6.20	121.33	111.66
8	H	269	THR	N-CA-C	6.19	118.03	111.28
6	F	101	PHE	N-CA-C	6.18	118.81	111.33
13	S	61	VAL	N-CA-C	-6.18	99.58	108.42
10	P	368	GLU	N-CA-CB	6.18	119.82	110.30
19	a	26	ILE	N-CA-C	-6.18	104.67	113.07
7	G	451	ILE	N-CA-C	-6.17	104.97	113.00
8	H	76	THR	N-CA-C	-6.17	104.56	111.28
7	G	420	LYS	N-CA-C	6.16	118.78	111.33
8	H	276	SER	N-CA-C	6.16	118.97	111.82
6	F	192	ASP	N-CA-C	6.15	118.97	109.07
18	Z	69	ILE	N-CA-CB	6.15	117.33	110.51
10	P	118	LYS	N-CA-C	6.14	118.94	111.82
6	F	415	ILE	N-CA-C	-6.13	104.37	110.62
7	G	418	ILE	N-CA-C	-6.13	103.46	112.04
4	D	291	VAL	N-CA-C	-6.13	103.43	111.09
7	G	325	ARG	N-CA-CB	6.11	118.83	109.91
6	F	212	LEU	N-CA-C	-6.07	104.66	111.28
13	S	87	VAL	N-CA-C	-6.06	104.44	110.62
8	H	185	TRP	N-CA-C	-6.05	104.03	112.45
7	G	353	ALA	N-CA-C	-6.04	104.62	112.23
7	G	508	ALA	N-CA-C	6.03	117.85	111.28
22	r	108	LYS	N-CA-C	6.03	117.93	111.36
8	H	7	LEU	N-CA-C	-6.02	104.34	111.03
7	G	638	THR	N-CA-C	-6.01	100.16	109.24
18	Z	65	LEU	N-CA-CB	6.01	119.06	110.16
8	H	24	GLU	N-CA-C	-6.01	104.10	112.45
18	Z	72	MET	CA-C-N	-6.00	113.00	119.24
18	Z	72	MET	C-N-CA	-6.00	113.00	119.24
2	B	196	PRO	N-CA-C	-5.97	101.83	111.03
4	D	352	PRO	N-CA-C	5.96	117.98	110.70
8	H	103	LEU	N-CA-C	-5.96	104.86	111.36
17	X	38	LYS	N-CA-C	-5.95	104.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	44	ILE	N-CA-C	-5.93	104.73	110.42
7	G	387	LEU	CB-CA-C	-5.91	101.75	111.68
6	F	127	ASP	N-CA-C	5.91	118.51	111.71
8	H	315	PRO	O-C-N	5.91	123.93	121.15
6	F	291	GLU	N-CA-C	5.91	118.17	110.43
17	X	97	PHE	N-CA-C	5.90	118.66	111.82
9	I	116	CYS	N-CA-C	-5.89	105.58	112.89
4	D	84	PHE	N-CA-C	-5.88	101.59	110.24
8	H	228	TYR	CB-CA-C	5.88	120.02	110.96
10	P	122	HIS	N-CA-C	5.87	120.14	112.92
4	D	258	VAL	N-CA-C	-5.87	103.93	110.62
13	S	86	GLU	N-CA-CB	5.87	118.84	110.16
14	T	94	ASP	N-CA-CB	-5.86	105.16	111.66
6	F	255	CYS	N-CA-C	-5.85	104.49	111.69
7	G	480	ALA	N-CA-C	-5.85	104.99	111.36
7	G	639	LEU	N-CA-C	5.83	118.58	111.82
21	q	65	THR	N-CA-C	5.83	119.17	110.14
3	C	209	LEU	N-CA-CB	-5.82	100.70	110.83
10	P	367	GLU	CB-CA-C	-5.81	99.51	110.67
15	V	19	THR	N-CA-CB	5.81	120.71	110.37
6	F	102	MET	CB-CA-C	-5.81	101.36	110.94
7	G	672	ALA	N-CA-C	-5.80	104.96	111.28
11	Q	164	PHE	N-CA-CB	5.80	119.81	110.42
8	H	116	ILE	N-CA-C	-5.79	104.86	110.42
17	X	36	CYS	CB-CA-C	-5.79	102.54	111.74
12	R	34	THR	N-CA-C	-5.77	106.86	112.97
21	q	7	LEU	N-CA-C	-5.77	104.90	111.07
2	B	135	GLY	CA-C-O	-5.76	117.97	122.52
10	P	234	LYS	CB-CA-C	-5.76	103.39	111.80
4	D	414	ASP	N-CA-C	-5.75	101.44	110.36
2	B	105	MET	N-CA-C	-5.74	104.23	111.11
10	P	119	ALA	N-CA-C	-5.73	104.95	111.14
10	P	272	LEU	N-CA-C	-5.73	101.80	110.28
6	F	299	LEU	N-CA-C	5.72	118.46	111.82
13	S	73	GLN	N-CA-C	-5.72	100.38	109.59
8	H	252	PRO	N-CA-CB	-5.71	98.03	103.51
6	F	176	ALA	N-CA-C	5.70	118.23	111.33
7	G	289	LYS	N-CA-C	5.69	117.48	111.28
6	F	393	ASN	N-CA-C	-5.69	104.98	111.07
11	Q	124	MET	CA-C-N	-5.68	114.91	122.98
11	Q	124	MET	C-N-CA	-5.68	114.91	122.98
5	E	119	THR	N-CA-C	-5.68	105.84	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	126	LYS	N-CA-C	5.68	117.47	111.28
12	R	35	GLY	N-CA-C	5.68	121.77	113.48
7	G	59	GLN	N-CA-C	5.67	118.03	107.99
7	G	540	ASN	CA-C-N	-5.67	114.54	120.38
7	G	540	ASN	C-N-CA	-5.67	114.54	120.38
6	F	457	HIS	N-CA-CB	-5.66	100.89	110.50
2	B	201	LEU	N-CA-C	-5.65	105.12	111.28
2	B	112	TYR	N-CA-C	5.65	122.83	110.80
6	F	416	SER	N-CA-C	5.64	117.88	111.11
7	G	599	THR	CA-C-N	-5.64	114.14	122.83
7	G	599	THR	C-N-CA	-5.64	114.14	122.83
2	B	91	TRP	CA-C-N	-5.64	114.79	120.31
2	B	91	TRP	C-N-CA	-5.64	114.79	120.31
2	B	71	ALA	N-CA-CB	-5.62	101.26	110.14
21	q	140	PRO	N-CA-C	-5.62	102.31	110.80
6	F	304	ALA	CB-CA-C	-5.62	110.08	116.54
12	R	52	GLN	N-CA-C	5.61	117.94	110.53
6	F	294	VAL	CA-C-N	-5.59	114.00	119.76
6	F	294	VAL	C-N-CA	-5.59	114.00	119.76
17	X	40	ASN	N-CA-C	-5.59	104.88	110.97
9	I	191	LEU	N-CA-C	-5.59	105.27	111.36
18	Z	64	ASP	N-CA-C	5.58	119.81	112.89
21	q	142	THR	N-CA-CB	5.58	119.89	109.68
5	E	183	PRO	N-CA-C	-5.58	102.17	111.26
7	G	530	TYR	N-CA-C	-5.57	102.04	110.28
6	F	118	ASP	N-CA-C	-5.55	102.06	110.28
22	r	94	ALA	N-CA-C	-5.55	101.63	109.96
21	q	68	MET	N-CA-C	5.55	119.31	112.54
19	a	25	TYR	N-CA-C	-5.53	107.79	114.75
7	G	615	LEU	N-CA-C	-5.52	106.32	113.16
21	q	71	LYS	N-CA-C	5.50	119.98	113.16
7	G	313	LEU	N-CA-C	5.49	118.51	109.72
7	G	363	SER	N-CA-C	-5.48	100.24	109.07
8	H	141	SER	N-CA-CB	5.47	117.94	110.01
10	P	86	CYS	N-CA-C	-5.47	103.16	110.55
7	G	127	ASP	CA-C-O	5.47	128.94	121.89
4	D	132	ALA	N-CA-C	-5.46	106.62	113.72
7	G	150	ARG	N-CA-CB	-5.46	102.77	111.62
8	H	46	LEU	N-CA-C	-5.46	106.62	113.28
4	D	200	PHE	CA-CB-CG	5.45	119.25	113.80
14	T	135	ALA	N-CA-CB	5.45	118.13	110.12
18	Z	50	MET	N-CA-C	-5.42	105.37	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	391	VAL	CA-C-N	-5.41	115.76	119.66
4	D	391	VAL	C-N-CA	-5.41	115.76	119.66
7	G	420	LYS	N-CA-CB	-5.41	101.94	110.06
7	G	682	ASP	CA-C-N	-5.41	114.19	119.76
7	G	682	ASP	C-N-CA	-5.41	114.19	119.76
14	T	92	LYS	N-CA-C	-5.41	106.27	112.92
8	H	94	PRO	N-CA-C	5.40	118.77	111.22
7	G	404	GLY	N-CA-C	5.39	121.35	113.48
5	E	48	PRO	N-CA-C	5.39	120.84	113.84
7	G	510	TRP	N-CA-C	-5.39	101.88	109.96
10	P	374	THR	N-CA-C	5.38	117.50	108.73
17	X	27	ALA	N-CA-C	-5.38	105.08	111.69
11	Q	163	ASN	CB-CA-C	-5.36	99.28	109.95
18	Z	55	GLN	N-CA-C	-5.36	105.44	111.28
4	D	201	PHE	N-CA-C	-5.33	105.55	111.36
21	q	131	ARG	N-CA-C	5.32	117.69	110.35
6	F	199	ARG	N-CA-C	5.31	117.39	109.59
1	A	101	GLY	N-CA-C	-5.30	106.35	112.50
8	H	252	PRO	CA-N-CD	5.29	119.41	112.00
10	P	339	GLY	N-CA-C	5.29	122.61	115.00
7	G	362	ASP	CA-CB-CG	5.28	117.88	112.60
5	E	74	GLN	N-CA-C	-5.28	107.50	114.04
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
21	q	6	VAL	CB-CA-C	-5.26	105.04	112.14
7	G	277	MET	N-CA-CB	-5.25	101.62	109.71
17	X	33	GLY	N-CA-C	-5.25	107.80	114.16
7	G	356	ASP	N-CA-C	-5.25	105.56	111.28
11	Q	164	PHE	N-CA-C	-5.25	106.85	113.20
6	F	300	ILE	N-CA-CB	5.24	119.31	110.56
8	H	146	MET	N-CA-C	-5.24	105.47	111.07
10	P	316	LYS	N-CA-C	-5.23	104.83	111.11
7	G	435	PRO	CB-CA-C	-5.23	105.86	111.56
22	r	25	GLN	N-CA-C	5.23	118.92	112.54
10	P	260	GLY	N-CA-C	-5.23	108.41	115.36
5	E	48	PRO	CB-CA-C	-5.22	104.43	111.85
15	V	84	ALA	N-CA-C	5.22	116.66	111.07
4	D	363	VAL	N-CA-C	5.22	116.30	111.81
3	C	164	TRP	N-CA-C	5.21	117.04	111.36
21	q	21	ARG	N-CA-C	5.20	117.62	111.33
7	G	63	PHE	CA-C-O	-5.20	115.03	121.06
7	G	556	THR	N-CA-C	-5.20	101.51	109.41
7	G	600	GLU	CB-CA-C	-5.20	103.00	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Q	72	ILE	N-CA-C	-5.20	108.44	113.53
22	r	107	SER	N-CA-C	-5.20	102.17	109.96
13	S	85	ASP	N-CA-C	5.19	117.84	111.82
8	H	310	PHE	N-CA-C	5.19	119.23	113.01
7	G	569	GLN	CB-CA-C	-5.18	104.17	112.05
7	G	713	ALA	N-CA-C	-5.18	105.53	111.07
8	H	277	TYR	N-CA-C	5.16	118.00	110.10
10	P	194	VAL	N-CA-CB	5.15	118.31	110.58
22	r	110	GLN	CA-C-N	-5.15	113.61	118.97
22	r	110	GLN	C-N-CA	-5.15	113.61	118.97
10	P	198	ALA	N-CA-C	-5.15	100.13	108.52
20	b	82	LYS	N-CA-C	-5.15	103.74	110.53
7	G	172	ILE	N-CA-C	-5.14	98.64	109.34
8	H	196	ALA	CA-C-N	-5.14	113.50	119.47
8	H	196	ALA	C-N-CA	-5.14	113.50	119.47
4	D	391	VAL	N-CA-C	5.14	113.80	109.02
7	G	458	GLY	N-CA-C	-5.14	108.22	115.32
8	H	90	PRO	CA-C-O	-5.14	117.42	121.38
1	A	48	ARG	N-CA-C	-5.14	106.56	114.16
7	G	387	LEU	N-CA-C	-5.13	98.33	107.98
21	q	5	GLU	N-CA-C	5.13	116.56	111.07
3	C	156	VAL	N-CA-C	-5.13	104.10	111.17
6	F	60	GLY	N-CA-C	-5.11	106.00	114.48
16	W	91	MET	N-CA-C	-5.10	105.91	111.82
1	A	66	ASP	N-CA-C	-5.10	105.63	111.14
3	C	109	SER	N-CA-C	5.09	118.12	109.76
8	H	101	GLY	N-CA-C	5.09	118.41	112.50
5	E	181	ASN	N-CA-C	-5.08	99.50	108.20
3	C	221	GLU	N-CA-C	-5.08	102.35	108.25
5	E	166	LYS	N-CA-C	-5.08	104.63	111.54
9	I	95	PRO	N-CA-C	5.08	121.18	113.81
7	G	393	GLY	N-CA-C	-5.08	107.74	115.66
23	s	38	HIS	N-CA-C	5.08	118.57	112.38
4	D	106	VAL	O-C-N	-5.07	116.75	122.94
17	X	112	LEU	N-CA-CB	5.07	117.42	110.07
7	G	280	ASP	N-CA-CB	-5.07	102.67	110.12
10	P	376	ASN	CB-CA-C	-5.06	102.25	110.85
4	D	224	ALA	CA-C-O	-5.04	115.50	120.90
12	R	43	TYR	N-CA-CB	-5.04	103.19	110.70
17	X	140	ASN	CA-C-N	-5.04	114.59	119.78
17	X	140	ASN	C-N-CA	-5.04	114.59	119.78
8	H	225	MET	N-CA-C	-5.04	105.49	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	130	LYS	N-CA-C	-5.03	105.69	111.07
6	F	366	ALA	N-CA-C	-5.03	105.49	110.97
8	H	254	LEU	N-CA-CB	5.03	118.07	110.28
14	T	140	CYS	N-CA-C	5.03	116.68	109.04
9	I	160	GLU	CB-CA-C	5.02	119.18	110.84
10	P	170	LEU	N-CA-C	5.02	117.00	110.43

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	200	0
2	B	1258	0	1270	198	0
3	C	1641	0	1596	134	0
4	D	3088	0	3059	336	0
5	E	1635	0	1626	177	0
6	F	3288	0	3243	343	0
7	G	5287	0	5323	554	0
8	H	2538	0	2627	510	0
9	I	1398	0	1359	149	0
10	P	2730	0	2747	240	0
11	Q	957	0	949	88	0
12	R	660	0	639	88	0
13	S	667	0	683	73	0
14	T	604	0	596	89	0
15	V	915	0	954	81	0
16	W	970	0	991	103	0
17	X	1164	0	1154	93	0
18	Z	1152	0	1148	100	0
19	a	540	0	550	84	0
20	b	620	0	617	69	0
21	q	1004	0	962	83	0
22	r	413	0	429	43	0
23	s	226	0	214	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	8	0	0	7	0
24	F	8	0	0	10	0
24	G	16	0	0	5	0
24	I	16	0	0	16	0
25	B	24	0	25	34	0
25	H	35	0	43	15	0
26	B	35	0	44	5	0
27	E	4	0	0	5	0
27	G	4	0	0	4	0
28	F	31	0	19	3	0
29	H	51	0	82	12	0
29	Z	46	0	69	3	0
30	P	48	0	26	4	0
31	R	1	0	0	0	0
32	W	32	0	0	7	0
All	All	34029	0	34001	3206	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 (3206) 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	1.47
1:A:51:PHE:HD1	4:D:80:MET:SD	1.36	1.47
1:A:51:PHE:CE1	4:D:80:MET:HE1	1.55	1.42
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
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.22
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.21
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.39	1.20
25:B:302:UQ9:C4M	4:D:189:THR:HG23	1.71	1.20
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
25:B:302:UQ9:H3M	4:D:92:HIS:CD2	1.77	1.17
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
2:B:101:ALA:HB1	25:B:302:UQ9:H1M	1.21	1.17
8:H:63:PRO:O	8:H:66:THR:HG22	1.42	1.17
1:A:18:ILE:CD1	8:H:76:THR:HG22	1.74	1.16
2:B:105:MET:HG2	25:B:302:UQ9:H7	1.18	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CZ	8:H:130:PHE:CE1	2.33	1.15
9:I:123:CYS:SG	24:I:301:SF4:FE1	1.40	1.13
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.13
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.12
6:F:382:CYS:SG	24:F:502:SF4:FE3	1.38	1.12
8:H:134:ARG:NH2	8:H:200:LEU:HD23	1.65	1.11
25:B:302:UQ9:H4M	4:D:189:THR:HG23	1.32	1.11
8:H:127:TYR:CE1	8:H:208:VAL:CG2	2.31	1.11
25:B:302:UQ9:C3M	4:D:92:HIS:HD2	1.63	1.11
2:B:95:PHE:HE1	2:B:97:LEU:HD11	1.18	1.09
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.34	1.09
6:F:379:CYS:SG	24:F:502:SF4:FE4	1.43	1.09
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.08
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
1:A:27:MET:CG	8:H:59:GLU:HG3	1.84	1.08
8:H:127:TYR:CD1	8:H:208:VAL:HG23	1.88	1.08
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.08
1:A:14:SER:O	1:A:18:ILE:HD12	1.52	1.08
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.31	1.07
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	1.72	1.07
2:B:105:MET:HE1	4:D:185:MET:HE1	1.37	1.07
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.07
9:I:152:CYS:SG	24:I:301:SF4:FE2	1.46	1.07
8:H:64:LEU:CG	10:P:362:LEU:HD11	1.85	1.07
8:H:127:TYR:CZ	8:H:208:VAL:CG2	2.37	1.07
25:B:302:UQ9:H3M	4:D:92:HIS:HD2	0.92	1.06
25:B:302:UQ9:C3M	4:D:92:HIS:CD2	2.38	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
1:A:18:ILE:HD13	8:H:76:THR:HG22	1.37	1.05
1:A:62:PHE:CE1	8:H:144:VAL:CG2	2.39	1.05
8:H:127:TYR:CZ	8:H:208:VAL:HG23	1.90	1.05
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.05
2:B:148:VAL:HG11	4:D:87:GLN:HE21	1.18	1.05
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.05
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.08	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.05
2:B:100:CYS:SG	24:B:301:SF4:FE4	1.48	1.05
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.38	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
12:R:88:HIS:CB	12:R:89:PRO:HD2	1.84	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.35	1.04
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	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:112:TYR:CE1	9:I:84:ILE:HD11	1.93	1.03
5:E:179:CYS:SG	27:E:301:FES:FE2	1.48	1.03
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.03
8:H:200:LEU:HD13	8:H:282:TYR:HA	1.39	1.03
1:A:51:PHE:CE1	4:D:80:MET:CE	2.42	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.02
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.02
1:A:27:MET:HG2	8:H:59:GLU:CG	1.89	1.02
1:A:27:MET:SD	8:H:60:PRO:HD2	1.99	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.01
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	1.01
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.01
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.22	1.01
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	1.01
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.40	1.01
9:I:155:CYS:SG	24:I:301:SF4:FE4	1.52	1.01
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.40	1.00
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.86	1.00
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.00
16:W:32:LYS:HG2	32:W:201:EHZ:C19	1.90	1.00
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	1.00
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.38	1.00
8:H:200:LEU:HD13	8:H:282:TYR:CA	1.92	1.00
11:Q:160:TYR:CZ	11:Q:164:PHE:CZ	2.49	0.99
8:H:172:MET:HE1	18:Z:46:GLY:CA	1.92	0.99
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.96	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.99
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	0.99
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.99
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.78	0.99
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.99
8:H:63:PRO:HB2	8:H:66:THR:HB	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.44	0.98
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.98
8:H:1:MET:HE3	19:a:29:PHE:CD1	1.98	0.98
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.97
1:A:18:ILE:HD11	8:H:76:THR:HG22	1.47	0.97
8:H:203:GLY:HA3	8:H:206:GLU:HB3	1.43	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
2:B:120:VAL:HG11	25:H:401:UQ9:H4MB	1.44	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.97
11:Q:160:TYR:CE2	11:Q:164:PHE:CE2	2.53	0.97
17:X:4:ILE:HG22	17:X:5:VAL:N	1.77	0.97
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.30	0.97
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.96
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.96
1:A:62:PHE:CD1	8:H:144:VAL:HG21	2.00	0.96
7:G:92:CYS:SG	27:G:803:FES:S1	2.62	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.96
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.96
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.96
1:A:62:PHE:CD1	8:H:144:VAL:CG2	2.48	0.96
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.95
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
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95
2:B:148:VAL:HG11	4:D:87:GLN:NE2	1.81	0.95
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.47	0.95
9:I:152:CYS:HG	24:I:301:SF4:FE2	0.69	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	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
8:H:134:ARG:CZ	8:H:200:LEU:CD2	2.44	0.94
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.94
1:A:27:MET:HG2	8:H:59:GLU:HG3	0.96	0.94
2:B:95:PHE:CE1	2:B:97:LEU:HD11	2.03	0.94
5:E:179:CYS:HG	27:E:301:FES:FE2	0.68	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:134:ARG:CZ	8:H:200:LEU:HD21	1.97	0.94
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.94
12:R:88:HIS:HB2	12:R:89:PRO:CD	1.97	0.94
11:Q:160:TYR:CE2	11:Q:164:PHE:HE2	1.86	0.93
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.32	0.93
17:X:53:PRO:HD2	18:Z:116:TRP:CD1	2.03	0.93
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.93
22:r:9:GLN:HA	22:r:12:ARG:HD3	1.50	0.93
1:A:51:PHE:CZ	8:H:130:PHE:CD1	2.57	0.93
9:I:113:CYS:SG	24:I:302:SF4:FE3	1.59	0.92
6:F:379:CYS:HG	24:F:502:SF4:FE4	0.74	0.92
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.92
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.33	0.92
10:P:262:THR:H	10:P:332:LEU:HD12	1.34	0.92
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.51	0.91
25:B:302:UQ9:H4MB	4:D:189:THR:HG23	1.49	0.91
6:F:425:CYS:HG	24:F:502:SF4:FE1	0.61	0.91
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.91
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.62	0.91
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.91
1:A:25:PRO:HB3	8:H:57:MET:O	1.69	0.91
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.91
8:H:134:ARG:NH2	8:H:200:LEU:CD2	2.34	0.91
1:A:51:PHE:CD1	4:D:80:MET:CE	2.52	0.90
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.90
1:A:33:LYS:HG2	8:H:61:MET:HE2	1.52	0.90
8:H:64:LEU:HG	10:P:362:LEU:HD11	1.51	0.90
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.51	0.90
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.90
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.05	0.90
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.51	0.90
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.90
7:G:226:CYS:HG	24:G:802:SF4:FE1	0.70	0.90
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.90
1:A:18:ILE:HD13	8:H:76:THR:CG2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CZ	8:H:130:PHE:HE1	1.81	0.89
6:F:110:PRO:HB3	6:F:152:ARG:CZ	2.03	0.89
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.89
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
7:G:32:ILE:HG23	7:G:98:LYS:HD2	1.55	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
1:A:51:PHE:HZ	8:H:130:PHE:HE1	0.95	0.89
6:F:382:CYS:HG	24:F:502:SF4:FE3	0.61	0.89
1:A:51:PHE:CD1	4:D:80:MET:HE1	2.08	0.89
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.89
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.88
1:A:51:PHE:HE1	4:D:80:MET:HE1	0.93	0.88
1:A:52:SER:O	4:D:103:GLY:HA3	1.72	0.88
2:B:81:LEU:HG	26:B:303:PC1:H261	1.52	0.88
8:H:96:ILE:HG12	18:Z:143:TYR:OH	1.74	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
10:P:192:ARG:HH22	10:P:198:ALA:HB3	1.36	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
1:A:62:PHE:HD1	8:H:144:VAL:HG21	1.35	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.87
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.53	0.87
2:B:95:PHE:CZ	2:B:141:MET:HE2	2.09	0.87
12:R:32:THR:HG22	12:R:36:GLN:H	1.40	0.87
6:F:292:MET:HG2	6:F:338:ASP:OD1	1.75	0.87
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.87
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.86
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
8:H:1:MET:CE	19:a:29:PHE:CE1	2.58	0.86
8:H:63:PRO:O	8:H:66:THR:CG2	2.23	0.86
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.57	0.86
8:H:64:LEU:HG	10:P:362:LEU:CD1	2.05	0.86
2:B:120:VAL:CG1	25:H:401:UQ9:H4MB	2.04	0.86
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.86
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:CYS:SG	27:G:803:FES:FE2	1.68	0.86
8:H:59:GLU:CD	8:H:61:MET:SD	2.58	0.85
9:I:162:CYS:HG	24:I:302:SF4:FE4	0.54	0.85
9:I:162:CYS:SG	24:I:302:SF4:FE4	1.68	0.85
6:F:44:ASN:HD21	6:F:51:TRP:HA	1.41	0.85
1:A:58:VAL:HG22	1:A:111:LEU:HD23	1.56	0.85
1:A:62:PHE:HE1	8:H:144:VAL:CG2	1.87	0.85
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.85
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.85
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.85
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.85
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.85
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.85
2:B:105:MET:HG2	25:B:302:UQ9:C7	2.03	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.85
1:A:39:CYS:HB3	4:D:85:GLY:HA3	1.56	0.85
8:H:200:LEU:CD1	8:H:282:TYR:N	2.40	0.85
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.11	0.85
1:A:18:ILE:CD1	8:H:76:THR:CG2	2.55	0.84
4:D:99:LEU:HD12	4:D:99:LEU:O	1.77	0.84
10:P:192:ARG:NH2	10:P:198:ALA:HB3	1.92	0.84
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.84
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	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
2:B:91:TRP:CZ2	8:H:51:ASP:CG	2.55	0.84
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.84
6:F:300:ILE:HD13	6:F:307:VAL:H	1.40	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	1.95	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.83
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.83
12:R:38:TYR:CE2	21:q:127:TYR:HB2	2.13	0.83
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.07	0.83
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.61	0.83
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.83
2:B:102:VAL:HG21	4:D:141:TYR:CD1	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:CYS:HG	27:G:803:FES:FE2	0.55	0.83
2:B:93:MET:CE	4:D:87:GLN:NE2	2.42	0.83
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.83
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.83
8:H:200:LEU:CD1	8:H:282:TYR:CA	2.56	0.83
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.42	0.83
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.44	0.83
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.93	0.82
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.79	0.82
8:H:303:TRP:HE3	20:b:29:ALA:HB2	1.43	0.82
1:A:41:PHE:HB3	16:W:102:GLN:NE2	1.93	0.82
3:C:172:MET:CE	3:C:187:LEU:HB2	2.09	0.82
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.82
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.60	0.82
25:B:302:UQ9:H4MB	4:D:189:THR:CG2	2.09	0.82
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
2:B:95:PHE:HE1	2:B:97:LEU:CD1	1.92	0.82
1:A:62:PHE:CE1	8:H:144:VAL:HG23	2.14	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.82
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.82
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.62	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
10:P:206:ILE:H	30:P:401:NDP:H71N	1.24	0.81
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.95	0.81
1:A:69:ILE:HD11	8:H:144:VAL:HG13	1.60	0.81
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.81
7:G:401:LEU:CD1	7:G:466:LEU:HD21	2.09	0.81
6:F:342:LEU:HB3	6:F:347:THR:HG23	1.63	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.21	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.81
1:A:21:ALA:O	8:H:60:PRO:HG3	1.79	0.81
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.81
2:B:95:PHE:CE1	2:B:97:LEU:HD21	2.15	0.81
2:B:95:PHE:HZ	2:B:141:MET:HE2	1.43	0.81
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.96	0.80
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.15	0.80
8:H:203:GLY:CA	8:H:206:GLU:HB3	2.11	0.80
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.11	0.80
9:I:113:CYS:HG	24:I:302:SF4:FE3	0.51	0.80
9:I:155:CYS:HG	24:I:301:SF4:FE4	0.94	0.80
6:F:392:MET:CE	6:F:416:SER:HA	2.11	0.80
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.80
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.63	0.80
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.80
8:H:64:LEU:CD2	10:P:362:LEU:HD11	2.11	0.80
1:A:41:PHE:CD2	16:W:102:GLN:NE2	2.49	0.80
1:A:62:PHE:HA	8:H:290:TRP:HH2	1.46	0.80
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.14	0.80
8:H:306:SER:HG	8:H:310:PHE:HE2	1.26	0.80
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.16	0.80
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.80
7:G:73:GLY:HA2	27:G:803:FES:S1	2.21	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
1:A:41:PHE:HD2	16:W:102:GLN:NE2	1.78	0.80
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.80
2:B:93:MET:HE2	4:D:87:GLN:CD	2.07	0.79
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.17	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.79
8:H:12:PRO:O	19:a:15:CYS:HB3	1.81	0.79
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.12	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.63	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.65	0.79
17:X:124:GLN:O	20:b:70:PRO:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
14:T:113:LEU:HD22	16:W:71:MET:HE2	1.63	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.78
2:B:102:VAL:HG21	4:D:141:TYR:CE1	2.18	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
6:F:174:ARG:HA	23:s:52:LEU:HD21	1.64	0.78
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.78
4:D:142:VAL:HG11	4:D:182:ASN:HA	1.65	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
21:q:9:ARG:HA	21:q:12:GLN:HG2	1.65	0.78
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.78
2:B:105:MET:CE	4:D:185:MET:HE1	2.13	0.78
25:B:302:UQ9:C10	4:D:200:PHE:CZ	2.66	0.78
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.19	0.78
5:E:178:ALA:HA	6:F:125:CYS:SG	2.24	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.78
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.65	0.78
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.78
4:D:91:ALA:C	4:D:93:GLY:H	1.91	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
8:H:172:MET:CE	18:Z:46:GLY:HA2	2.14	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.77
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.50	0.77
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.49	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
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.77
12:R:89:PRO:HG3	12:R:106:TYR:CE1	2.20	0.77
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:HB3	16:W:102:GLN:HE21	1.49	0.77
1:A:51:PHE:CE1	4:D:103:GLY:HA2	2.20	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.76
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.76
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.76
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.76
8:H:52:ALA:HB2	25:H:401:UQ9:H16	1.65	0.76
18:Z:58:ARG:NH2	20:b:49:THR:HG21	2.00	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.68	0.76
1:A:62:PHE:CE1	8:H:144:VAL:HG22	2.19	0.76
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.67	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.26	0.76
9:I:123:CYS:HG	24:I:301:SF4:FE1	0.47	0.76
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.76
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.76
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.68	0.76
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.21	0.76
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
2:B:102:VAL:CG2	4:D:141:TYR:CE1	2.69	0.76
8:H:134:ARG:NH1	8:H:200:LEU:HD21	1.99	0.76
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.76
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.13	0.76
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.75
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.75
8:H:1:MET:HB3	19:a:26:ILE:CG2	2.16	0.75
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.75
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.75
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.75
10:P:355:ARG:HH21	10:P:356:HIS:CE1	2.03	0.75
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.69	0.75
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.11	0.75
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
2:B:68:ARG:HD3	2:B:70:ARG:HG2	1.69	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
6:F:425:CYS:SG	24:F:502:SF4:FE1	1.78	0.74
8:H:171:HIS:HB3	18:Z:49:ARG:HD3	1.68	0.74
11:Q:160:TYR:CD2	11:Q:164:PHE:HE2	2.03	0.74
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.02	0.74
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.74
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.69	0.74
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.74
4:D:141:TYR:CE1	4:D:142:VAL:HG23	2.22	0.74
4:D:141:TYR:CE2	4:D:457:VAL:HG13	2.21	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
16:W:28:LEU:HG	16:W:32:LYS:HE3	1.69	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.87	0.74
1:A:41:PHE:CB	16:W:102:GLN:NE2	2.50	0.74
8:H:64:LEU:HD21	10:P:362:LEU:CD1	2.16	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
25:B:302:UQ9:C4M	4:D:189:THR:CG2	2.59	0.74
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.74
8:H:64:LEU:CD2	10:P:362:LEU:CD1	2.66	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.69	0.74
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.74
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.53	0.73
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.73
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.73
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.69	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.70	0.73
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.69	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
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.73
12:R:89:PRO:CG	12:R:106:TYR:CZ	2.72	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
2:B:91:TRP:CZ2	8:H:51:ASP:OD1	2.41	0.73
3:C:102:HIS:HE1	15:V:48:THR:CG2	1.99	0.73
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.73
8:H:64:LEU:CD1	10:P:362:LEU:HD11	2.19	0.73
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.28	0.73
16:W:32:LYS:HE2	32:W:201:EHZ:C19	2.18	0.73
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.54	0.73
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.23	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
8:H:64:LEU:CG	10:P:362:LEU:CD1	2.62	0.73
1:A:62:PHE:HE1	8:H:144:VAL:HG23	1.50	0.73
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.73
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.04	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.69	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.89	0.73
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.72
8:H:96:ILE:HG23	18:Z:143:TYR:CZ	2.24	0.72
25:B:302:UQ9:H10A	4:D:200:PHE:CZ	2.24	0.72
5:E:240:PRO:HG3	6:F:57:LEU:O	1.88	0.72
7:G:651:PRO:HG3	13:S:57:GLU:H	1.51	0.72
12:R:89:PRO:HG3	12:R:106:TYR:CZ	2.23	0.72
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.72
1:A:68:GLU:CD	1:A:98:LEU:HG	2.13	0.72
6:F:210:THR:HB	6:F:224:ARG:HB2	1.70	0.72
8:H:99:ASN:CG	19:a:40:ARG:HG3	2.13	0.72
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	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
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.54	0.72
17:X:37:ASP:OD2	20:b:70:PRO:HD3	1.90	0.72
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.24	0.72
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.72
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.72
1:A:17:LEU:HD21	8:H:56:PHE:CZ	2.24	0.72
9:I:200:GLU:OE2	21:q:93:MET:SD	2.48	0.72
10:P:192:ARG:NH1	10:P:192:ARG:HA	2.05	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.20	0.72
8:H:200:LEU:CD1	8:H:282:TYR:HB2	2.19	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
16:W:101:LYS:NZ	16:W:109:PHE:CE2	2.58	0.72
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.20	0.72
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.72
2:B:112:TYR:OH	9:I:91:GLY:CA	2.28	0.72
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.72
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.72
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	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
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
4:D:142:VAL:CG1	4:D:182:ASN:HA	2.19	0.71
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.71
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.71
1:A:14:SER:C	1:A:18:ILE:HD12	2.16	0.71
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.71
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.55	0.71
8:H:99:ASN:OD1	19:a:40:ARG:HG3	1.90	0.71
2:B:105:MET:CG	25:B:302:UQ9:H7	2.09	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.71
8:H:5:ASN:ND2	19:a:23:THR:HA	2.05	0.71
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.71
2:B:105:MET:HG3	25:B:302:UQ9:H1MA	1.73	0.71
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.71
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.73	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.71
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.70
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
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.71	0.70
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.71	0.70
8:H:1:MET:HB2	19:a:30:THR:CG2	2.21	0.70
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.21	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
10:P:169:HIS:H	10:P:184:LYS:HE3	1.54	0.70
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.70
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.73	0.70
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.73	0.70
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.70
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.70
29:Z:401:3PE:H2E1	29:Z:401:3PE:H2I2	1.74	0.70
4:D:99:LEU:HD13	4:D:101:LEU:CD1	2.20	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.27	0.70
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.70
4:D:99:LEU:CD1	4:D:101:LEU:HD13	2.19	0.70
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	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
8:H:187:ILE:HD12	29:H:402:3PE:H242	1.72	0.69
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.69
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.06	0.69
1:A:44:THR:HG22	16:W:99:VAL:HG13	1.73	0.69
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.73	0.69
8:H:224:PHE:CD2	25:H:401:UQ9:H10B	2.27	0.69
21:q:3:LEU:HD12	21:q:6:VAL:CG2	2.22	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.69
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.69
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.69
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:MET:HB3	19:a:26:ILE:HG23	1.75	0.69
9:I:92:PRO:HA	21:q:91:HIS:O	1.93	0.69
4:D:280:ALA:CB	15:V:11:LEU:HG	2.22	0.69
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.69
5:E:192:TYR:CE2	5:E:215:PRO:HA	2.27	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.69
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.75	0.69
8:H:227:GLU:O	8:H:231:ILE:HG13	1.92	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
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.68
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
8:H:63:PRO:HB2	8:H:66:THR:CB	2.21	0.68
8:H:64:LEU:HD21	10:P:362:LEU:HD11	1.71	0.68
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.55	0.68
8:H:65:THR:O	8:H:124:ASN:HB3	1.93	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
20:b:8:PHE:HA	20:b:11:ASN:HD21	1.58	0.68
3:C:107:PHE:CD1	3:C:133:SER:HB2	2.28	0.68
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.68
17:X:50:GLU:HG3	17:X:56:CYS:SG	2.33	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
2:B:114:MET:HB2	2:B:119:VAL:HG23	1.76	0.68
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.68
6:F:228:PRO:HG3	11:Q:160:TYR:HD2	1.59	0.68
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.75	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
8:H:203:GLY:HA3	8:H:206:GLU:CB	2.20	0.68
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	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
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
10:P:192:ARG:NH2	10:P:200:ILE:HD11	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.68
1:A:41:PHE:HA	16:W:102:GLN:HE22	1.58	0.68
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.68
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.76	0.68
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.09	0.68
8:H:5:ASN:CG	19:a:23:THR:HA	2.19	0.68
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.67
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.67
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.59	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.67
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.92	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.67
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.29	0.67
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.74	0.67
8:H:1:MET:HE2	19:a:29:PHE:CE1	2.30	0.67
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.67
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.77	0.67
4:D:94:VAL:O	4:D:115:LEU:HD22	1.94	0.67
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.67
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.67
6:F:300:ILE:HD13	6:F:307:VAL:HG23	1.77	0.67
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.77	0.67
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.67
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.67
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.60	0.66
6:F:41:ILE:HG23	6:F:253:THR:HG21	1.76	0.66
6:F:297:LYS:HB2	6:F:333:GLU:HA	1.76	0.66
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.66
9:I:93:LEU:O	21:q:93:MET:HG2	1.94	0.66
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
16:W:32:LYS:CG	32:W:201:EHZ:C19	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CZ	4:D:103:GLY:HA2	2.30	0.66
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
1:A:61:THR:O	1:A:62:PHE:C	2.35	0.66
2:B:91:TRP:CZ2	8:H:51:ASP:OD2	2.48	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
2:B:82:ILE:HA	8:H:57:MET:HE1	1.77	0.66
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.77	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
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.66
3:C:79:CYS:O	3:C:80:LEU:HB2	1.96	0.66
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.76	0.66
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.66
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.66
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.77	0.66
2:B:93:MET:CE	4:D:87:GLN:CD	2.68	0.66
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.76	0.66
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.66
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.66
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.66
25:H:401:UQ9:H11	25:H:401:UQ9:H15	1.76	0.66
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
8:H:63:PRO:HD2	8:H:66:THR:HG21	1.76	0.66
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.66
1:A:106:TRP:CD1	8:H:291:LYS:HD3	2.31	0.66
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.66
11:Q:160:TYR:CE2	11:Q:164:PHE:CZ	2.80	0.66
1:A:27:MET:HE3	8:H:59:GLU:HG2	1.78	0.66
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.66
2:B:105:MET:HE2	25:B:302:UQ9:C6	2.26	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.65
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.65
2:B:173:TYR:O	3:C:203:LEU:HD22	1.95	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	1.77	0.65
8:H:200:LEU:HD13	8:H:282:TYR:CB	2.26	0.65
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.65
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.65
8:H:65:THR:HB	8:H:124:ASN:ND2	2.10	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
16:W:42:TRP:CH2	16:W:93:LEU:HA	2.31	0.65
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.65
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.65
10:P:192:ARG:HH22	10:P:198:ALA:CB	2.07	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
1:A:73:LEU:N	1:A:74:PRO:HD2	2.11	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
8:H:9:LEU:HA	19:a:19:PRO:HB3	1.78	0.65
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.65
12:R:32:THR:HG22	12:R:36:GLN:N	2.10	0.65
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.26	0.65
10:P:169:HIS:H	10:P:184:LYS:CE	2.09	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.97	0.65
1:A:15:LEU:HA	1:A:18:ILE:HD13	1.79	0.65
2:B:105:MET:CE	25:B:302:UQ9:C1	2.75	0.65
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.32	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.65
10:P:59:PHE:HB2	10:P:130:ILE:HD11	1.78	0.65
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:5:ASN:OD1	19:a:23:THR:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
10:P:191:VAL:HG13	10:P:192:ARG:NH2	2.12	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.77	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.64
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.27	0.64
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.31	0.64
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	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
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.63	0.64
1:A:104:TYR:CZ	1:A:108:GLN:HG3	2.32	0.64
9:I:79:ARG:HG2	22:r:12:ARG:HH21	1.62	0.64
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.79	0.64
2:B:104:MET:O	2:B:105:MET:C	2.40	0.64
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.64
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.64
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.19	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
18:Z:86:ILE:HA	18:Z:128:ARG:HH21	1.62	0.64
1:A:105:GLU:HG3	1:A:110:GLY:HA3	1.78	0.64
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.79	0.64
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.32	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
8:H:131:GLY:CA	8:H:207:LEU:HD11	2.28	0.64
4:D:79:ASN:HB2	4:D:100:GLU:HB3	1.80	0.64
4:D:375:MET:HE1	7:G:126:LEU:HA	1.79	0.64
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.64
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.64
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.64
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.64
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.64
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.33	0.63
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.63
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.63	0.63
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.63
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.78	0.63
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.33	0.63
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.78	0.63
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.28	0.63
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.79	0.63
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.63
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.63
16:W:101:LYS:NZ	16:W:109:PHE:HE2	1.94	0.63
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	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
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.63
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
8:H:65:THR:HB	8:H:124:ASN:HD22	1.63	0.63
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
4:D:141:TYR:CD1	4:D:142:VAL:N	2.67	0.63
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	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:228:PRO:HG3	11:Q:160:TYR:CD2	2.33	0.63
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.29	0.63
10:P:262:THR:N	10:P:332:LEU:HD12	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.66	0.63
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.96	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.63
8:H:15:ILE:HG22	19:a:15:CYS:SG	2.38	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.99	0.62
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.62
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.62
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.62
8:H:64:LEU:HD11	10:P:362:LEU:HD11	1.81	0.62
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.29	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.62
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.81	0.62
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.62
10:P:180:SER:O	10:P:184:LYS:HG3	1.98	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:421:SER:CB	7:G:427:LEU:CD1	2.77	0.62
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.62
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.29	0.62
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.14	0.62
21:q:6:VAL:HA	21:q:9:ARG:HG2	1.79	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
5:E:71:GLU:HB2	23:s:59:GLN:HB3	1.82	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
8:H:19:PHE:CE2	19:a:11:ILE:HG21	2.35	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.62
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.62
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.81	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.34	0.62
8:H:176:LEU:O	18:Z:43:LEU:HD23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.62
1:A:44:THR:HA	16:W:99:VAL:HG11	1.82	0.62
2:B:93:MET:HE1	4:D:87:GLN:NE2	2.14	0.62
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.62
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	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
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
8:H:94:PRO:O	19:a:27:HIS:HE1	1.82	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.62
1:A:27:MET:HE3	8:H:59:GLU:CG	2.29	0.62
2:B:105:MET:HE2	25:B:302:UQ9:C1	2.29	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
8:H:310:PHE:CB	20:b:33:PRO:HA	2.29	0.62
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.62
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.82	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.62
7:G:399:VAL:CG2	7:G:462:PHE:HZ	2.12	0.62
7:G:617:ARG:NH1	16:W:129:HIS:HA	2.14	0.62
8:H:15:ILE:CG2	19:a:15:CYS:SG	2.88	0.62
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.62
1:A:38:GLU:HG2	4:D:83:ASN:OD1	2.00	0.61
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.61
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.35	0.61
8:H:228:TYR:O	8:H:229:THR:C	2.41	0.61
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.61
12:R:89:PRO:CG	12:R:106:TYR:CE1	2.83	0.61
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.61
5:E:230:LEU:HD11	6:F:48:ARG:HE	1.64	0.61
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.81	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.61
16:W:42:TRP:CZ2	16:W:93:LEU:CB	2.83	0.61
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.61
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:11:ASN:HB2	20:b:15:LYS:HE3	1.81	0.61
21:q:3:LEU:HD12	21:q:6:VAL:HG21	1.81	0.61
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.22	0.61
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.48	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.30	0.61
1:A:51:PHE:CE1	8:H:130:PHE:CD1	2.88	0.61
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
8:H:99:ASN:HD21	19:a:40:ARG:HA	1.65	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
1:A:65:PHE:O	1:A:69:ILE:HG13	2.00	0.61
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.61
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.61
10:P:333:PRO:HB2	10:P:337:ASP:CB	2.25	0.61
1:A:39:CYS:SG	8:H:208:VAL:CG2	2.89	0.61
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.81	0.61
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.82	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.82	0.61
10:P:192:ARG:HA	10:P:192:ARG:CZ	2.30	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
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.54	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
12:R:32:THR:HA	12:R:55:VAL:HG23	1.83	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.61
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.61
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.83	0.61
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.65	0.60
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.60
8:H:134:ARG:HB3	8:H:282:TYR:CE1	2.35	0.60
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.60
21:q:3:LEU:O	21:q:6:VAL:HG22	2.01	0.60
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.83	0.60
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.60
10:P:263:PHE:HD2	10:P:333:PRO:O	1.83	0.60
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.31	0.60
23:s:57:LEU:HG	23:s:58:PRO:HD2	1.83	0.60
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.83	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.36	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
1:A:51:PHE:HE1	4:D:80:MET:CE	1.87	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.30	0.60
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.60
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.60
8:H:200:LEU:CD1	8:H:282:TYR:CB	2.79	0.60
10:P:191:VAL:HG13	10:P:192:ARG:HH21	1.66	0.60
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
3:C:80:LEU:HD21	4:D:157:LYS:O	2.02	0.60
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.60
6:F:119:GLU:HB3	6:F:124:THR:CG2	2.32	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.60
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.01	0.60
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.60
10:P:318:LYS:O	10:P:322:ILE:HG13	2.02	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.14	0.60
1:A:41:PHE:CB	16:W:102:GLN:HE22	2.14	0.60
2:B:101:ALA:HB1	25:B:302:UQ9:C1M	2.13	0.60
4:D:95:LEU:HG	4:D:96:ARG:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
8:H:127:TYR:HE1	8:H:207:LEU:C	2.09	0.60
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.60
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.60
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.60
6:F:416:SER:O	6:F:419:ILE:HG22	2.01	0.60
8:H:5:ASN:HD21	19:a:23:THR:HA	1.65	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.32	0.60
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.60
16:W:53:MET:SD	16:W:106:VAL:HG21	2.42	0.60
2:B:100:CYS:SG	24:B:301:SF4:S2	2.99	0.59
2:B:114:MET:HB2	2:B:119:VAL:CG2	2.32	0.59
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.59
9:I:51:LYS:HA	18:Z:33:TYR:CE2	2.37	0.59
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.59
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.59
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
3:C:70:LYS:O	15:V:103:LEU:HD12	2.02	0.59
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.59
8:H:51:ASP:OD2	25:H:401:UQ9:H12	2.02	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.02	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.59
5:E:182:ALA:O	5:E:183:PRO:C	2.42	0.59
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
8:H:200:LEU:HD11	8:H:282:TYR:HB2	1.84	0.59
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.59
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.59
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.59
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.59
1:A:12:LEU:O	1:A:13:LEU:C	2.44	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:315:THR:O	10:P:316:LYS:C	2.45	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
1:A:4:TYR:CE2	29:Z:401:3PE:H231	2.38	0.59
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.37	0.59
3:C:186:ILE:HG13	3:C:187:LEU:N	2.18	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59
5:E:164:PRO:C	5:E:166:LYS:H	2.11	0.59
6:F:235:VAL:HG22	6:F:236:PHE:HD2	1.68	0.59
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.59
4:D:81:THR:HA	4:D:100:GLU:HA	1.85	0.59
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	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
10:P:178:SER:O	10:P:182:ARG:HG2	2.02	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.59
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.59
1:A:2:ASN:HB2	18:Z:143:TYR:CZ	2.38	0.59
1:A:52:SER:O	4:D:103:GLY:CA	2.49	0.59
2:B:120:VAL:CG1	25:H:401:UQ9:C4M	2.80	0.59
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.59
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.59
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.59
23:s:35:LEU:HB3	23:s:38:HIS:HB2	1.85	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.58
4:D:95:LEU:HD22	4:D:458:PHE:HZ	1.68	0.58
4:D:141:TYR:CE1	4:D:142:VAL:CG2	2.86	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.58
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.58
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.58
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.33	0.58
8:H:93:HIS:CE1	19:a:24:ALA:HB1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:127:TYR:CE1	8:H:207:LEU:C	2.82	0.58
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
7:G:126:LEU:HD12	12:R:89:PRO:HB2	1.84	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.85	0.58
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.58
17:X:134:ASP:O	17:X:135:ARG:C	2.45	0.58
6:F:382:CYS:SG	24:F:502:SF4:S1	3.02	0.58
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.58
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.85	0.58
1:A:106:TRP:CD1	8:H:291:LYS:CD	2.87	0.58
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.69	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
8:H:5:ASN:HA	19:a:26:ILE:HD12	1.85	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.58
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.58
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.36	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	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
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.58
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.58
8:H:172:MET:CE	18:Z:46:GLY:CA	2.73	0.58
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.33	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
6:F:44:ASN:HB3	6:F:134:ASP:HB2	1.85	0.58
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
8:H:1:MET:HE3	19:a:29:PHE:CG	2.39	0.58
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.32	0.58
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.58
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.58
6:F:48:ARG:NH1	6:F:48:ARG:HA	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.58
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.58
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.58
1:A:41:PHE:CA	16:W:102:GLN:HE22	2.16	0.57
2:B:154:GLU:O	10:P:89:TYR:OH	2.20	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:90:PRO:HG3	8:H:162:LEU:HB3	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
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.57
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.57
17:X:141:PRO:O	17:X:142:TYR:HB2	2.04	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.86	0.57
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.57
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
1:A:92:PHE:O	1:A:93:ILE:C	2.46	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
8:H:200:LEU:HD13	8:H:282:TYR:HB2	1.85	0.57
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.87	0.57
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.57
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.57
1:A:15:LEU:HD23	8:H:76:THR:HG21	1.86	0.57
1:A:18:ILE:HG13	8:H:222:LEU:HD21	1.86	0.57
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.35	0.57
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.86	0.57
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.57
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
16:W:42:TRP:CZ2	32:W:201:EHZ:O1	2.58	0.57
2:B:124:SER:O	2:B:125:PRO:C	2.42	0.57
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.87	0.57
6:F:39:ASP:HA	6:F:261:TRP:HZ2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
2:B:120:VAL:HG11	25:H:401:UQ9:C4M	2.28	0.57
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.87	0.57
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.86	0.57
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.57
25:H:401:UQ9:H4MA	25:H:401:UQ9:H3MB	1.85	0.57
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.57
21:q:68:MET:SD	21:q:81:MET:HB3	2.44	0.57
2:B:99:CYS:HB3	4:D:141:TYR:HB3	1.87	0.57
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.57
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.57
1:A:33:LYS:HA	2:B:150:ASP:O	2.04	0.57
2:B:91:TRP:HZ2	8:H:51:ASP:CG	2.12	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.57
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.57
17:X:52:ASP:OD2	17:X:55:ARG:HG3	2.04	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	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
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.57
1:A:39:CYS:SG	8:H:208:VAL:HG21	2.45	0.56
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.87	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
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.70	0.56
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.56
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.53	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
10:P:145:PHE:O	10:P:149:PRO:HG2	2.05	0.56
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
2:B:194:CYS:HB2	9:I:153:ILE:O	2.06	0.56
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.56
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.89	0.56
10:P:140:ASP:OD1	10:P:142:GLU:HB2	2.06	0.56
10:P:188:GLU:O	10:P:192:ARG:HG2	2.05	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
17:X:137:LEU:HD23	17:X:138:PRO:O	2.05	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
1:A:26:GLN:O	2:B:154:GLU:HG2	2.05	0.56
3:C:80:LEU:HD22	4:D:157:LYS:HB3	1.88	0.56
4:D:128:THR:H	4:D:131:GLN:NE2	2.01	0.56
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.56
10:P:192:ARG:CZ	10:P:198:ALA:HB3	2.34	0.56
10:P:320:GLU:O	10:P:324:ILE:HG12	2.05	0.56
16:W:104:THR:O	16:W:108:ARG:HG3	2.05	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
1:A:102:LEU:HD22	8:H:294:LEU:HD23	1.86	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
12:R:59:PHE:O	12:R:63:LEU:HG	2.06	0.56
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.56
2:B:114:MET:HE1	2:B:121:PHE:CZ	2.41	0.56
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.56
3:C:184:ARG:HA	16:W:91:MET:SD	2.46	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:401:LEU:HD11	7:G:462:PHE:HE2	1.71	0.56
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.56
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.21	0.56
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.56
2:B:81:LEU:HD22	26:B:303:PC1:H352	1.87	0.56
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.56
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.36	0.56
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.40	0.56
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.56
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.56
26:B:303:PC1:H131	8:H:39:ILE:HD11	1.87	0.56
6:F:293:SER:N	6:F:338:ASP:OD1	2.38	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.56
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.41	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
22:r:7:VAL:O	22:r:11:LEU:HG	2.06	0.56
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.56
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
22:r:9:GLN:O	22:r:12:ARG:HB2	2.06	0.56
1:A:15:LEU:HA	1:A:18:ILE:CD1	2.36	0.55
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.20	0.55
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.19	0.55
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.55
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.55
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.55
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.55
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.55
1:A:69:ILE:HG22	1:A:73:LEU:HD21	1.88	0.55
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.55
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.69	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
8:H:5:ASN:CB	19:a:26:ILE:HD12	2.36	0.55
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.55
1:A:68:GLU:HG3	1:A:69:ILE:N	2.21	0.55
2:B:93:MET:HE2	4:D:87:GLN:OE1	2.06	0.55
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.32	0.55
21:q:6:VAL:HG23	21:q:7:LEU:N	2.21	0.55
1:A:41:PHE:HD2	16:W:102:GLN:CD	2.14	0.55
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.42	0.55
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.89	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
6:F:382:CYS:SG	24:F:502:SF4:S4	3.05	0.55
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.37	0.55
8:H:203:GLY:C	8:H:206:GLU:HB3	2.31	0.55
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.55
12:R:88:HIS:O	12:R:89:PRO:C	2.45	0.55
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.55
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.55
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.55
21:q:13:GLN:HB3	21:q:33:ILE:HG22	1.87	0.55
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.88	0.55
8:H:171:HIS:CB	18:Z:49:ARG:HD3	2.35	0.55
16:W:35:VAL:HG21	32:W:201:EHZ:N2	2.22	0.55
1:A:33:LYS:HZ3	8:H:61:MET:HE1	1.72	0.55
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.46	0.55
6:F:293:SER:HB3	6:F:338:ASP:OD2	2.06	0.55
9:I:75:SER:O	22:r:12:ARG:HG2	2.07	0.55
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.50	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
4:D:142:VAL:HG11	4:D:182:ASN:HD22	1.71	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.55
6:F:300:ILE:HD11	6:F:311:TRP:HD1	1.72	0.55
7:G:35:PHE:O	7:G:101:ASN:HA	2.07	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.88	0.55
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.88	0.55
16:W:23:ILE:HG13	16:W:80:ARG:HG2	1.87	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
1:A:94:LEU:O	1:A:97:ILE:HG12	2.07	0.55
4:D:84:PHE:CD2	4:D:99:LEU:HD23	2.42	0.55
6:F:299:LEU:CD1	6:F:300:ILE:HG23	2.37	0.55
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.55
17:X:49:GLU:OE1	20:b:58:ARG:NH2	2.39	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.55
8:H:5:ASN:CA	19:a:26:ILE:HD12	2.37	0.55
29:H:402:3PE:H331	9:I:63:TRP:CZ2	2.42	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.54
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.89	0.54
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.54
8:H:168:THR:HG23	18:Z:50:MET:HE1	1.89	0.54
9:I:49:ASP:HB3	9:I:52:SER:HB3	1.89	0.54
11:Q:160:TYR:OH	11:Q:164:PHE:HZ	1.89	0.54
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.54
2:B:105:MET:HE2	25:B:302:UQ9:C5	2.37	0.54
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.54
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.07	0.54
6:F:170:GLN:HB3	23:s:48:LEU:HD22	1.89	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
7:G:617:ARG:HH12	16:W:128:GLY:C	2.16	0.54
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.56	0.54
16:W:42:TRP:CZ2	16:W:93:LEU:CA	2.89	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
21:q:17:HIS:NE2	21:q:33:ILE:HG23	2.23	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
5:E:162:THR:HG22	5:E:166:LYS:HA	1.89	0.54
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.07	0.54
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.54
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.54
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.71	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.89	0.54
2:B:92:PRO:HG2	2:B:121:PHE:CD1	2.41	0.54
2:B:114:MET:SD	2:B:121:PHE:CE1	3.01	0.54
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.54
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:131:GLY:HA3	8:H:207:LEU:HD11	1.90	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.90	0.54
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.54
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.54
8:H:316:PRO:HB3	18:Z:58:ARG:HD2	1.88	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	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
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
2:B:174:SER:HA	3:C:203:LEU:CD2	2.37	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	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:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
21:q:9:ARG:HA	21:q:12:GLN:CG	2.37	0.54
1:A:39:CYS:SG	8:H:208:VAL:HG22	2.47	0.54
6:F:80:MET:HE2	6:F:95:THR:HG21	1.89	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.54
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.54
4:D:144:MET:HG2	4:D:223:HIS:H	1.72	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.54
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.54
8:H:21:THR:HG22	8:H:228:TYR:CE2	2.43	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
9:I:123:CYS:SG	24:I:301:SF4:S3	3.06	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
16:W:25:SER:HB3	16:W:30:GLU:HB3	1.88	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.54
2:B:95:PHE:CE1	2:B:97:LEU:CD2	2.90	0.54
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.06	0.54
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ARG:HB3	6:F:289:GLU:OE2	2.07	0.54
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.54
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.54
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.54
10:P:172:ALA:H	10:P:202:ARG:NH2	2.06	0.54
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.54
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
20:b:13:TRP:HA	20:b:13:TRP:CE3	2.42	0.54
1:A:65:PHE:O	1:A:68:GLU:HG2	2.08	0.54
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	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:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
10:P:85:ARG:HE	30:P:401:NDP:C2A	2.21	0.54
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.54
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.54
16:W:53:MET:HB2	16:W:55:LEU:HG	1.89	0.54
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.54
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
2:B:114:MET:HE1	2:B:121:PHE:CE1	2.43	0.53
6:F:119:GLU:HG3	6:F:127:ASP:OD2	2.07	0.53
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.53
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.91	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:109:GLY:O	12:R:63:LEU:HD12	2.08	0.53
10:P:316:LYS:O	10:P:320:GLU:HG2	2.08	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.53
4:D:91:ALA:C	4:D:93:GLY:N	2.52	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.08	0.53
6:F:339:PHE:HA	6:F:349:LEU:HB2	1.90	0.53
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
2:B:138:THR:HG21	4:D:116:LEU:HA	1.91	0.53
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.53
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.53
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.43	0.53
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.53
8:H:179:TRP:CD1	18:Z:43:LEU:CD2	2.91	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	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
1:A:61:THR:O	1:A:64:LEU:N	2.41	0.53
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.53
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.53
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.53
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.90	0.53
6:F:48:ARG:HA	6:F:48:ARG:HH11	1.72	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
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.53
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.91	0.53
8:H:133:LEU:O	8:H:136:VAL:HG12	2.08	0.53
8:H:206:GLU:O	8:H:207:LEU:C	2.49	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.53
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.53
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:5:ASN:ND2	19:a:23:THR:HG23	2.22	0.53
8:H:206:GLU:O	8:H:208:VAL:N	2.41	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
1:A:19:LEU:O	1:A:20:VAL:C	2.48	0.53
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.53
5:E:199:ASP:O	5:E:203:ILE:HG13	2.08	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
4:D:95:LEU:HD13	4:D:458:PHE:CE1	2.44	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:126:LYS:HG3	6:F:275:LEU:CB	2.39	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:43:TYR:CE2	21:q:27:PHE:HZ	2.27	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.91	0.53
8:H:16:ALA:HB2	19:a:15:CYS:CB	2.39	0.53
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.53
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.74	0.53
2:B:105:MET:HE3	25:B:302:UQ9:C1	2.39	0.53
2:B:194:CYS:O	24:B:301:SF4:S2	2.67	0.53
3:C:73:GLN:NE2	15:V:112:TRP:HE1	2.07	0.53
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.07	0.53
6:F:294:VAL:HG12	6:F:337:MET:HB2	1.90	0.53
6:F:329:LYS:HA	6:F:332:CYS:SG	2.49	0.53
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.53
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.23	0.53
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.53
21:q:73:THR:HA	21:q:76:ASP:OD1	2.09	0.53
1:A:49:LEU:HD23	1:A:49:LEU:H	1.72	0.53
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.27	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.90	0.53
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.24	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.53
8:H:131:GLY:HA2	8:H:207:LEU:HD11	1.89	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
1:A:75:LEU:O	1:A:79:ILE:HG12	2.09	0.52
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.52
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.52
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.52
1:A:39:CYS:CB	4:D:85:GLY:HA3	2.36	0.52
1:A:53:MET:HE3	1:A:55:PHE:CE1	2.45	0.52
2:B:105:MET:HE1	4:D:185:MET:CE	2.24	0.52
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.70	0.52
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.90	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.92	0.52
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.90	0.52
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.52
1:A:15:LEU:O	1:A:16:THR:C	2.51	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.10	0.52
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.25	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.52
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
8:H:5:ASN:HD21	19:a:23:THR:CG2	2.21	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:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	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
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.52
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.52
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.33	0.52
6:F:411:SER:HA	6:F:414:GLU:CD	2.34	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.52
7:G:372:PHE:H	7:G:532:PRO:HB2	1.74	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
3:C:170:TRP:CZ2	16:W:91:MET:HE1	2.44	0.52
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.24	0.52
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.52
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.52
3:C:234:LEU:O	4:D:387:GLU:HG3	2.09	0.52
4:D:145:MET:O	4:D:148:GLU:N	2.43	0.52
5:E:65:ILE:HA	5:E:68:ASN:ND2	2.24	0.52
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.52
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
17:X:91:TYR:OH	19:a:28:LYS:HE2	2.10	0.52
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.43	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.52
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:331:VAL:O	6:F:335:VAL:HG23	2.10	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.52
7:G:617:ARG:HH12	16:W:129:HIS:N	2.07	0.52
8:H:224:PHE:CG	25:H:401:UQ9:H10B	2.44	0.52
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.73	0.52
14:T:100:VAL:O	14:T:141:PRO:HD2	2.09	0.52
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.52
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.52
4:D:142:VAL:CG1	4:D:182:ASN:HD22	2.23	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.75	0.52
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.52
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.75	0.52
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.52
8:H:316:PRO:HG3	18:Z:57:ARG:CB	2.39	0.52
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.52
10:P:192:ARG:NH1	10:P:198:ALA:HB3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.52
2:B:170:TYR:OH	4:D:131:GLN:O	2.28	0.52
5:E:164:PRO:C	5:E:166:LYS:N	2.64	0.52
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.74	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
9:I:50:MET:HB3	18:Z:33:TYR:OH	2.10	0.52
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
19:a:2:TRP:O	19:a:3:PHE:C	2.53	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
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
8:H:1:MET:HB2	19:a:30:THR:HG21	1.92	0.52
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.92	0.52
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.52
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
1:A:2:ASN:HB3	18:Z:143:TYR:OH	2.10	0.51
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.51
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.75	0.51
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.91	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
7:G:364:ASP:C	7:G:364:ASP:OD1	2.52	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:64:LEU:CD2	10:P:362:LEU:HD13	2.39	0.51
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.51
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.51
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.51
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.51
1:A:33:LYS:HG3	2:B:150:ASP:O	2.11	0.51
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.39	0.51
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.25	0.51
5:E:177:GLY:O	27:E:301:FES:S1	2.68	0.51
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.51
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.85	0.51
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.51
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.51
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:MET:CE	19:a:29:PHE:CZ	2.93	0.51
8:H:93:HIS:CE1	19:a:24:ALA:CB	2.93	0.51
25:H:401:UQ9:C8	25:H:401:UQ9:C1M	2.88	0.51
9:I:71:GLY:O	22:r:15:ALA:HB1	2.11	0.51
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.29	0.51
1:A:73:LEU:O	1:A:76:PRO:HD2	2.10	0.51
3:C:241:PHE:H	7:G:146:PHE:HE1	1.58	0.51
6:F:225:LEU:N	11:Q:160:TYR:OH	2.39	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:399:VAL:HG21	7:G:462:PHE:CZ	2.44	0.51
8:H:12:PRO:HB2	19:a:19:PRO:HG3	1.93	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.51
6:F:40:ARG:HB3	6:F:289:GLU:CD	2.35	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.51
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.24	0.51
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.51
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.51
8:H:15:ILE:HD11	25:H:401:UQ9:H26A	1.92	0.51
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.75	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.54	0.51
6:F:225:LEU:HB2	11:Q:160:TYR:CZ	2.45	0.51
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.51
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:195:ARG:O	8:H:199:ASP:HB2	2.10	0.51
9:I:49:ASP:HB3	9:I:52:SER:CB	2.40	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
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.51
2:B:87:ARG:HH11	26:B:303:PC1:P	2.34	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	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
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.51
17:X:137:LEU:HG	17:X:138:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.92	0.51
2:B:93:MET:SD	4:D:87:GLN:NE2	2.84	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.51
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.25	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.51
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.51
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.51
9:I:155:CYS:SG	24:I:301:SF4:S2	3.08	0.51
10:P:108:TRP:CZ2	30:P:401:NDP:H2A	2.46	0.51
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	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
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.51
1:A:25:PRO:HG2	8:H:60:PRO:HD3	1.93	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.51
8:H:218:GLY:O	8:H:219:PRO:C	2.54	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
1:A:68:GLU:O	1:A:69:ILE:C	2.53	0.51
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.51
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.51
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	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	2.36	0.51
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.51
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.50
5:E:196:THR:O	5:E:197:PRO:C	2.54	0.50
5:E:245:GLN:HB3	6:F:256:ARG:O	2.11	0.50
6:F:343:VAL:O	6:F:344:GLN:C	2.54	0.50
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:651:PRO:HD2	13:S:56:ARG:HD2	1.93	0.50
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.50
2:B:126:ARG:HD3	2:B:151:GLN:O	2.12	0.50
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.50
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.50
8:H:75:PRO:HB2	8:H:222:LEU:CB	2.41	0.50
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.50
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.50
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.50
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.50
8:H:221:ALA:O	8:H:222:LEU:C	2.52	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
16:W:65:LYS:HE3	16:W:69:MET:HE2	1.92	0.50
19:a:3:PHE:O	19:a:6:LEU:HG	2.11	0.50
1:A:42:ASP:OD1	1:A:42:ASP:N	2.45	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.50
2:B:91:TRP:CH2	8:H:51:ASP:OD2	2.63	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
8:H:135:ALA:HA	8:H:201:THR:OG1	2.12	0.50
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.50
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.50
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.50
5:E:174:GLU:HG2	6:F:369:ARG:NH1	2.14	0.50
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.50
8:H:273:ILE:HD11	29:H:402:3PE:H2A1	1.93	0.50
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.50
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.50
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.47	0.50
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.50
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.50
8:H:69:SER:C	8:H:71:PHE:N	2.68	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.50
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.50
1:A:49:LEU:HD11	4:D:80:MET:HA	1.93	0.50
2:B:95:PHE:CE1	2:B:97:LEU:CG	2.94	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	1.94	0.50
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.50
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.50
6:F:185:ASN:HA	6:F:189:SER:O	2.11	0.50
6:F:342:LEU:HD12	6:F:349:LEU:CA	2.42	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	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	2.11	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:135:GLU:CG	10:P:140:ASP:HA	2.41	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.50
18:Z:58:ARG:NH2	20:b:49:THR:CG2	2.72	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	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:387:LEU:CD1	7:G:514:ASN:CG	2.73	0.50
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.50
8:H:1:MET:CE	19:a:29:PHE:CD1	2.82	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
10:P:172:ALA:H	10:P:202:ARG:HH21	1.59	0.50
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.50
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.50
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
2:B:164:CYS:SG	24:B:301:SF4:S4	3.10	0.50
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.64	0.50
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.50
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.50
8:H:187:ILE:CD1	29:H:402:3PE:H242	2.41	0.50
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:58:ARG:CZ	20:b:49:THR:HG21	2.41	0.50
2:B:100:CYS:HG	24:B:301:SF4:FE4	1.18	0.49
5:E:70:PRO:HB3	23:s:60:PRO:HG3	1.92	0.49
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.49
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.49
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.49
10:P:157:LYS:O	10:P:158:GLU:C	2.53	0.49
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.49
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.49
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.49
20:b:11:ASN:O	20:b:15:LYS:HG2	2.11	0.49
1:A:104:TYR:CE2	1:A:108:GLN:HG3	2.47	0.49
1:A:108:GLN:C	1:A:110:GLY:N	2.68	0.49
3:C:79:CYS:O	3:C:80:LEU:CB	2.60	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.41	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.49
1:A:113:TRP:HH2	8:H:282:TYR:CE2	2.30	0.49
2:B:102:VAL:CG2	4:D:141:TYR:CD1	2.89	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.49
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.49
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	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:150:ARG:O	10:P:151:ALA:C	2.55	0.49
10:P:315:THR:H	10:P:318:LYS:HB3	1.76	0.49
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.49
16:W:32:LYS:CD	32:W:201:EHZ:C19	2.90	0.49
17:X:49:GLU:HB3	17:X:138:PRO:HG3	1.93	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.49
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.47	0.49
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.94	0.49
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.49
8:H:99:ASN:ND2	19:a:40:ARG:O	2.45	0.49
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.49
2:B:68:ARG:HD3	2:B:70:ARG:CG	2.41	0.49
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.94	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
6:F:427:LEU:HB2	28:F:501:FMN:C7M	2.43	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.49
17:X:25:LEU:HB3	18:Z:71:LEU:HD22	1.93	0.49
17:X:130:LYS:HG2	20:b:67:PRO:HA	1.95	0.49
1:A:34:ALA:HB1	8:H:64:LEU:H	1.77	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
2:B:95:PHE:HE1	2:B:97:LEU:CG	2.23	0.49
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.12	0.49
4:D:304:LYS:HE2	9:I:35:THR:N	2.27	0.49
5:E:39:VAL:HG11	7:G:163:LYS:HZ3	1.75	0.49
6:F:49:HIS:O	6:F:50:ASP:C	2.54	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.95	0.49
8:H:19:PHE:CE2	19:a:11:ILE:CG2	2.95	0.49
8:H:172:MET:SD	18:Z:49:ARG:HB3	2.53	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
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.49
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.49
16:W:42:TRP:CE2	16:W:93:LEU:HD12	2.47	0.49
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.49
1:A:108:GLN:O	1:A:110:GLY:N	2.45	0.49
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.77	0.49
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.31	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.95	0.49
6:F:126:LYS:HG3	6:F:275:LEU:HB3	1.94	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.49
8:H:20:LEU:HA	19:a:12:MET:SD	2.52	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.61	0.49
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.49
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.42	0.49
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.49
10:P:191:VAL:CG1	10:P:192:ARG:HH21	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.49
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.49
4:D:79:ASN:O	4:D:80:MET:C	2.55	0.49
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.95	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
6:F:379:CYS:SG	24:F:502:SF4:S1	3.11	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
8:H:220:PHE:O	8:H:221:ALA:C	2.54	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	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
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.49
6:F:299:LEU:HD11	6:F:300:ILE:HG23	1.95	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	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:200:LEU:HD11	8:H:282:TYR:N	2.25	0.49
10:P:192:ARG:CZ	10:P:200:ILE:HD11	2.42	0.49
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.49
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.95	0.49
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.48
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.69	0.48
4:D:375:MET:HE1	7:G:126:LEU:CA	2.42	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	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
1:A:113:TRP:CH2	8:H:282:TYR:CE2	3.01	0.48
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.48
3:C:176:PHE:CE1	16:W:87:ILE:HG21	2.48	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
8:H:19:PHE:CZ	19:a:11:ILE:HD12	2.48	0.48
8:H:127:TYR:CE2	8:H:208:VAL:CG2	2.94	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.37	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
2:B:68:ARG:HG2	2:B:69:SER:N	2.28	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.48
5:E:39:VAL:HG21	7:G:163:LYS:HZ2	1.78	0.48
8:H:75:PRO:HB2	8:H:222:LEU:CD2	2.42	0.48
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.48
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.48
4:D:83:ASN:O	4:D:84:PHE:C	2.56	0.48
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.48
7:G:33:GLU:OE2	7:G:40:SER:HA	2.14	0.48
7:G:117:MET:HE3	7:G:142:GLN:C	2.38	0.48
7:G:179:CYS:HG	24:G:802:SF4:FE3	1.28	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.48	0.48
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.13	0.48
4:D:95:LEU:CG	4:D:96:ARG:N	2.75	0.48
4:D:117:HIS:HD2	4:D:462:ASP:O	1.96	0.48
4:D:136:PHE:HA	4:D:139:LEU:HG	1.95	0.48
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	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	2.41	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:59:GLU:OE2	8:H:61:MET:SD	2.71	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
10:P:170:LEU:HG	10:P:171:ASN:N	2.29	0.48
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.95	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.48
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.60	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.96	0.48
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.48
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:126:LYS:HE2	6:F:274:LYS:NZ	2.27	0.48
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.48
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.94	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.14	0.48
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.48
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.49	0.48
4:D:279:THR:HA	15:V:12:VAL:HG13	1.96	0.48
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.48
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.48
18:Z:62:ILE:HG12	20:b:49:THR:HA	1.94	0.48
1:A:14:SER:C	1:A:18:ILE:CD1	2.87	0.48
2:B:126:ARG:HB2	8:H:213:VAL:O	2.14	0.48
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.49	0.48
3:C:209:LEU:HD21	16:W:108:ARG:NH1	2.29	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.48
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.79	0.48
7:G:688:GLN:HA	7:G:693:ASP:CB	2.44	0.48
8:H:64:LEU:HD21	10:P:362:LEU:HD13	1.95	0.48
8:H:68:MET:O	8:H:71:PHE:HB2	2.13	0.48
25:H:401:UQ9:C8	25:H:401:UQ9:H1MA	2.44	0.48
9:I:62:MET:HG3	18:Z:35:MET:SD	2.54	0.48
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.30	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.48
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.48
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.48
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.48
3:C:70:LYS:HB2	15:V:99:PRO:O	2.14	0.47
4:D:84:PHE:CE2	4:D:99:LEU:CD2	2.97	0.47
4:D:95:LEU:HD22	4:D:458:PHE:CZ	2.48	0.47
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.97	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.14	0.47
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.79	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.47
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.13	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
25:B:302:UQ9:H4MB	25:B:302:UQ9:H3MA	1.95	0.47
4:D:197:MET:HE1	8:H:274:ARG:HE	1.79	0.47
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.47
5:E:221:ARG:HH21	5:E:227:ALA:HB2	1.79	0.47
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.47
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.96	0.47
9:I:171:PRO:HB3	21:q:93:MET:CE	2.38	0.47
10:P:360:ARG:HD3	10:P:360:ARG:O	2.14	0.47
17:X:7:LEU:O	18:Z:88:ARG:NH1	2.47	0.47
17:X:139:GLU:O	17:X:140:ASN:C	2.57	0.47
1:A:44:THR:HG22	16:W:99:VAL:CG1	2.41	0.47
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.47
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.49	0.47
6:F:110:PRO:O	6:F:238:CYS:HB3	2.14	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.47
6:F:383:THR:O	6:F:384:PRO:C	2.55	0.47
8:H:131:GLY:HA3	8:H:207:LEU:CD1	2.43	0.47
8:H:296:LEU:HD21	29:H:402:3PE:H351	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:59:PHE:CB	10:P:130:ILE:HD11	2.42	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.47
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.47
3:C:151:PRO:HG2	16:W:23:ILE:HG23	1.96	0.47
4:D:84:PHE:CD2	4:D:97:LEU:HD12	2.49	0.47
4:D:88:HIS:NE2	8:H:207:LEU:O	2.47	0.47
6:F:270:ASN:ND2	6:F:338:ASP:HB3	2.29	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.96	0.47
12:R:89:PRO:HG2	12:R:106:TYR:CE2	2.49	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.47
16:W:71:MET:C	16:W:73:ASN:N	2.70	0.47
2:B:105:MET:HE1	25:B:302:UQ9:H3MB	1.97	0.47
2:B:140:LYS:O	2:B:143:PRO:HD2	2.15	0.47
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.48	0.47
7:G:557:ARG:CG	7:G:579:MET:HE3	2.32	0.47
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	1.95	0.47
11:Q:160:TYR:CD2	11:Q:164:PHE:CE2	2.91	0.47
12:R:88:HIS:HE1	12:R:91:VAL:HG22	1.80	0.47
4:D:87:GLN:O	4:D:88:HIS:C	2.58	0.47
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.47
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.47
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.47
6:F:44:ASN:ND2	6:F:133:HIS:O	2.48	0.47
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.97	0.47
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.95	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:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.47
10:P:131:GLY:HA3	30:P:401:NDP:O3D	2.15	0.47
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.47
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:69:ILE:HG23	20:b:54:PRO:HD3	1.95	0.47
1:A:47:ALA:HB1	8:H:126:LYS:N	2.30	0.47
2:B:97:LEU:HB2	2:B:134:ALA:O	2.15	0.47
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.47
4:D:95:LEU:HD12	4:D:96:ARG:H	1.79	0.47
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.47
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.47
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.47
7:G:496:MET:O	7:G:500:ILE:HG13	2.14	0.47
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.47
8:H:93:HIS:CE1	19:a:24:ALA:HA	2.50	0.47
8:H:140:ILE:HG13	8:H:141:SER:N	2.29	0.47
9:I:209:TYR:CG	12:R:86:LEU:HD21	2.50	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
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	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:48:TYR:OH	21:q:83:PRO:HD2	2.14	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47
2:B:135:GLY:HA2	24:B:301:SF4:S3	2.54	0.47
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.47
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.47
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.48	0.47
1:A:48:ARG:HG3	1:A:48:ARG:O	2.14	0.47
1:A:111:LEU:HB2	8:H:291:LYS:NZ	2.30	0.47
2:B:105:MET:HE2	25:B:302:UQ9:C3	2.45	0.47
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.47
6:F:51:TRP:HZ2	23:s:36:GLN:HG3	1.80	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
9:I:106:TYR:O	9:I:107:PRO:C	2.55	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
18:Z:26:PRO:HG3	22:r:17:GLY:O	2.15	0.47
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.47
1:A:102:LEU:CD2	8:H:295:PRO:HG3	2.45	0.47
5:E:222:PHE:O	5:E:223:CYS:C	2.56	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.96	0.47
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.50	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:66:GLY:O	10:P:69:VAL:N	2.48	0.47
1:A:24:LEU:N	1:A:25:PRO:CD	2.78	0.46
25:B:302:UQ9:H3MA	4:D:189:THR:HG21	1.97	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
6:F:35:LEU:HG	6:F:39:ASP:HB2	1.97	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.50	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:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.46
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.46
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.29	0.46
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.96	0.46
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	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
9:I:123:CYS:SG	24:I:301:SF4:S4	3.13	0.46
10:P:192:ARG:HH12	10:P:198:ALA:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.46
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.46
1:A:2:ASN:CB	18:Z:143:TYR:CZ	2.98	0.46
2:B:105:MET:SD	4:D:185:MET:HE1	2.55	0.46
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.80	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
6:F:39:ASP:CA	6:F:261:TRP:HZ2	2.28	0.46
6:F:425:CYS:SG	24:F:502:SF4:S4	3.13	0.46
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.46
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.46
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.50	0.46
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.46
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.58	0.46
18:Z:86:ILE:CG2	18:Z:128:ARG:HE	2.16	0.46
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	0.46
23:s:55:PHE:O	23:s:56:ARG:C	2.57	0.46
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.50	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:251:SER:N	6:F:252:PRO:HD2	2.30	0.46
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.46
8:H:200:LEU:HD12	8:H:282:TYR:N	2.25	0.46
8:H:312:ALA:CB	20:b:38:TYR:HB3	2.45	0.46
9:I:79:ARG:HG2	22:r:12:ARG:NH2	2.29	0.46
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.16	0.46
4:D:95:LEU:HD13	4:D:458:PHE:HE1	1.80	0.46
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.46
6:F:136:HIS:O	6:F:137:LYS:C	2.55	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:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.46
8:H:51:ASP:OD1	8:H:54:LYS:HE3	2.15	0.46
8:H:51:ASP:OD2	25:H:401:UQ9:C12	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:123:GLY:HA2	18:Z:66:GLU:OE2	2.15	0.46
21:q:8:LYS:HG2	21:q:12:GLN:HE21	1.79	0.46
21:q:14:VAL:HA	21:q:23:LEU:HD13	1.97	0.46
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.95	0.46
1:A:87:MET:HE3	1:A:87:MET:HB3	1.84	0.46
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.80	0.46
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.46
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:75:PRO:HB2	8:H:222:LEU:HD22	1.98	0.46
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.46
12:R:32:THR:HA	12:R:55:VAL:CG2	2.45	0.46
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
2:B:97:LEU:O	2:B:98:ALA:C	2.56	0.46
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.96	0.46
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.46
8:H:215:TYR:O	8:H:220:PHE:HB2	2.16	0.46
9:I:51:LYS:HA	18:Z:33:TYR:HE2	1.77	0.46
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.74	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.46
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.46
23:s:52:LEU:HB3	23:s:56:ARG:HH11	1.81	0.46
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.45	0.46
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.15	0.46
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:45:GLU:O	5:E:50:THR:HG21	2.15	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.46
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.46
6:F:213:ILE:CG2	6:F:224:ARG:HH21	2.27	0.46
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.46
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	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
3:C:75:VAL:HG23	3:C:83:LEU:HD11	1.98	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
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
16:W:71:MET:O	16:W:72:LYS:C	2.59	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.46
1:A:48:ARG:HH11	8:H:124:ASN:HA	1.81	0.46
1:A:51:PHE:CE1	8:H:130:PHE:CE1	2.97	0.46
1:A:72:LEU:C	1:A:74:PRO:HD2	2.40	0.46
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.51	0.46
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.46
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.46
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.46
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.46
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
10:P:315:THR:HB	10:P:318:LYS:HB2	1.98	0.46
12:R:33:HIS:HE1	12:R:56:ASN:HD22	1.64	0.46
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.46
1:A:41:PHE:CG	16:W:102:GLN:NE2	2.84	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
6:F:358:ASP:C	6:F:360:SER:H	2.22	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.45
8:H:168:THR:CG2	18:Z:50:MET:HE1	2.45	0.45
10:P:235:THR:HG22	10:P:323:HIS:O	2.15	0.45
12:R:32:THR:HG21	21:q:129:THR:HG23	1.98	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
20:b:16:GLU:C	20:b:18:VAL:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HG13	8:H:222:LEU:CD2	2.46	0.45
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	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
29:H:402:3PE:H241	29:H:402:3PE:H272	1.60	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.51	0.45
1:A:56:PHE:O	1:A:57:LEU:C	2.58	0.45
1:A:73:LEU:HA	8:H:151:LEU:HD13	1.98	0.45
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.96	0.45
5:E:133:VAL:HG22	5:E:185:VAL:CG1	2.45	0.45
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.51	0.45
6:F:137:LYS:HG2	6:F:249:ALA:HB1	1.98	0.45
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.99	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
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.81	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
9:I:92:PRO:HB3	21:q:92:CYS:HB2	1.98	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.45
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.45
17:X:53:PRO:HG2	18:Z:116:TRP:NE1	2.31	0.45
1:A:18:ILE:HD11	8:H:76:THR:CG2	2.31	0.45
1:A:37:TYR:CE1	2:B:125:PRO:HD2	2.52	0.45
1:A:37:TYR:HE2	8:H:208:VAL:HG11	1.82	0.45
1:A:102:LEU:HD23	8:H:295:PRO:HG3	1.97	0.45
1:A:108:GLN:C	1:A:110:GLY:H	2.24	0.45
2:B:105:MET:CE	25:B:302:UQ9:C2	2.94	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
3:C:134:LEU:H	3:C:134:LEU:HD12	1.81	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
5:E:59:TYR:O	5:E:62:ILE:HB	2.17	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:122:HIS:HB3	12:R:46:VAL:HG12	1.98	0.45
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.45
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.51	0.45
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.97	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:O	8:H:160:TYR:OH	2.35	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.44	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:92:HIS:HE2	4:D:141:TYR:HH	1.65	0.45
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.97	0.45
5:E:163:THR:O	5:E:166:LYS:HD3	2.16	0.45
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.46	0.45
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.31	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
9:I:90:LYS:HG2	21:q:90:LEU:HD21	1.97	0.45
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.45
12:R:91:VAL:HG11	12:R:106:TYR:HE2	1.82	0.45
2:B:114:MET:O	2:B:119:VAL:HG22	2.16	0.45
2:B:125:PRO:O	2:B:126:ARG:C	2.58	0.45
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.31	0.45
5:E:48:PRO:C	5:E:50:THR:N	2.74	0.45
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.99	0.45
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.45
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.99	0.45
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.44	0.45
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.76	0.45
1:A:62:PHE:CD1	8:H:144:VAL:HG23	2.43	0.45
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.32	0.45
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.80	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
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.16	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:48:TRP:CE3	20:b:55:VAL:HG21	2.51	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.45
5:E:162:THR:CG2	5:E:166:LYS:HA	2.46	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
6:F:249:ALA:O	6:F:252:PRO:HD2	2.16	0.45
7:G:401:LEU:HD11	7:G:462:PHE:CE2	2.51	0.45
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.45
8:H:203:GLY:O	8:H:206:GLU:HB3	2.17	0.45
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.45
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.32	0.45
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.45
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.45
16:W:32:LYS:CE	32:W:201:EHZ:C19	2.90	0.45
1:A:62:PHE:HE1	8:H:144:VAL:HG22	1.65	0.45
2:B:93:MET:HE3	2:B:93:MET:HB2	1.76	0.45
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.45
25:B:302:UQ9:H10	4:D:200:PHE:CZ	2.49	0.45
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.45
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.45
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:293:PHE:CE1	29:H:402:3PE:H32	2.52	0.45
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	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
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.90	0.45
4:D:97:LEU:HD23	4:D:111:PRO:HA	1.98	0.45
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.45
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.52	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
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.45
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.45
8:H:71:PHE:O	8:H:75:PRO:HD2	2.16	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	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
9:I:50:MET:O	9:I:54:THR:HG23	2.17	0.45
23:s:52:LEU:O	23:s:56:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:MET:HE3	1:A:55:PHE:CD1	2.52	0.44
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.44
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.44
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.44
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.44
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.44
5:E:222:PHE:H	5:E:225:GLU:CD	2.25	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.98	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	2.00	0.44
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:450:LYS:CD	7:G:453:GLN:HG3	2.32	0.44
8:H:127:TYR:HD1	8:H:207:LEU:HB3	1.82	0.44
8:H:303:TRP:HE3	20:b:29:ALA:CB	2.24	0.44
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.44
11:Q:160:TYR:CE1	11:Q:164:PHE:HZ	2.25	0.44
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.44
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
1:A:60:ILE:O	1:A:61:THR:C	2.57	0.44
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.98	0.44
3:C:170:TRP:CE2	16:W:91:MET:HE1	2.52	0.44
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.44
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.44
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.44
8:H:167:THR:O	18:Z:53:TRP:NE1	2.46	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.97	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.97	0.44
1:A:97:ILE:HG13	1:A:98:LEU:N	2.32	0.44
3:C:98:PHE:HB2	15:V:94:MET:CE	2.47	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.44
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.44
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.52	0.44
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.80	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
9:I:78:PHE:HB2	22:r:12:ARG:HG2	2.00	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.44
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.44
6:F:224:ARG:HG2	11:Q:164:PHE:CZ	2.52	0.44
6:F:398:ARG:HH12	6:F:408:GLU:CD	2.25	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
8:H:93:HIS:HE1	19:a:24:ALA:HB1	1.81	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	2.18	0.44
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.44
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.44
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.44
3:C:70:LYS:O	15:V:103:LEU:HA	2.18	0.44
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.80	0.44
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:163:THR:HG23	5:E:168:PHE:O	2.17	0.44
7:G:259:SER:HA	7:G:281:ILE:HD13	1.98	0.44
7:G:450:LYS:HG3	7:G:450:LYS:O	2.18	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
8:H:202:GLU:HA	8:H:210:GLY:HA3	2.00	0.44
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44
17:X:127:LYS:HD2	20:b:70:PRO:O	2.18	0.44
21:q:21:ARG:O	21:q:25:ARG:HG3	2.17	0.44
1:A:53:MET:HE2	1:A:56:PHE:N	2.32	0.44
1:A:91:ALA:O	1:A:94:LEU:HB3	2.17	0.44
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.44
6:F:126:LYS:O	6:F:129:GLU:HG2	2.18	0.44
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.44
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.44
8:H:277:TYR:CE2	29:H:402:3PE:H271	2.53	0.44
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.44
12:R:79:CYS:O	12:R:88:HIS:CE1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.44
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
1:A:93:ILE:O	1:A:97:ILE:HG23	2.18	0.44
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.06	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
6:F:294:VAL:CG1	6:F:337:MET:HG3	2.48	0.44
6:F:299:LEU:C	6:F:299:LEU:CD1	2.91	0.44
6:F:427:LEU:HB2	28:F:501:FMN:HM73	2.00	0.44
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.48	0.44
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	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:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.44
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.44
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
1:A:38:GLU:CD	1:A:43:PRO:HA	2.42	0.44
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.44
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.44
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.44
6:F:300:ILE:HD13	6:F:307:VAL:N	2.21	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
9:I:90:LYS:HG3	21:q:90:LEU:CD2	2.48	0.44
10:P:355:ARG:NH2	10:P:356:HIS:CE1	2.80	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.44
1:A:15:LEU:O	1:A:18:ILE:N	2.51	0.44
1:A:67:LEU:O	1:A:70:ALA:HB3	2.18	0.44
1:A:97:ILE:O	1:A:98:LEU:C	2.57	0.44
25:B:302:UQ9:O5	25:B:302:UQ9:C8	2.66	0.44
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.44
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.44
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
8:H:99:ASN:ND2	19:a:40:ARG:HA	2.32	0.44
8:H:186:PHE:CE2	29:H:402:3PE:H2B1	2.52	0.44
10:P:310:PHE:O	10:P:311:GLU:C	2.59	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.44
21:q:4:VAL:HG23	21:q:5:GLU:N	2.33	0.44
1:A:34:ALA:HB1	8:H:64:LEU:N	2.33	0.43
2:B:105:MET:HE2	25:B:302:UQ9:C4	2.48	0.43
4:D:137:ASP:OD1	4:D:148:GLU:HG3	2.17	0.43
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.43
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.83	0.43
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.43
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.43
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.43
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
13:S:85:ASP:O	13:S:89:ARG:N	2.41	0.43
20:b:11:ASN:OD1	20:b:12:ALA:N	2.50	0.43
2:B:90:LEU:HD22	2:B:130:VAL:HG21	1.99	0.43
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:119:GLU:HB3	6:F:124:THR:HG22	2.00	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
8:H:1:MET:HE3	19:a:29:PHE:CZ	2.50	0.43
8:H:227:GLU:O	8:H:228:TYR:C	2.60	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.43
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.43
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.00	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.43
1:A:21:ALA:O	8:H:60:PRO:CG	2.61	0.43
3:C:221:GLU:OE1	16:W:114:GLU:HB2	2.18	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.34	0.43
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.43
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.43
7:G:466:LEU:HD13	7:G:500:ILE:HD13	2.00	0.43
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:253:GLU:O	8:H:257:THR:N	2.43	0.43
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.43
10:P:73:LEU:HD23	10:P:73:LEU:HA	1.89	0.43
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.47	0.43
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.43
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.43
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.43
16:W:120:ASP:HB3	16:W:123:SER:OG	2.18	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.43
7:G:303:THR:HB	7:G:614:GLY:HA3	1.99	0.43
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.43
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.43
8:H:127:TYR:HE1	8:H:207:LEU:O	2.00	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:78:PHE:HB2	22:r:12:ARG:CG	2.48	0.43
10:P:130:ILE:N	10:P:130:ILE:HD12	2.33	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.43
21:q:22:GLY:O	21:q:26:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.43
1:A:37:TYR:CE1	2:B:125:PRO:CD	3.02	0.43
2:B:77:LYS:HD3	2:B:77:LYS:HA	1.64	0.43
3:C:160:ILE:HB	4:D:286:TYR:CE1	2.54	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
5:E:192:TYR:OH	5:E:213:PRO:HD2	2.18	0.43
5:E:195:LEU:HD21	5:E:218:ARG:HG2	1.99	0.43
6:F:38:GLU:HG3	6:F:39:ASP:N	2.34	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
12:R:88:HIS:ND1	12:R:89:PRO:O	2.50	0.43
16:W:71:MET:O	16:W:74:ALA:N	2.39	0.43
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.43
1:A:41:PHE:HE1	4:D:86:PRO:CG	2.32	0.43
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.83	0.43
6:F:126:LYS:HE2	6:F:274:LYS:HZ3	1.84	0.43
6:F:235:VAL:O	6:F:236:PHE:C	2.62	0.43
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.18	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
8:H:228:TYR:N	8:H:228:TYR:CD1	2.87	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
9:I:162:CYS:SG	24:I:302:SF4:S2	3.17	0.43
9:I:197:TRP:CZ3	21:q:84:PRO:HA	2.53	0.43
11:Q:160:TYR:OH	11:Q:164:PHE:CZ	2.69	0.43
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43
21:q:79:GLY:O	21:q:82:VAL:HG22	2.19	0.43
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.43
1:A:65:PHE:CD2	8:H:294:LEU:HD21	2.53	0.43
2:B:123:ALA:O	2:B:124:SER:C	2.61	0.43
3:C:186:ILE:HB	4:D:113:ILE:HD11	2.01	0.43
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.43
6:F:173:ILE:HD13	6:F:195:VAL:CG1	2.48	0.43
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.43
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.43
8:H:1:MET:CB	19:a:30:THR:CG2	2.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.43
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
11:Q:55:VAL:HG21	16:W:78:ASP:OD1	2.19	0.43
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.43
18:Z:72:MET:O	18:Z:73:PRO:C	2.59	0.43
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.43
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.19	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.43
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.43
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.43
8:H:94:PRO:O	19:a:27:HIS:CE1	2.68	0.43
8:H:96:ILE:HG12	18:Z:143:TYR:HH	1.77	0.43
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.43
8:H:179:TRP:HE1	18:Z:43:LEU:HG	1.84	0.43
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
21:q:25:ARG:O	21:q:26:VAL:C	2.62	0.43
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.43
1:A:18:ILE:CG1	8:H:222:LEU:HD21	2.47	0.43
1:A:84:THR:CG2	20:b:46:ASN:HD21	2.32	0.43
1:A:113:TRP:CH2	8:H:286:MET:SD	3.12	0.43
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
4:D:376:GLU:HG2	7:G:121:LEU:HD12	2.00	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:419:ILE:HG23	6:F:432:ALA:HB2	2.01	0.43
7:G:36:VAL:O	7:G:39:GLN:HG2	2.19	0.43
7:G:466:LEU:O	7:G:467:LYS:C	2.61	0.43
8:H:7:LEU:HD13	8:H:7:LEU:HA	1.75	0.43
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.43
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.43
18:Z:86:ILE:HA	18:Z:128:ARG:NH2	2.33	0.43
1:A:42:ASP:O	1:A:43:PRO:C	2.61	0.43
4:D:143:SER:HA	4:D:178:THR:CG2	2.49	0.43
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.01	0.43
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.43
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:19:PHE:CB	19:a:12:MET:HG3	2.48	0.43
8:H:138:GLN:HG3	8:H:139:THR:N	2.34	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.43
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.43
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.43
1:A:27:MET:HE1	8:H:60:PRO:O	2.19	0.42
1:A:74:PRO:C	1:A:76:PRO:HD2	2.44	0.42
3:C:136:PHE:O	3:C:137:ASN:C	2.60	0.42
5:E:198:LYS:HE2	5:E:198:LYS:HB2	1.91	0.42
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.42
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.53	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.48	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.19	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
21:q:5:GLU:HG3	21:q:9:ARG:HE	1.84	0.42
22:r:20:LEU:C	22:r:20:LEU:CD1	2.89	0.42
2:B:81:LEU:CD2	26:B:303:PC1:H352	2.48	0.42
2:B:146:ARG:NH2	3:C:211:TYR:CZ	2.86	0.42
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.42
4:D:264:ASN:O	9:I:65:GLU:OE1	2.37	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:179:CYS:SG	27:E:301:FES:S1	3.18	0.42
6:F:340:ASP:O	6:F:343:VAL:HB	2.19	0.42
7:G:169:VAL:HG11	7:G:231:LEU:HD13	2.00	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:5:ASN:HD21	19:a:23:THR:CA	2.32	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.42
10:P:237:LYS:HE3	10:P:322:ILE:O	2.19	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.42
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.42
1:A:71:LEU:HB2	1:A:94:LEU:HD21	2.01	0.42
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.42
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.48	0.42
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.00	0.42
5:E:221:ARG:HB2	5:E:225:GLU:HG2	2.01	0.42
6:F:224:ARG:HD3	11:Q:164:PHE:CD1	2.55	0.42
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.42
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
7:G:664:TYR:OH	13:S:23:LEU:HD11	2.20	0.42
8:H:204:GLU:O	8:H:205:SER:HB2	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.19	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.54	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.42
4:D:95:LEU:HB2	4:D:458:PHE:CE1	2.55	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
6:F:47:GLY:N	6:F:133:HIS:ND1	2.68	0.42
6:F:166:ALA:HB1	23:s:45:PHE:HD2	1.84	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:617:ARG:NH1	16:W:129:HIS:N	2.67	0.42
29:H:402:3PE:H3I2	20:b:28:LEU:CD2	2.49	0.42
9:I:59:ARG:O	9:I:59:ARG:HG2	2.20	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.42
12:R:31:ILE:HG22	12:R:55:VAL:HG21	2.02	0.42
12:R:51:ARG:NH2	21:q:125:VAL:HG12	2.24	0.42
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.42
29:Z:401:3PE:H2E1	29:Z:401:3PE:C2I	2.46	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
2:B:101:ALA:O	25:B:302:UQ9:H1MA	2.19	0.42
4:D:139:LEU:HD13	4:D:424:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.34	0.42
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.42
5:E:137:THR:HG22	6:F:370:LEU:HD21	2.02	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.42
6:F:333:GLU:HG2	6:F:334:THR:N	2.34	0.42
6:F:398:ARG:NH1	6:F:408:GLU:CD	2.78	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
8:H:1:MET:HB3	19:a:26:ILE:HG22	1.96	0.42
9:I:152:CYS:SG	24:I:301:SF4:S1	3.17	0.42
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.00	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
21:q:9:ARG:CA	21:q:12:GLN:HG2	2.43	0.42
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.49	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.81	0.42
5:E:94:ILE:HD13	7:G:209:TYR:CE2	2.53	0.42
6:F:113:LEU:HD13	6:F:149:MET:SD	2.59	0.42
6:F:228:PRO:CG	11:Q:160:TYR:HD2	2.30	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:283:GLU:O	7:G:283:GLU:CG	2.51	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
17:X:142:TYR:HA	18:Z:115:ARG:HD3	2.01	0.42
23:s:53:SER:HA	23:s:56:ARG:HG2	2.02	0.42
1:A:108:GLN:OE1	1:A:108:GLN:HA	2.19	0.42
1:A:112:GLU:O	1:A:113:TRP:HB2	2.18	0.42
2:B:69:SER:O	2:B:70:ARG:C	2.61	0.42
3:C:64:VAL:HG11	3:C:85:ILE:HD13	2.02	0.42
4:D:84:PHE:CE2	4:D:99:LEU:HD23	2.55	0.42
4:D:92:HIS:O	4:D:92:HIS:CG	2.72	0.42
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.42
6:F:416:SER:O	6:F:419:ILE:CG2	2.65	0.42
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:200:LEU:HD11	8:H:282:TYR:CB	2.47	0.42
11:Q:160:TYR:CE1	11:Q:164:PHE:CZ	3.02	0.42
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:29:ALA:HB2	18:Z:71:LEU:CD1	2.43	0.42
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.42
1:A:24:LEU:H	1:A:25:PRO:HD3	1.84	0.42
2:B:112:TYR:HE1	9:I:84:ILE:HD11	1.72	0.42
2:B:122:ARG:HD2	2:B:122:ARG:HA	1.66	0.42
4:D:82:LEU:HG	4:D:83:ASN:N	2.35	0.42
4:D:91:ALA:O	4:D:93:GLY:N	2.52	0.42
4:D:144:MET:HE2	4:D:144:MET:HB2	1.93	0.42
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:32:ILE:CG2	7:G:98:LYS:HA	2.50	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.42
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.83	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.42
21:q:64:TYR:CD1	21:q:77:VAL:HG11	2.54	0.42
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.02	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
5:E:136:THR:HB	27:E:301:FES:S2	2.60	0.42
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.47	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.34	0.42
6:F:208:GLU:OE1	6:F:210:THR:N	2.52	0.42
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.50	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
8:H:59:GLU:OE1	8:H:61:MET:SD	2.78	0.42
8:H:90:PRO:O	8:H:91:MET:C	2.60	0.42
8:H:157:ASN:ND2	8:H:164:THR:OG1	2.49	0.42
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:152:CYS:SG	24:I:301:SF4:S3	3.17	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
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.42
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.81	0.42
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.42
2:B:116:ARG:NH2	9:I:86:TYR:H	2.18	0.42
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.42
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.42
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.42
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.42
6:F:70:LEU:O	6:F:71:LYS:C	2.63	0.42
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.42
6:F:315:LEU:HD23	6:F:315:LEU:O	2.20	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
8:H:20:LEU:CD2	8:H:228:TYR:CD2	3.02	0.42
8:H:99:ASN:HD21	19:a:40:ARG:CA	2.32	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
12:R:81:GLY:HA3	12:R:88:HIS:CD2	2.55	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	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
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
23:s:35:LEU:HA	23:s:37:HIS:CE1	2.55	0.42
1:A:49:LEU:HD23	1:A:49:LEU:N	2.34	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
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
1:A:99:SER:O	1:A:100:LEU:C	2.63	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:160:ILE:CD1	4:D:286:TYR:HE1	2.28	0.41
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.41
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.41
6:F:410:ASP:OD1	6:F:411:SER:N	2.53	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
8:H:93:HIS:CE1	19:a:28:LYS:NZ	2.88	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:H:402:3PE:H3H2	29:H:402:3PE:H3E1	1.90	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
10:P:331:ASP:CG	10:P:332:LEU:H	2.28	0.41
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.41
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.41
17:X:52:ASP:O	17:X:53:PRO:C	2.61	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
21:q:85:GLU:HG2	21:q:98:PRO:HB3	2.01	0.41
1:A:46:SER:O	1:A:47:ALA:HB3	2.21	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
4:D:375:MET:HE2	4:D:375:MET:HB2	1.67	0.41
5:E:69:TYR:HB3	5:E:70:PRO:CD	2.50	0.41
6:F:47:GLY:C	6:F:49:HIS:H	2.27	0.41
6:F:126:LYS:HG3	6:F:275:LEU:HB2	2.01	0.41
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.41
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.41
8:H:5:ASN:OD1	19:a:23:THR:CA	2.67	0.41
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.38	0.41
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
19:a:17:VAL:O	19:a:18:ILE:C	2.62	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:112:GLU:C	1:A:113:TRP:HD1	2.28	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
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:86:PRO:HG3	4:D:115:LEU:CD2	2.50	0.41
4:D:88:HIS:CE1	4:D:90:ALA:HB3	2.55	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.50	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.45	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.41
9:I:49:ASP:OD2	9:I:51:LYS:HB2	2.20	0.41
10:P:315:THR:HB	10:P:318:LYS:H	1.85	0.41
10:P:316:LYS:C	10:P:316:LYS:HD3	2.46	0.41
12:R:88:HIS:CB	12:R:89:PRO:CD	2.65	0.41
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
1:A:37:TYR:CE1	2:B:125:PRO:CG	3.04	0.41
2:B:95:PHE:CE1	2:B:97:LEU:CD1	2.81	0.41
4:D:144:MET:SD	4:D:222:MET:HB2	2.60	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.41
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:172:MET:HB3	18:Z:49:ARG:HD2	2.03	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.55	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.41
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.21	0.41
20:b:25:VAL:O	20:b:26:TRP:C	2.64	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.21	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
4:D:142:VAL:HG11	4:D:182:ASN:ND2	2.35	0.41
4:D:144:MET:HG2	4:D:222:MET:HB2	2.03	0.41
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.41
6:F:363:ILE:O	6:F:364:VAL:C	2.64	0.41
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:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.55	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:231:LEU:HD12	10:P:231:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:CYS:HB3	4:D:85:GLY:CA	2.40	0.41
1:A:113:TRP:N	1:A:113:TRP:CD1	2.87	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.41
2:B:121:PHE:CD1	2:B:121:PHE:N	2.88	0.41
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.41
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
11:Q:55:VAL:HG21	16:W:80:ARG:HH11	1.85	0.41
16:W:38:LEU:HG	16:W:70:PHE:HZ	1.84	0.41
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.41
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.35	0.41
6:F:311:TRP:CH2	6:F:333:GLU:HB3	2.55	0.41
7:G:496:MET:HG2	7:G:500:ILE:HD11	2.01	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.41
8:H:135:ALA:HB2	8:H:201:THR:HG23	2.02	0.41
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.41
10:P:146:VAL:HG13	10:P:147:ASN:OD1	2.21	0.41
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.41
10:P:231:LEU:CD1	10:P:290:PRO:HB2	2.51	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
1:A:57:LEU:C	1:A:57:LEU:HD23	2.46	0.41
1:A:112:GLU:C	1:A:113:TRP:CD1	2.99	0.41
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.85	0.41
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.41
5:E:192:TYR:CD2	5:E:203:ILE:HD13	2.56	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:119:GLU:OE1	6:F:119:GLU:HA	2.21	0.41
6:F:232:ASP:OD1	6:F:232:ASP:N	2.54	0.41
6:F:299:LEU:HD12	6:F:300:ILE:HG23	2.01	0.41
6:F:300:ILE:CD1	6:F:307:VAL:HG23	2.49	0.41
6:F:337:MET:HE2	6:F:337:MET:HA	2.02	0.41
6:F:337:MET:O	6:F:338:ASP:OD1	2.38	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.41
7:G:339:ALA:CB	7:G:537:ILE:CD1	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:PRO:HD2	8:H:45:ILE:CD1	2.51	0.41
8:H:71:PHE:HA	8:H:215:TYR:OH	2.19	0.41
8:H:220:PHE:O	8:H:223:PHE:N	2.53	0.41
8:H:296:LEU:CD2	29:H:402:3PE:H351	2.50	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
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.56	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
22:r:10:LYS:O	22:r:11:LEU:C	2.62	0.41
1:A:69:ILE:O	1:A:73:LEU:HG	2.20	0.41
1:A:103:ALA:O	1:A:106:TRP:HB3	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
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.85	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
3:C:72:VAL:O	3:C:72:VAL:HG23	2.20	0.41
3:C:241:PHE:CD2	7:G:146:PHE:CZ	3.09	0.41
4:D:119:GLY:O	4:D:123:LEU:HD23	2.21	0.41
4:D:141:TYR:HE2	4:D:457:VAL:HG13	1.82	0.41
4:D:269:ARG:O	4:D:273:VAL:HG23	2.21	0.41
4:D:279:THR:HA	15:V:12:VAL:CG1	2.51	0.41
5:E:109:MET:HE2	7:G:196:GLY:CA	2.51	0.41
5:E:165:ASP:O	5:E:166:LYS:C	2.62	0.41
6:F:61:ASP:O	6:F:256:ARG:NH2	2.54	0.41
6:F:119:GLU:CD	28:F:501:FMN:HN3	2.28	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:312:GLY:O	21:q:143:PRO:HA	2.21	0.41
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.41
7:G:476:LEU:CD2	7:G:481:LEU:HD21	2.50	0.41
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.41
8:H:89:LEU:HD12	8:H:89:LEU:HA	1.87	0.41
8:H:124:ASN:O	8:H:124:ASN:CG	2.62	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
9:I:164:VAL:O	9:I:165:ASP:C	2.59	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:227:PRO:O	10:P:228:LEU:HD23	2.21	0.41
11:Q:64:LEU:HD11	16:W:85:LEU:HG	2.03	0.41
13:S:21:VAL:HG22	13:S:91:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
16:W:72:LYS:HE2	16:W:72:LYS:HB3	1.93	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
21:q:3:LEU:O	21:q:6:VAL:CG2	2.66	0.41
4:D:116:LEU:O	4:D:118:ARG:HG3	2.21	0.41
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.97	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
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:404:GLY:HA3	7:G:684:LEU:CD1	2.34	0.41
8:H:35:LYS:HE3	8:H:38:ASN:HD21	1.86	0.41
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.41
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.41
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.20	0.40
25:B:302:UQ9:H3MB	4:D:92:HIS:CD2	2.44	0.40
4:D:158:LEU:O	4:D:392:PRO:HG2	2.21	0.40
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.40
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.36	0.40
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.86	0.40
6:F:102:MET:HE2	6:F:149:MET:HB2	2.03	0.40
6:F:210:THR:CB	6:F:224:ARG:H	2.35	0.40
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.40
7:G:49:VAL:HB	7:G:91:ALA:HA	2.03	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:173:SER:C	10:P:175:LYS:N	2.79	0.40
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.40
11:Q:160:TYR:HH	11:Q:164:PHE:HZ	1.69	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
21:q:64:TYR:CE2	21:q:81:MET:HB2	2.56	0.40
1:A:18:ILE:CD1	8:H:222:LEU:HD21	2.51	0.40
1:A:110:GLY:O	1:A:111:LEU:C	2.64	0.40
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.40
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.84	0.40
25:B:302:UQ9:O3	4:D:92:HIS:HA	2.20	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.40
7:G:169:VAL:HG12	7:G:231:LEU:HB2	2.03	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:544:MET:HG3	7:G:565:PHE:HD2	1.87	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.40
9:I:107:PRO:O	9:I:108:SER:C	2.64	0.40
10:P:221:ARG:CG	10:P:286:ARG:HD3	2.52	0.40
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.02	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.46	0.40
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.40
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.40
1:A:113:TRP:CZ2	8:H:286:MET:SD	3.15	0.40
2:B:91:TRP:CE2	8:H:51:ASP:OD1	2.75	0.40
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.40
3:C:102:HIS:CE1	15:V:48:THR:CG2	2.89	0.40
4:D:213:PHE:O	4:D:214:TYR:C	2.65	0.40
5:E:61:ARG:O	5:E:65:ILE:HG13	2.21	0.40
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.40
6:F:315:LEU:HA	6:F:359:ARG:CZ	2.52	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
7:G:598:ASN:ND2	7:G:600:GLU:OE2	2.51	0.40
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.02	0.40
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.40
10:P:105:PHE:C	10:P:106:LEU:HD12	2.47	0.40
16:W:28:LEU:O	16:W:32:LYS:HG3	2.20	0.40
21:q:39:VAL:CG1	21:q:97:PRO:HB3	2.52	0.40
21:q:97:PRO:HA	21:q:98:PRO:HD3	1.98	0.40
25:B:302:UQ9:C10	4:D:200:PHE:HZ	2.31	0.40
3:C:139:ARG:NH1	4:D:306:GLN:OE1	2.44	0.40
4:D:313:GLN:HE21	4:D:313:GLN:HB2	1.67	0.40
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.40
5:E:81:VAL:HG21	5:E:104:LEU:HD21	2.04	0.40
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.37	0.40
6:F:177:TYR:O	6:F:178:GLU:C	2.64	0.40
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.40
7:G:177:ILE:HG12	7:G:228:VAL:CG2	2.51	0.40
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.40
7:G:356:ASP:OD2	7:G:645:ARG:NE	2.51	0.40
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:TYR:CE2	21:q:27:PHE:CZ	3.08	0.40
8:H:145:THR:HG22	8:H:289:LEU:HD11	2.03	0.40
8:H:199:ASP:C	8:H:201:THR:O	2.65	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:360:ARG:C	10:P:362:LEU:N	2.78	0.40
16:W:117:ARG:HA	16:W:118:PRO:HD3	1.94	0.40
17:X:135:ARG:HE	17:X:135:ARG:HB3	1.72	0.40
1:A:49:LEU:H	1:A:49:LEU:CD2	2.34	0.40
2:B:99:CYS:HB2	4:D:141:TYR:HB2	2.04	0.40
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	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:32:ILE:HG22	7:G:33:GLU:N	2.36	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.10	0.40
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
8:H:25:ARG:HD2	25:H:401:UQ9:H1MB	2.02	0.40
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.03	0.40
8:H:85:LEU:HB2	8:H:233:LEU:HD22	2.04	0.40
9:I:89:GLU:CG	21:q:61:TRP:HB3	2.50	0.40
9:I:90:LYS:CG	21:q:90:LEU:CD2	3.00	0.40
10:P:300:TRP:CE2	10:P:304:LEU:HD21	2.57	0.40
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.40
13:S:45:LYS:O	13:S:46:LYS:C	2.64	0.40
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.40
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.40
16:W:122:LEU:HG	16:W:126:TYR:CE2	2.56	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
20:b:13:TRP:HA	20:b:13:TRP:HE3	1.85	0.40
20:b:43:SER:O	20:b:47:LYS:HB2	2.22	0.40
21:q:68:MET:SD	21:q:81:MET:CB	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/115 (96%)	100 (90%)	10 (9%)	1 (1%)	14	47
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%)	192 (92%)	16 (8%)	0	100	100
6	F	424/464 (91%)	405 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	630 (92%)	55 (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%)	312 (92%)	26 (8%)	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%)	77 (95%)	4 (5%)	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%)	110 (98%)	2 (2%)	0	100	100
17	X	140/172 (81%)	130 (93%)	10 (7%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
21	q	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
22	r	46/113 (41%)	44 (96%)	2 (4%)	0	100	100
23	s	24/104 (23%)	24 (100%)	0	0	100	100
All	All	4163/5036 (83%)	3920 (94%)	240 (6%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
1	A	109	LYS
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%)	132 (99%)	1 (1%)	73	77
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%)	340 (100%)	1 (0%)	86	83
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%)	295 (99%)	2 (1%)	76	78
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	56/60 (93%)	56 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	108/131 (82%)	108 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	26/95 (27%)	26 (100%)	0	100	100
All	All	3653/4292 (85%)	3638 (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	104	MET
4	D	94	VAL
4	D	232	VAL
5	E	244	VAL
6	F	337	MET
7	G	271	MET
8	H	229	THR
10	P	192	ARG
10	P	242	VAL
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) 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	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	87	GLN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN

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Mol	Chain	Res	Type
5	E	68	ASN
5	E	132	GLN
5	E	152	GLN
5	E	245	GLN
6	F	44	ASN
6	F	49	HIS
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	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	260	ASN
7	G	278	HIS
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	169	GLN
8	H	212	ASN
8	H	258	ASN
8	H	292	ASN
10	P	43	HIS
10	P	71	ASN
10	P	154	GLN
10	P	166	HIS
10	P	216	HIS

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Mol	Chain	Res	Type
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	56	ASN
15	V	41	HIS
15	V	50	GLN
16	W	54	GLN
16	W	102	GLN
17	X	30	HIS
17	X	77	HIS
19	a	27	HIS
19	a	31	ASN
20	b	69	HIS
20	b	83	ASN
21	q	12	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	9	GLN
22	r	21	GLN
22	r	110	GLN
23	s	59	GLN

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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
30	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.67	11 (16%)
24	SF4	I	302	9	0,12,12	-	-	-		
25	UQ9	H	401	-	35,35,58	0.80	2 (5%)	42,45,73	0.63	0
26	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.15	3 (7%)
28	FMN	F	501	-	33,33,33	1.38	4 (12%)	48,50,50	1.21	7 (14%)
25	UQ9	B	302	-	24,24,58	1.14	3 (12%)	29,32,73	0.86	1 (3%)
27	FES	E	301	5	0,4,4	-	-	-		
24	SF4	I	301	9	0,12,12	-	-	-		
29	3PE	H	402	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
29	3PE	Z	401	-	45,45,50	0.97	2 (4%)	48,50,55	0.98	2 (4%)
32	EHZ	W	201	-	27,31,37	1.90	7 (25%)	37,41,47	1.86	11 (29%)
24	SF4	G	801	7	0,12,12	-	-	-		
27	FES	G	803	7	0,4,4	-	-	-		
24	SF4	G	802	7	0,12,12	-	-	-		
24	SF4	B	301	2	0,12,12	-	-	-		
24	SF4	F	502	6	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
24	SF4	I	302	9	-	-	0/6/5/5
28	FMN	F	501	-	-	3/18/18/18	0/3/3/3
25	UQ9	H	401	-	-	13/30/54/81	0/1/1/1
26	PC1	B	303	-	-	11/38/38/57	-
25	UQ9	B	302	-	-	9/17/41/81	0/1/1/1
29	3PE	H	402	-	-	17/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	3PE	Z	401	-	-	16/49/49/54	-
32	EHZ	W	201	-	-	21/39/39/45	-
24	SF4	F	502	6	-	-	0/6/5/5
24	SF4	I	301	9	-	-	0/6/5/5
27	FES	E	301	5	-	-	0/1/1/1
24	SF4	G	801	7	-	-	0/6/5/5
27	FES	G	803	7	-	-	0/1/1/1
24	SF4	G	802	7	-	-	0/6/5/5
24	SF4	B	301	2	-	-	0/6/5/5
30	NDP	P	401	-	-	3/34/77/77	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	201	EHZ	C15-N2	5.40	1.45	1.33
32	W	201	EHZ	C12-N1	5.16	1.45	1.33
28	F	501	FMN	C9A-C5A	4.80	1.49	1.41
30	P	401	NDP	C5A-C4A	4.24	1.46	1.39
29	Z	401	3PE	O21-C21	4.19	1.46	1.34
26	B	303	PC1	O31-C31	4.19	1.45	1.33
29	Z	401	3PE	O31-C31	4.17	1.45	1.33
29	H	402	3PE	O31-C31	4.09	1.45	1.33
26	B	303	PC1	O21-C21	4.01	1.45	1.34
29	H	402	3PE	O21-C21	3.98	1.45	1.34
30	P	401	NDP	C6N-C5N	3.31	1.39	1.33
28	F	501	FMN	C8-C7	3.09	1.48	1.40
25	B	302	UQ9	C3-C2	-2.85	1.40	1.48
25	B	302	UQ9	O4-C4M	-2.83	1.38	1.45
28	F	501	FMN	C4-N3	-2.67	1.33	1.38
25	H	401	UQ9	C3-C2	-2.65	1.41	1.48
32	W	201	EHZ	P1-O7	2.55	1.64	1.54
32	W	201	EHZ	O4-C15	-2.50	1.18	1.23
30	P	401	NDP	C5A-C6A	2.48	1.48	1.41
25	H	401	UQ9	C4-C5	-2.44	1.41	1.48
32	W	201	EHZ	C9-S1	2.43	1.82	1.76
30	P	401	NDP	C5A-N7A	-2.42	1.34	1.39
32	W	201	EHZ	O3-C12	-2.40	1.18	1.23
30	P	401	NDP	C8A-N7A	2.38	1.36	1.31
28	F	501	FMN	C5A-N5	-2.32	1.35	1.39
25	B	302	UQ9	C4-C5	-2.28	1.42	1.48
32	W	201	EHZ	P1-OP3	-2.25	1.46	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	201	EHZ	C8-C9-S1	6.34	121.48	113.63
30	P	401	NDP	C5A-C4A-N3A	-6.13	118.75	126.75
30	P	401	NDP	N3A-C4A-N9A	4.81	135.00	127.08
30	P	401	NDP	C2A-N3A-C4A	3.90	120.96	111.75
26	B	303	PC1	O21-C21-C22	3.75	119.58	111.50
29	Z	401	3PE	O21-C21-C22	3.71	119.49	111.50
29	H	402	3PE	O21-C21-C22	3.67	119.42	111.50
30	P	401	NDP	PN-O3-PA	-3.65	120.29	132.83
30	P	401	NDP	C4A-C5A-N7A	-3.21	106.70	110.62
30	P	401	NDP	N3A-C2A-N1A	-3.21	123.58	128.60
25	B	302	UQ9	C4M-O4-C4	-3.09	105.51	116.47
32	W	201	EHZ	C13-C12-N1	3.06	121.57	116.42
32	W	201	EHZ	C14-C13-C12	-3.04	107.29	112.36
32	W	201	EHZ	OP3-P1-O9	-2.90	99.34	110.68
32	W	201	EHZ	C7-C8-C9	-2.86	107.36	113.89
26	B	303	PC1	O31-C31-C32	2.79	120.67	111.91
30	P	401	NDP	C4A-N9A-C8A	2.77	108.73	105.73
30	P	401	NDP	C5A-N7A-C8A	2.74	107.41	103.51
26	B	303	PC1	C2-O21-C21	-2.70	111.15	117.79
29	H	402	3PE	O31-C31-C32	2.67	120.29	111.91
28	F	501	FMN	C4A-C10-N1	-2.55	118.81	124.73
28	F	501	FMN	C4-C4A-N5	2.43	121.69	118.23
28	F	501	FMN	O4-C4-C4A	-2.42	120.19	126.60
32	W	201	EHZ	C5-C6-C7	-2.37	108.03	114.85
29	Z	401	3PE	O31-C31-C32	2.33	119.23	111.91
32	W	201	EHZ	C10-S1-C9	2.27	108.93	101.87
28	F	501	FMN	O2-C2-N1	-2.23	118.14	121.83
30	P	401	NDP	N9A-C8A-N7A	-2.19	110.92	113.91
30	P	401	NDP	C3D-C2D-C1D	2.19	105.58	101.43
30	P	401	NDP	C6A-C5A-N7A	2.19	136.09	132.02
32	W	201	EHZ	C11-N1-C12	-2.17	118.80	122.84
32	W	201	EHZ	O2-C9-S1	-2.17	119.80	122.61
28	F	501	FMN	C4A-C10-N10	2.16	119.64	116.48
28	F	501	FMN	C10-N1-C2	2.13	121.17	116.90
32	W	201	EHZ	O6-P1-O9	2.11	112.41	106.47
32	W	201	EHZ	O3-C12-N1	-2.11	119.04	123.01
29	H	402	3PE	O31-C31-O32	-2.03	118.47	123.59
29	H	402	3PE	C2-O21-C21	-2.02	112.81	117.79
28	F	501	FMN	C4A-C4-N3	2.01	118.28	113.19

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	302	UQ9	C15-C14-C16-C17
25	B	302	UQ9	C13-C14-C16-C17
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
25	H	401	UQ9	C17-C18-C19-C21
25	H	401	UQ9	C17-C18-C19-C20
25	H	401	UQ9	C1-C6-C7-C8
25	H	401	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
28	F	501	FMN	C5'-O5'-P-O2P
28	F	501	FMN	C5'-O5'-P-O3P
29	H	402	3PE	C11-O13-P-O12
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	C2B-O2B-P2B-O2X
32	W	201	EHZ	O1-C7-C8-C9
32	W	201	EHZ	C6-C7-C8-C9
32	W	201	EHZ	C7-C8-C9-S1
32	W	201	EHZ	S1-C10-C11-N1
32	W	201	EHZ	C11-C10-S1-C9
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
26	B	303	PC1	O22-C21-O21-C2
25	B	302	UQ9	C12-C11-C9-C10
25	H	401	UQ9	C20-C19-C21-C22
25	B	302	UQ9	C12-C11-C9-C8
25	H	401	UQ9	C18-C19-C21-C22
25	H	401	UQ9	C14-C16-C17-C18
29	H	402	3PE	C32-C31-O31-C3
25	H	401	UQ9	C12-C13-C14-C15
29	H	402	3PE	O32-C31-O31-C3
29	H	402	3PE	C1-O11-P-O13
29	H	402	3PE	C11-O13-P-O11
29	Z	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
29	Z	401	3PE	C11-O13-P-O11
29	Z	401	3PE	C22-C21-O21-C2
29	Z	401	3PE	O22-C21-O21-C2
29	H	402	3PE	C22-C21-O21-C2
29	Z	401	3PE	C3-C2-O21-C21
28	F	501	FMN	C5'-O5'-P-O1P
29	H	402	3PE	C24-C25-C26-C27
29	H	402	3PE	O22-C21-O21-C2
26	B	303	PC1	C2-C1-O11-P
26	B	303	PC1	C32-C33-C34-C35
25	H	401	UQ9	C12-C13-C14-C16
32	W	201	EHZ	N2-C15-C16-C17
32	W	201	EHZ	C3-C4-C5-C6
32	W	201	EHZ	C5-C6-C7-O1
26	B	303	PC1	C32-C31-O31-C3
32	W	201	EHZ	O2-C9-S1-C10
29	Z	401	3PE	C31-C32-C33-C34
29	Z	401	3PE	C2-C1-O11-P
26	B	303	PC1	O32-C31-O31-C3
29	H	402	3PE	C1-O11-P-O12
29	H	402	3PE	C1-O11-P-O14
29	H	402	3PE	C11-O13-P-O14
29	Z	401	3PE	C1-O11-P-O12
29	Z	401	3PE	C1-O11-P-O14
29	Z	401	3PE	C11-O13-P-O14
25	H	401	UQ9	C5-C4-O4-C4M
30	P	401	NDP	O4D-C1D-N1N-C6N
26	B	303	PC1	O13-C11-C12-N
29	H	402	3PE	O21-C2-C3-O31
32	W	201	EHZ	O4-C15-C16-O5
32	W	201	EHZ	C19-C17-C20-O6
32	W	201	EHZ	C2-C3-C4-C5
30	P	401	NDP	PN-O3-PA-O2A
26	B	303	PC1	C34-C35-C36-C37
29	H	402	3PE	C37-C38-C39-C3A
29	Z	401	3PE	C2E-C2F-C2G-C2H
29	H	402	3PE	C35-C36-C37-C38
29	H	402	3PE	C33-C34-C35-C36
29	Z	401	3PE	O13-C11-C12-N
25	H	401	UQ9	C11-C12-C13-C14
32	W	201	EHZ	N2-C15-C16-O5
32	W	201	EHZ	C18-C17-C20-O6

Continued on next page...

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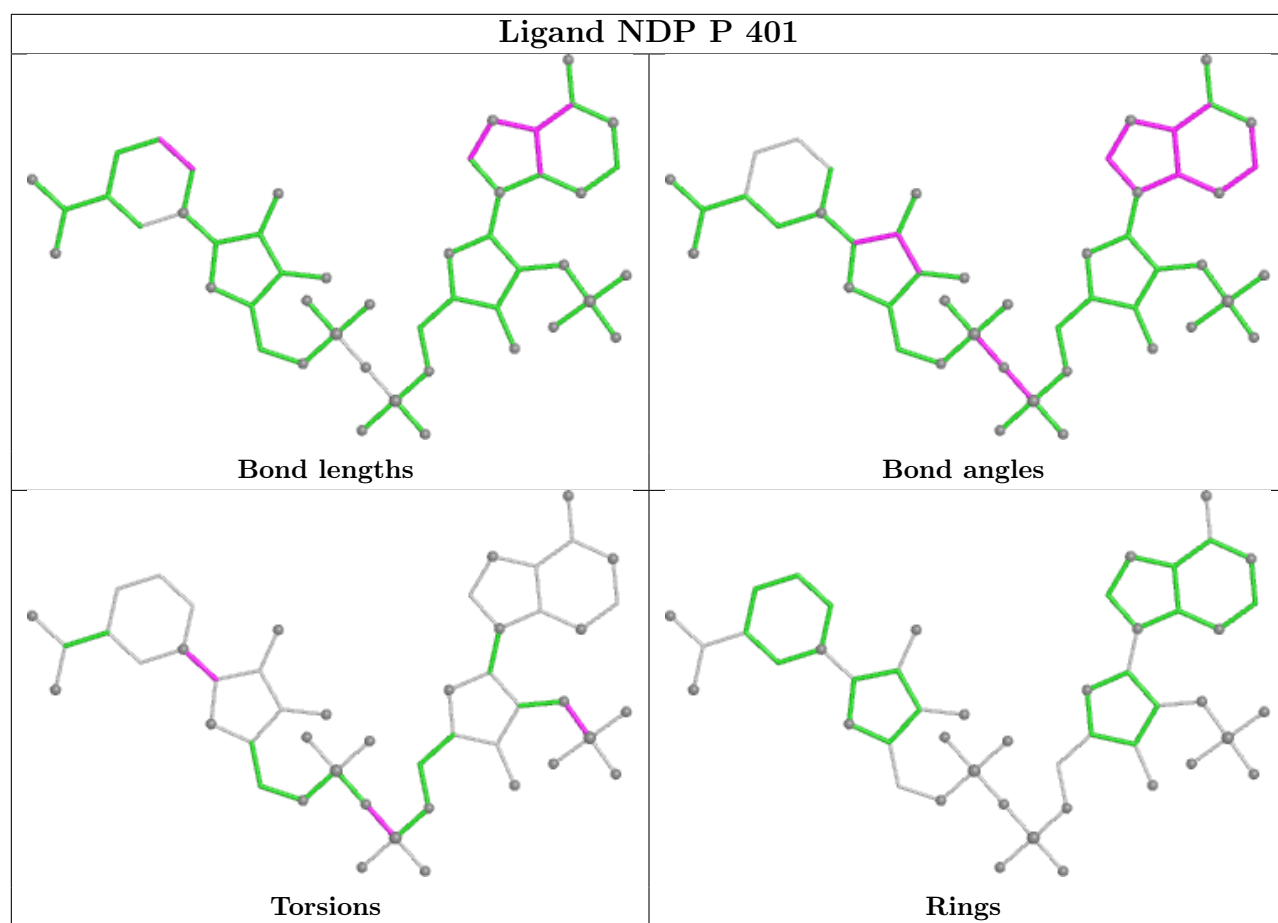
Mol	Chain	Res	Type	Atoms
32	W	201	EHZ	C15-C16-C17-C18
32	W	201	EHZ	O5-C16-C17-C18
25	H	401	UQ9	C3-C4-O4-C4M
25	B	302	UQ9	C2-C3-O3-C3M
29	H	402	3PE	C1-C2-C3-O31
29	Z	401	3PE	C25-C26-C27-C28
32	W	201	EHZ	O4-C15-C16-C17
25	H	401	UQ9	C21-C22-C23-C24
29	H	402	3PE	C2-C1-O11-P

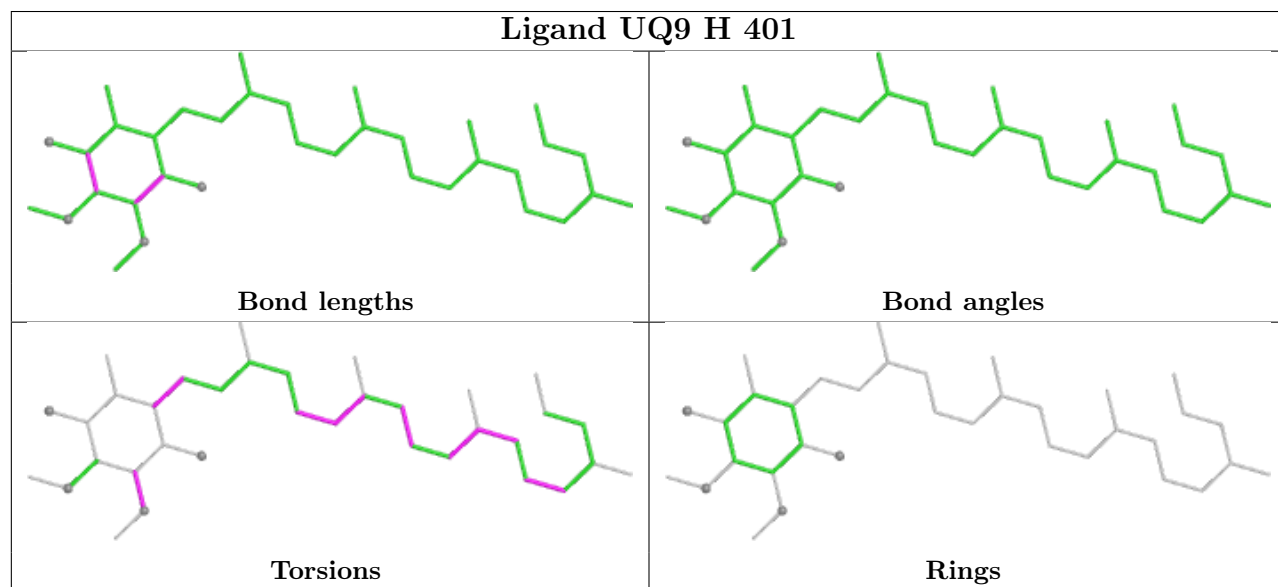
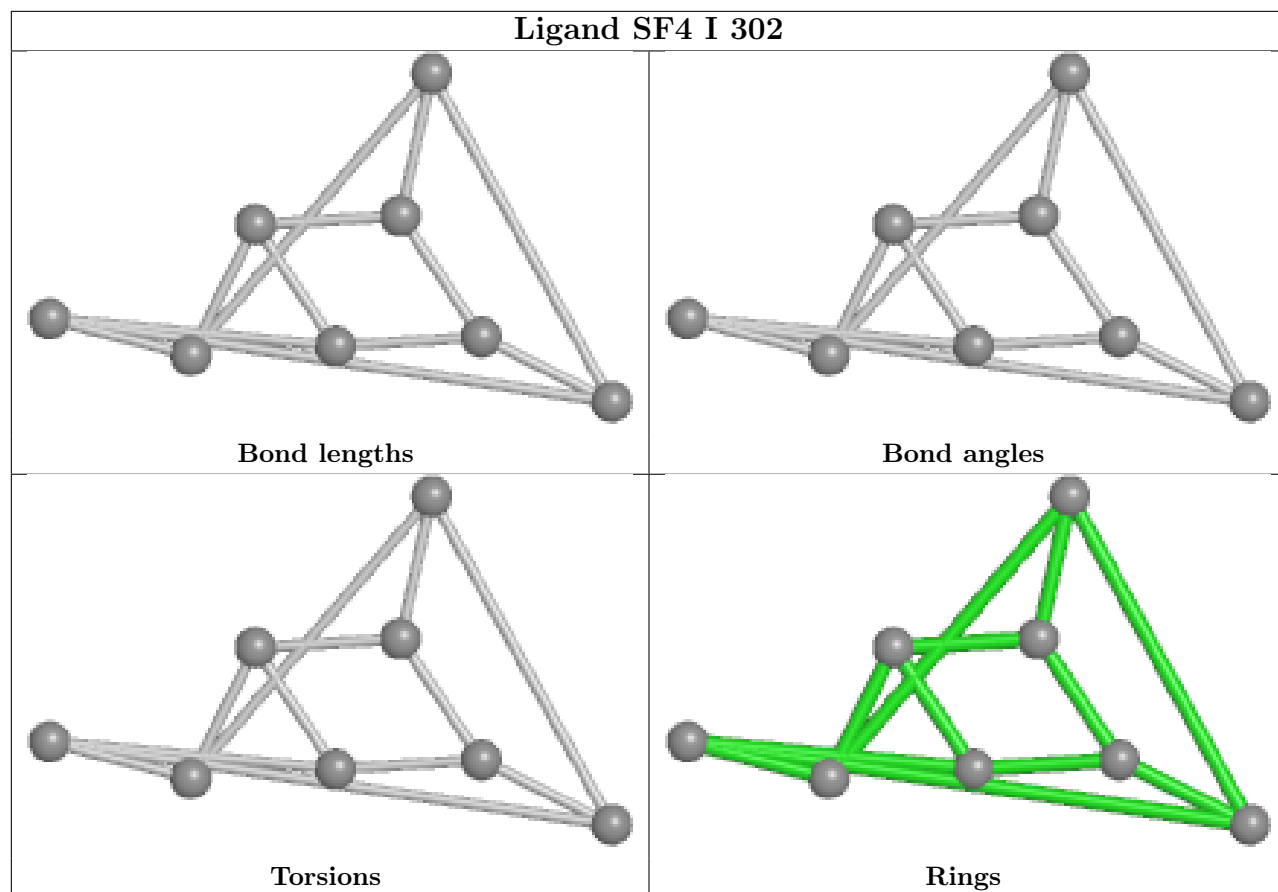
There are no ring outliers.

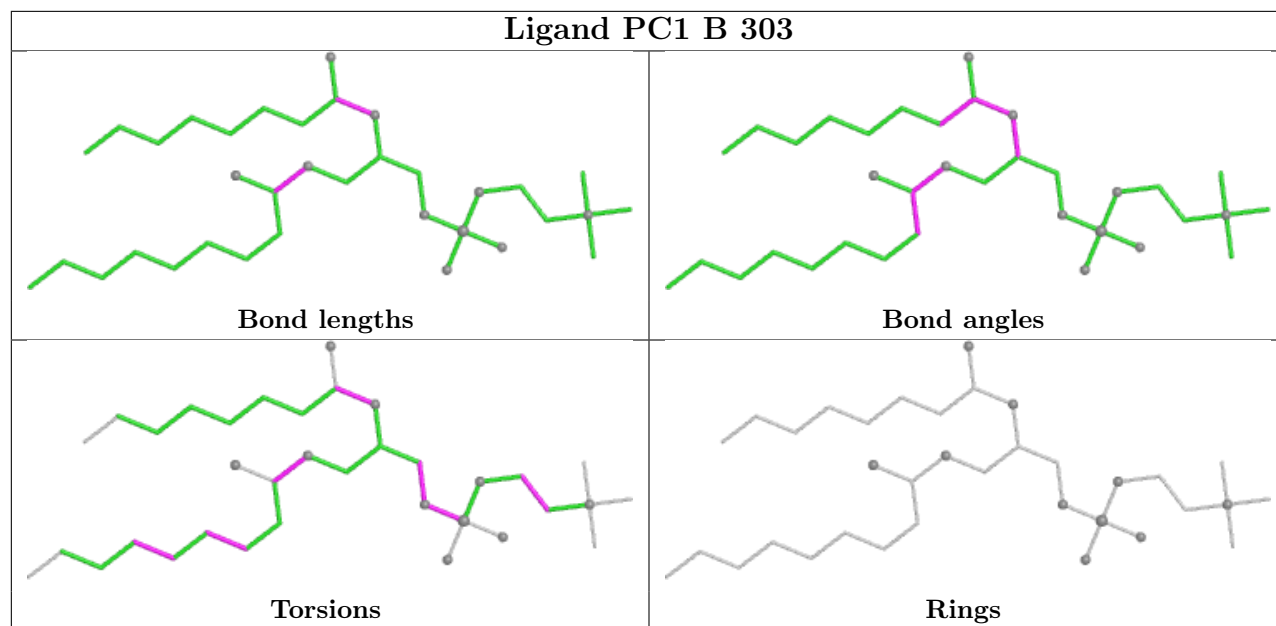
15 monomers are involved in 130 short contacts:

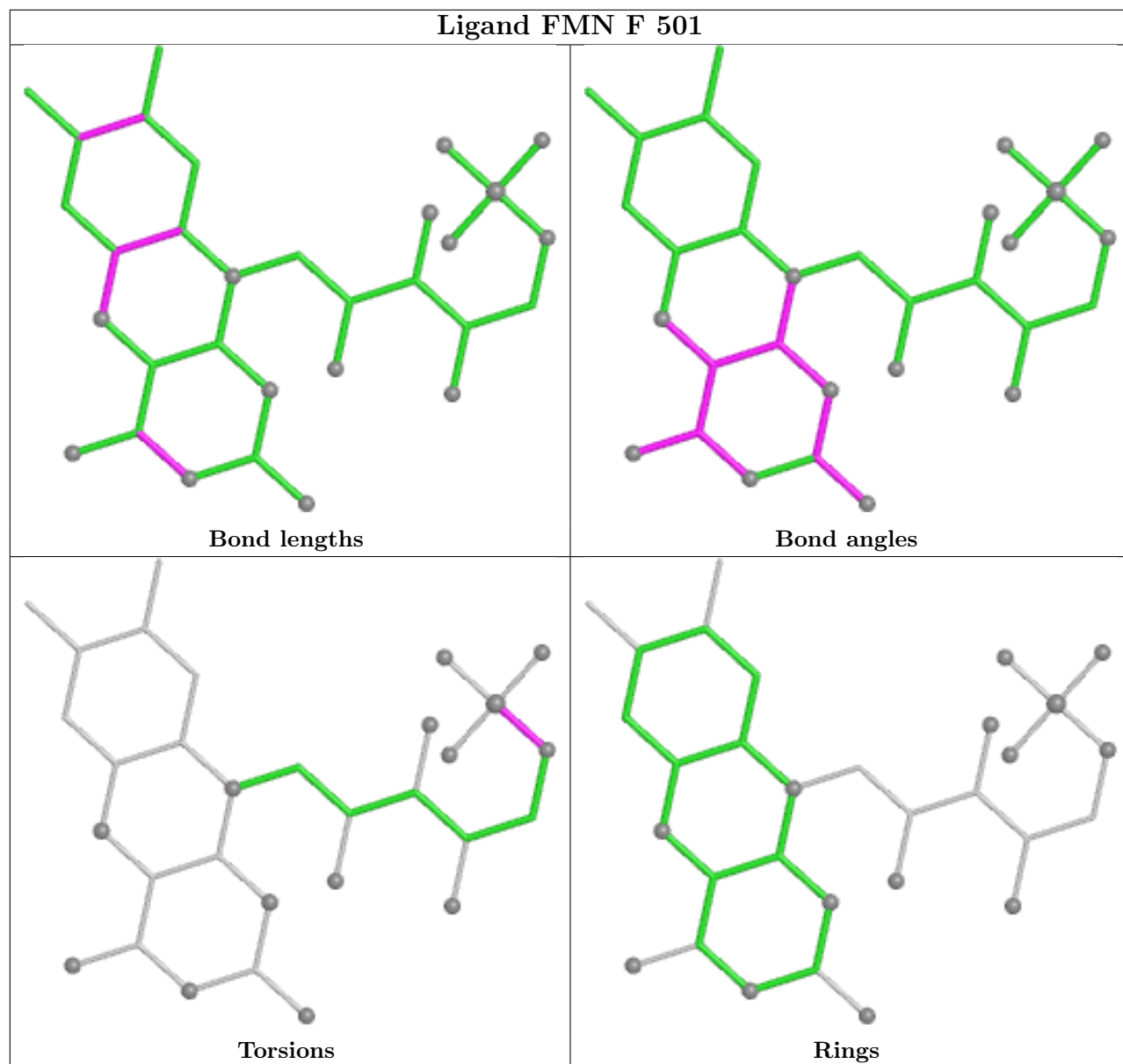
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	P	401	NDP	4	0
24	I	302	SF4	5	0
25	H	401	UQ9	15	0
26	B	303	PC1	5	0
28	F	501	FMN	3	0
25	B	302	UQ9	34	0
27	E	301	FES	5	0
24	I	301	SF4	11	0
29	H	402	3PE	12	0
29	Z	401	3PE	3	0
32	W	201	EHZ	7	0
27	G	803	FES	4	0
24	G	802	SF4	5	0
24	B	301	SF4	7	0
24	F	502	SF4	10	0

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

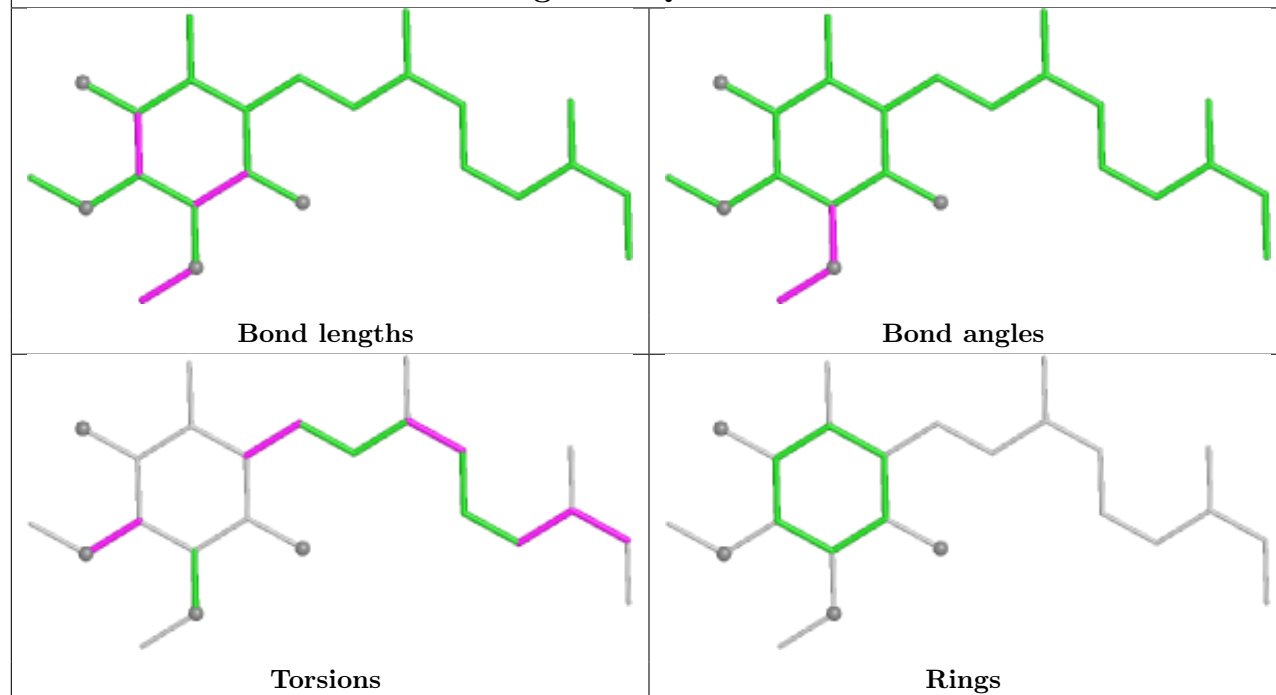




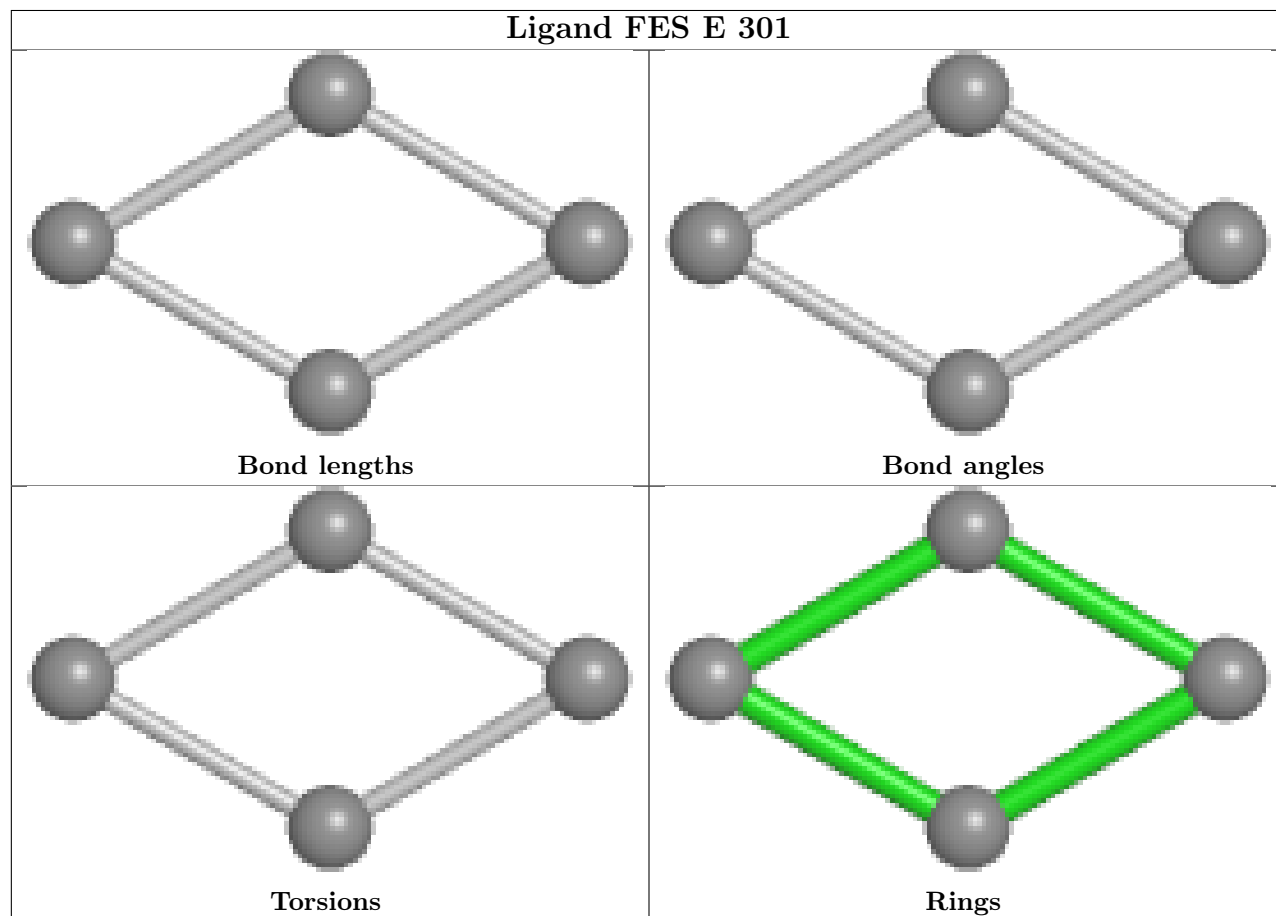


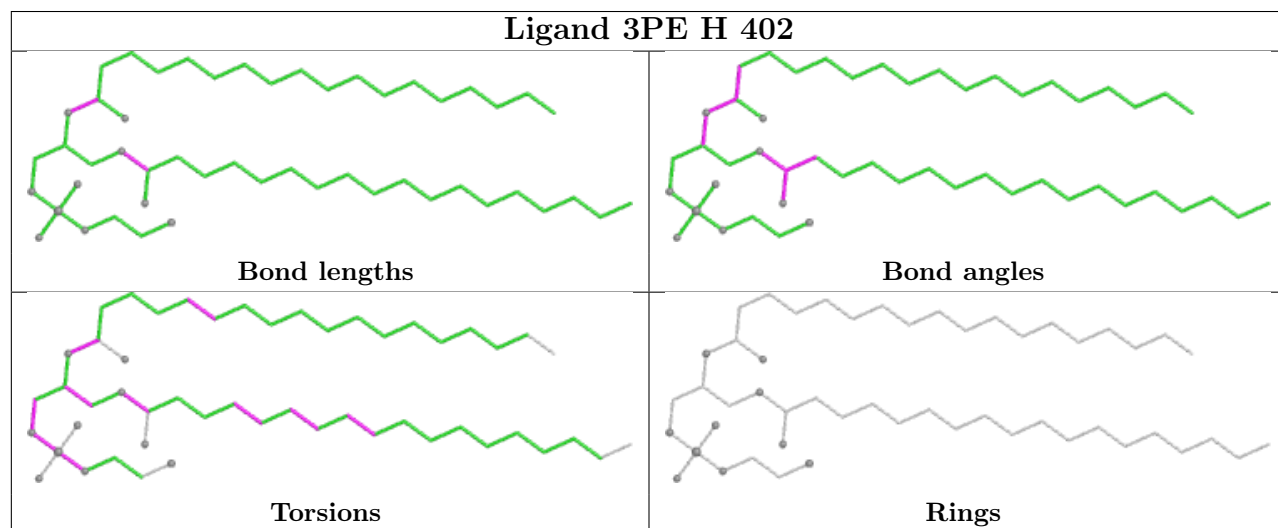
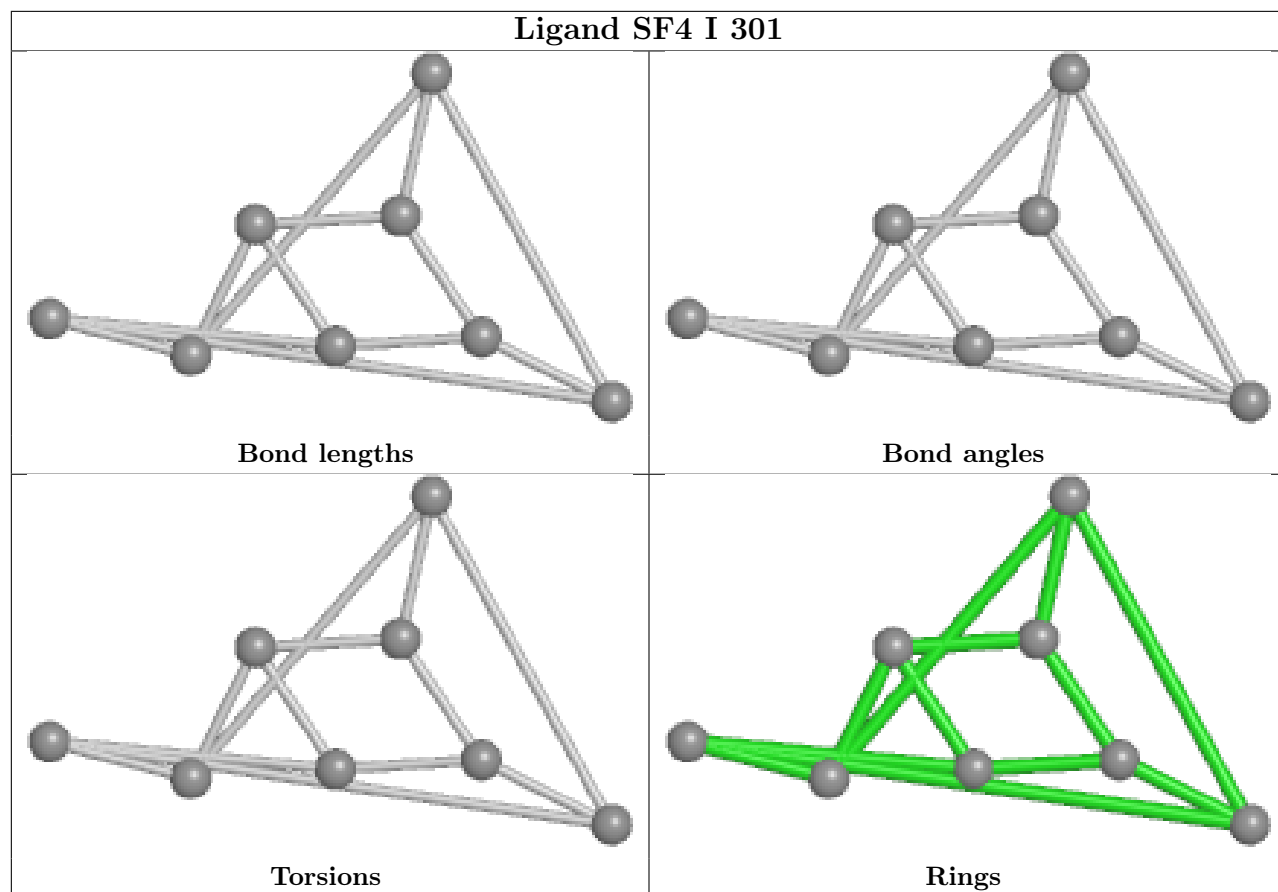


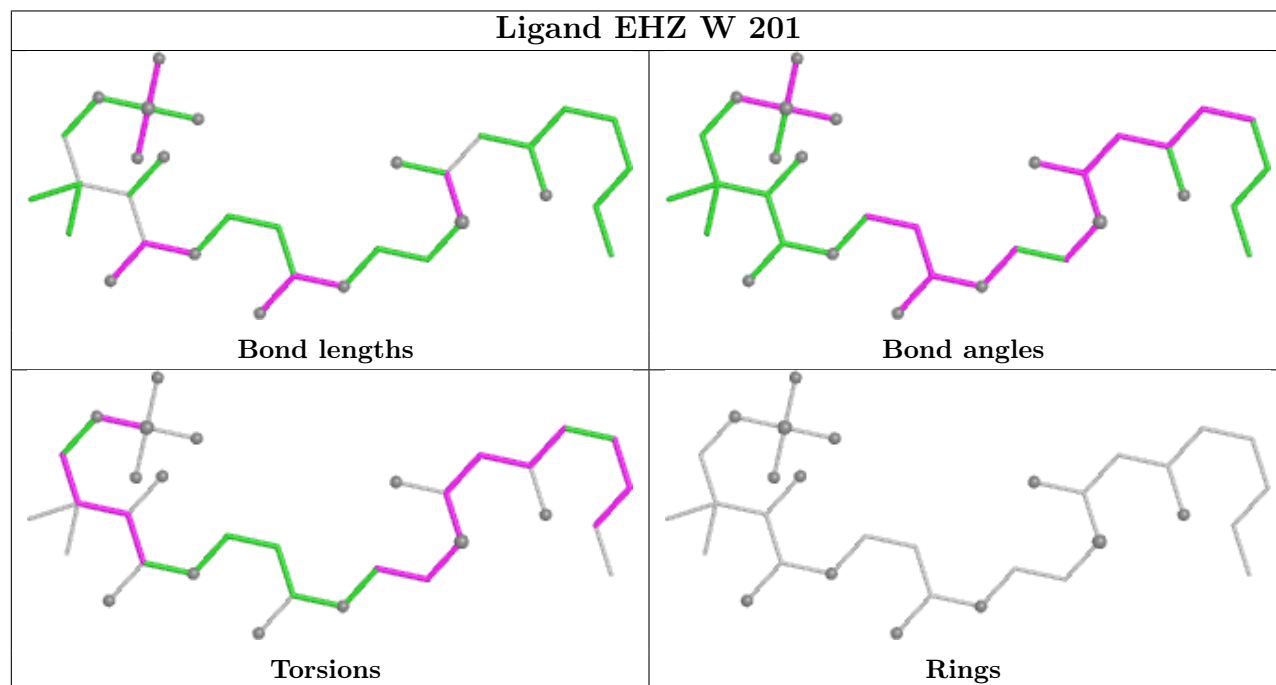
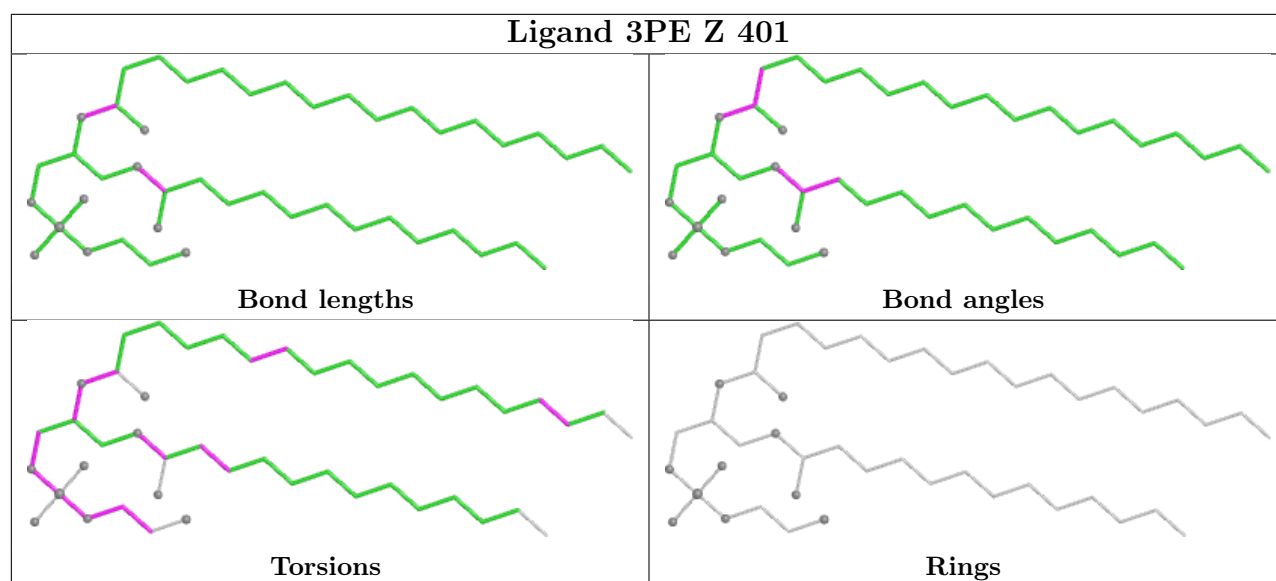
Ligand UQ9 B 302

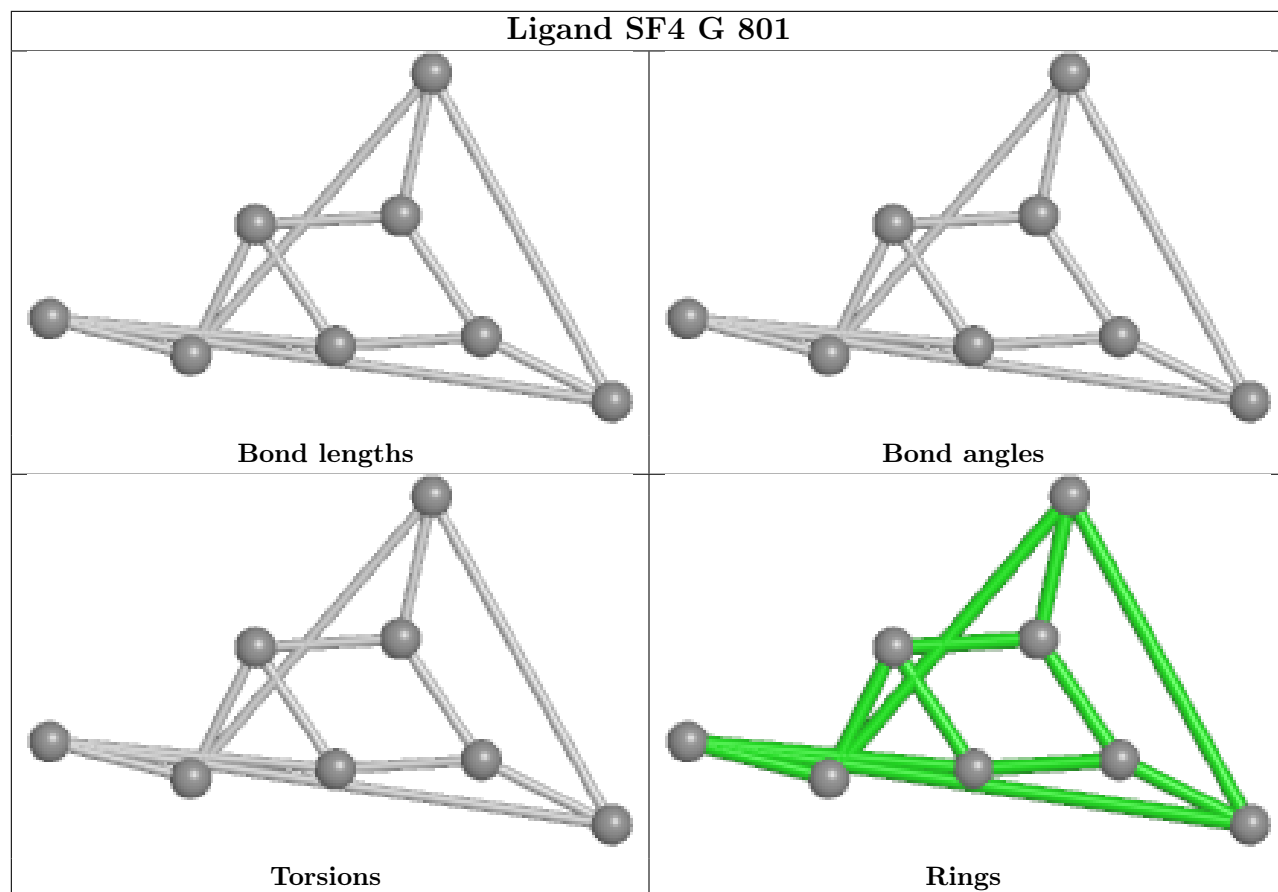


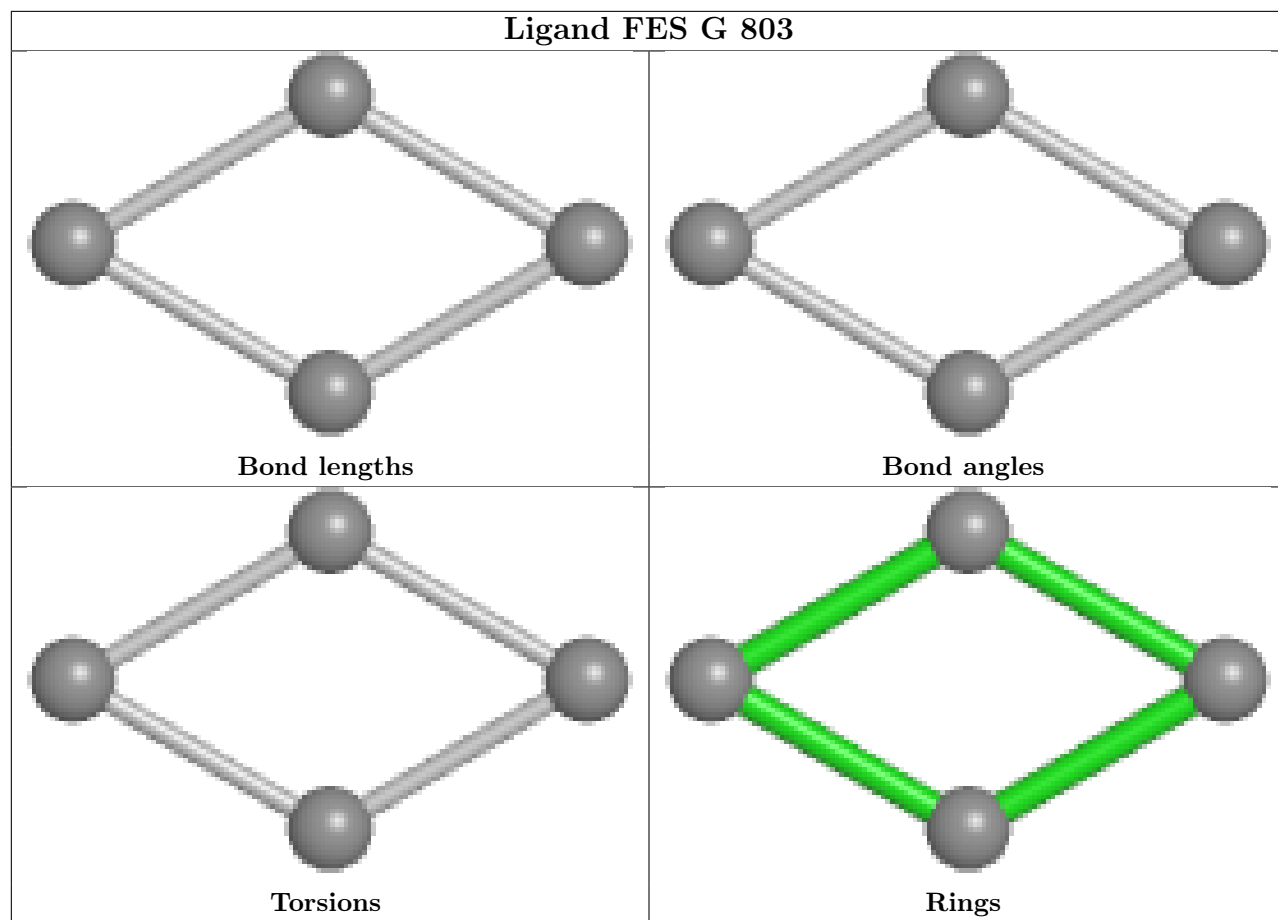
Ligand FES E 301

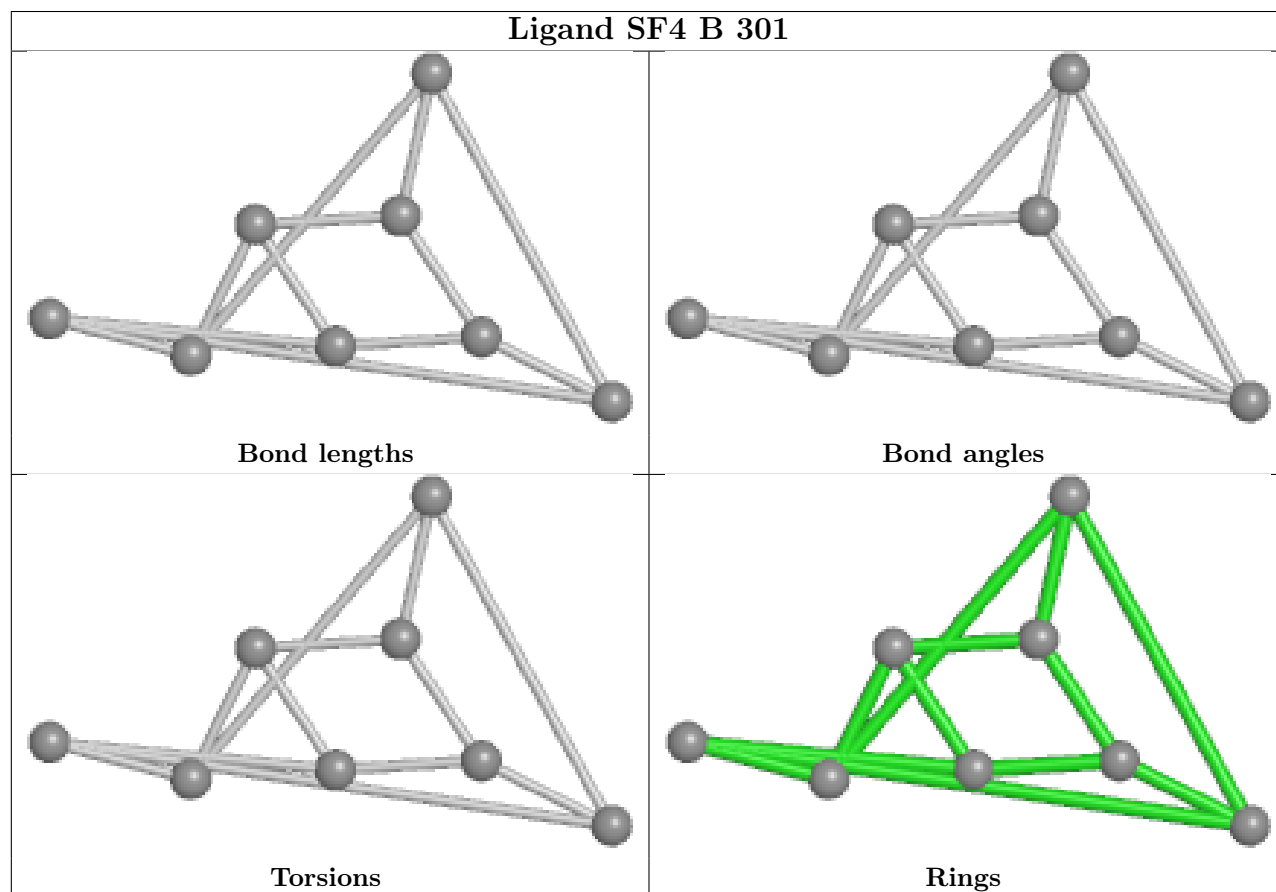
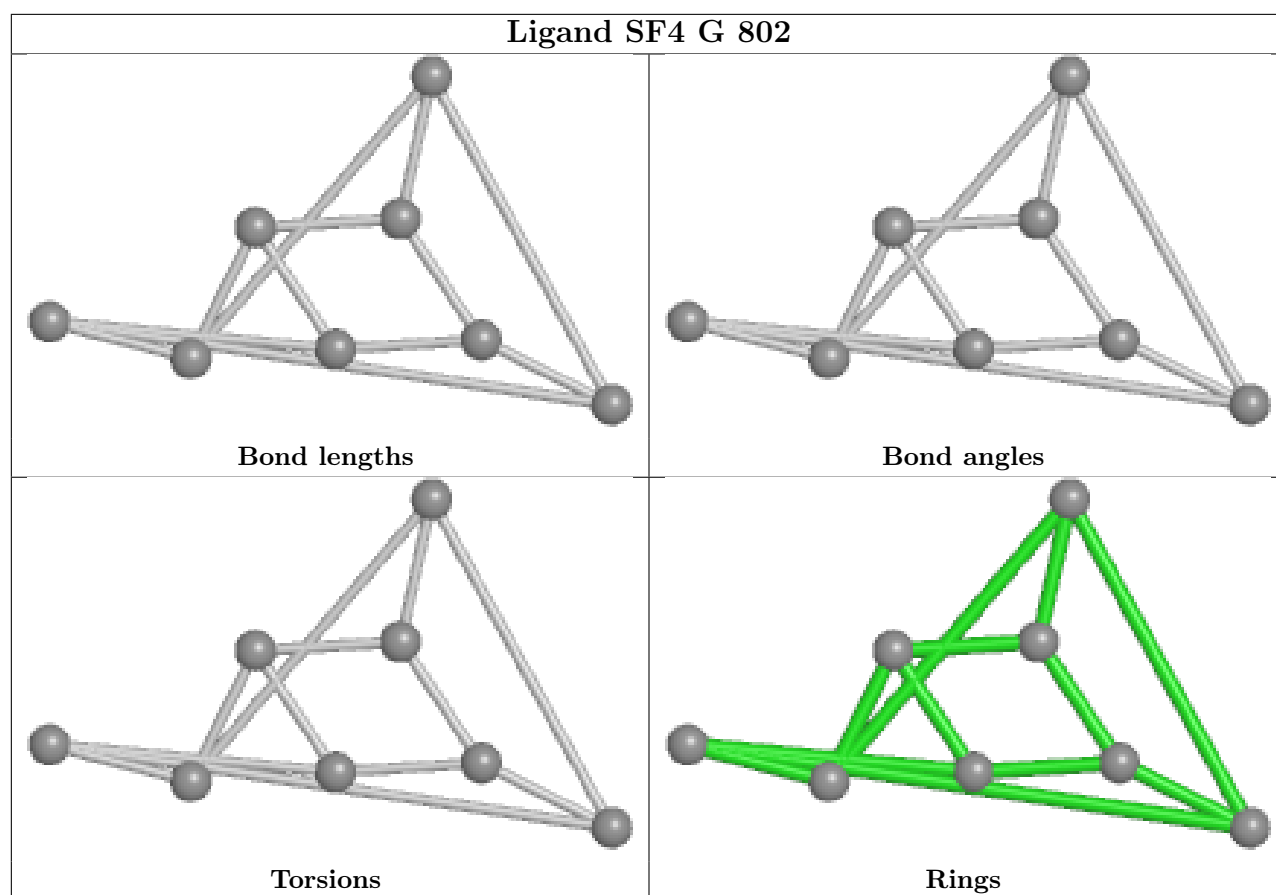


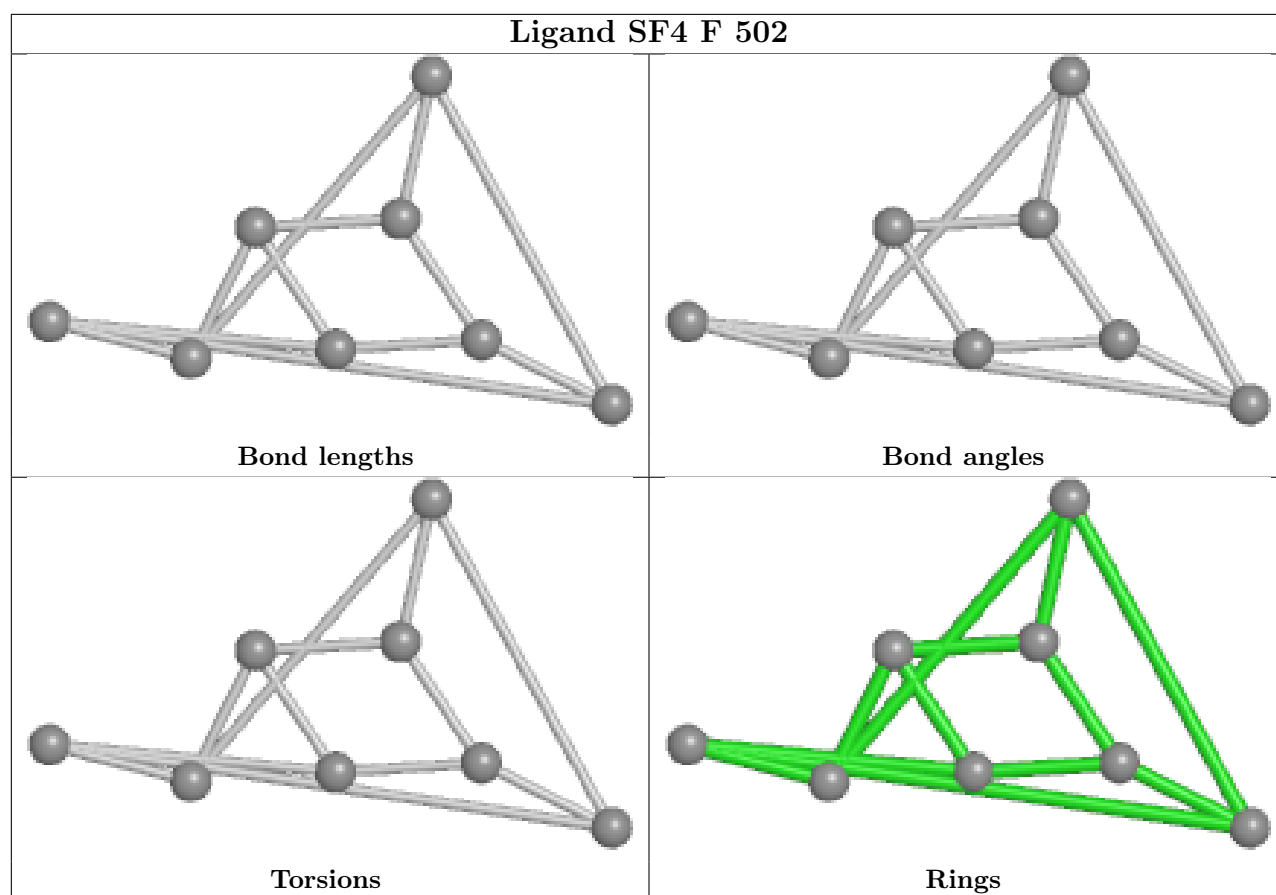












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

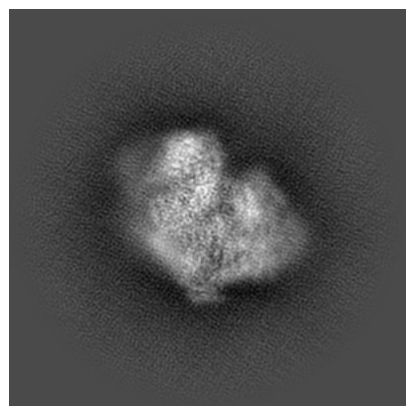
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38513. These allow visual inspection of the internal detail of the map and identification of artifacts.

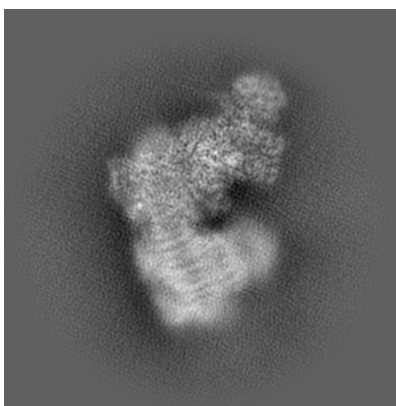
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

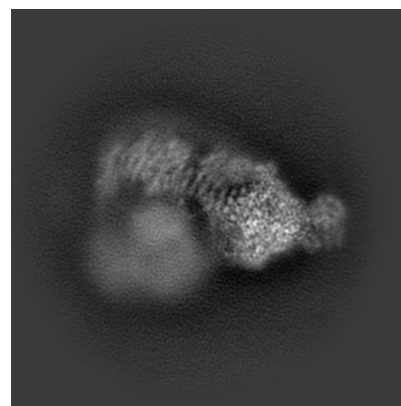
6.1.1 Primary map



X

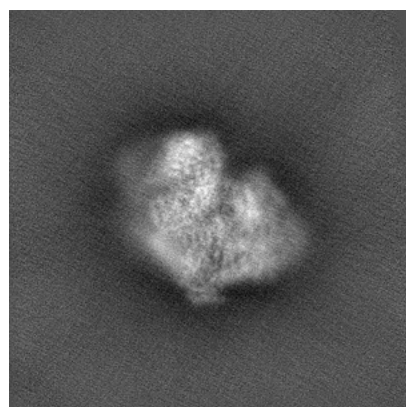


Y

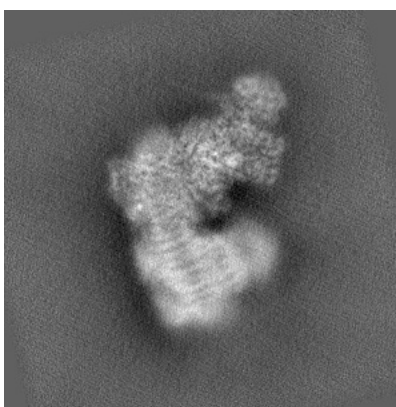


Z

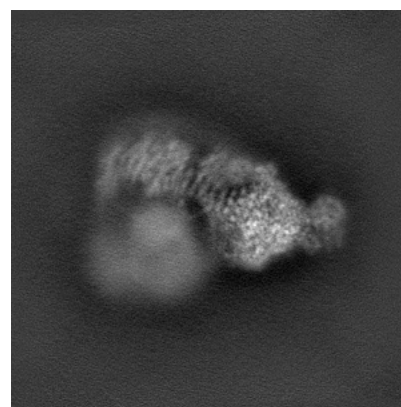
6.1.2 Raw map



X



Y

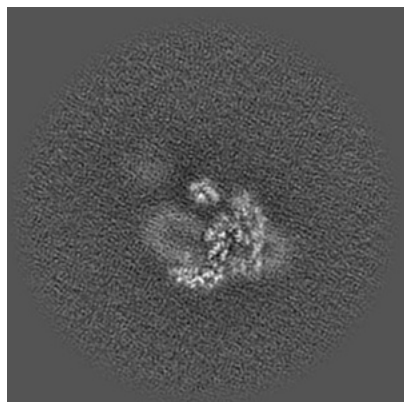


Z

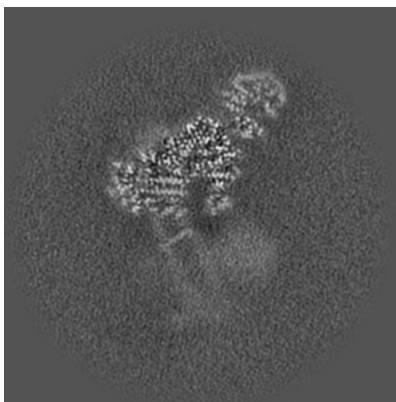
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

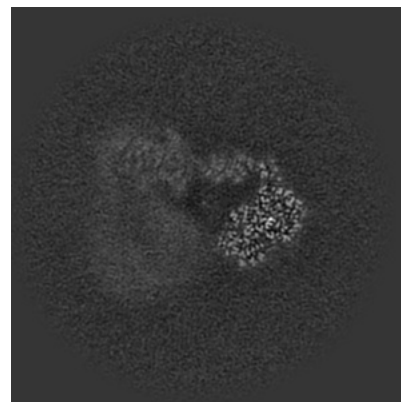
6.2.1 Primary map



X Index: 192

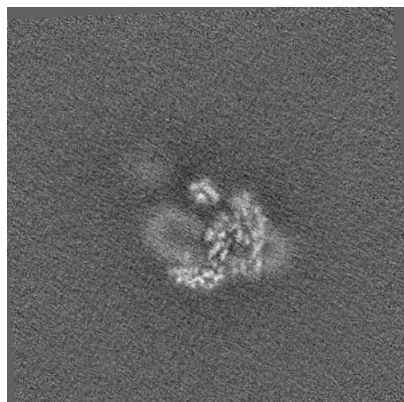


Y Index: 192

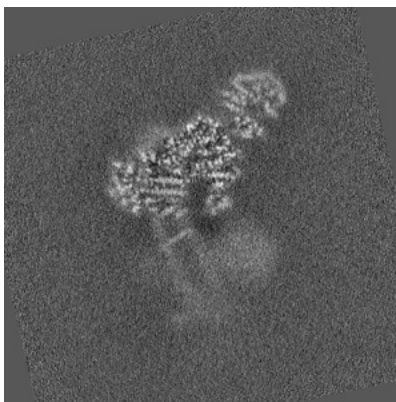


Z Index: 192

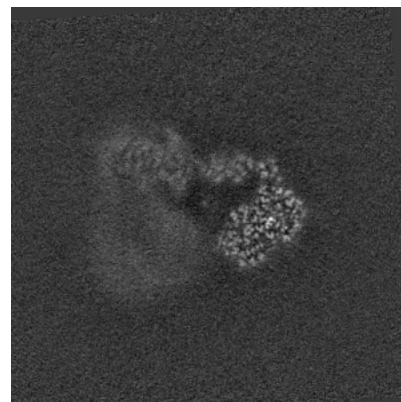
6.2.2 Raw map



X Index: 192



Y Index: 192

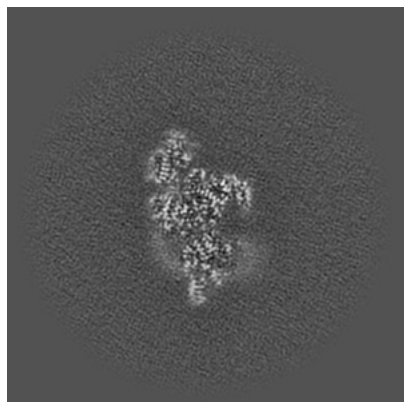


Z Index: 192

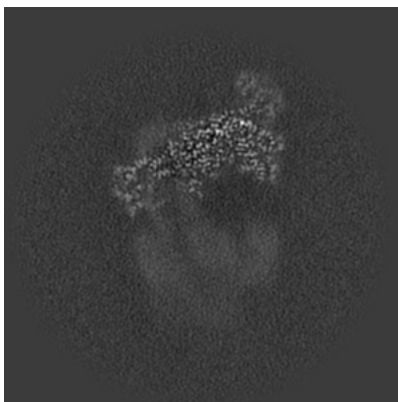
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

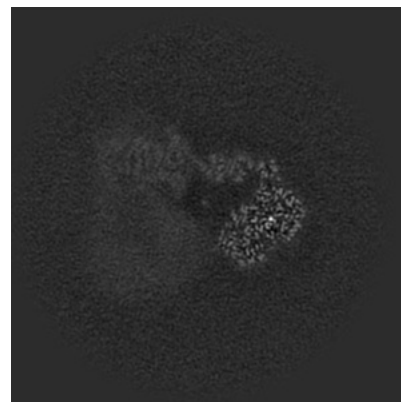
6.3.1 Primary map



X Index: 236

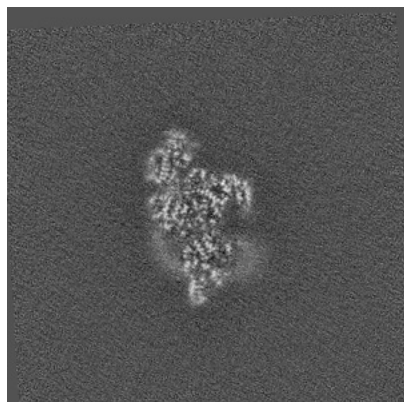


Y Index: 171

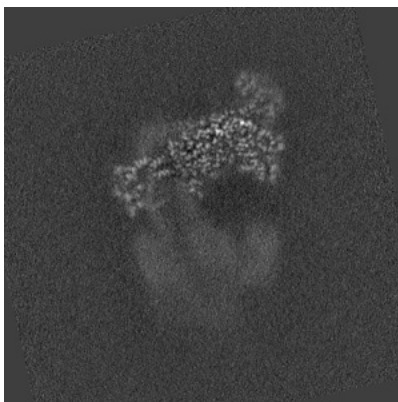


Z Index: 191

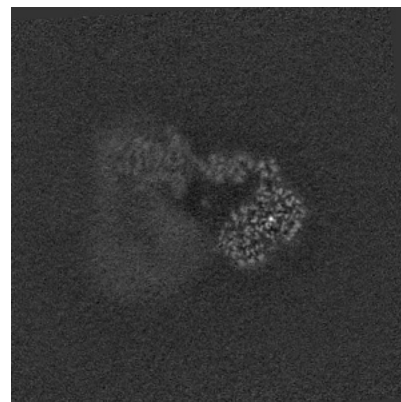
6.3.2 Raw map



X Index: 236



Y Index: 171

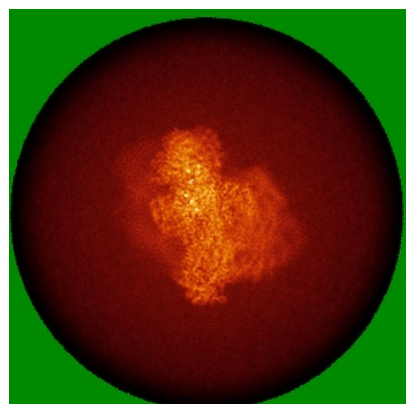


Z Index: 191

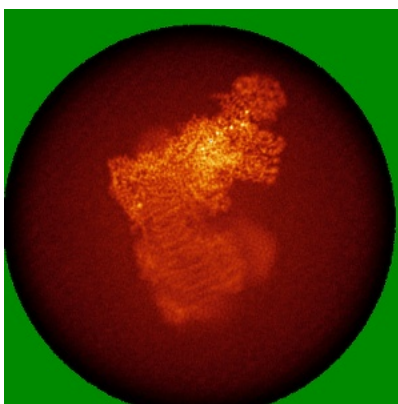
The images above show the largest variance slices of the map in three orthogonal directions.

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

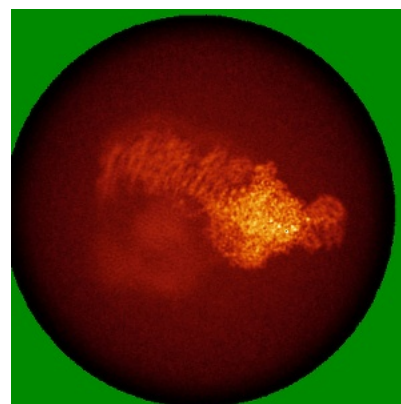
6.4.1 Primary map



X

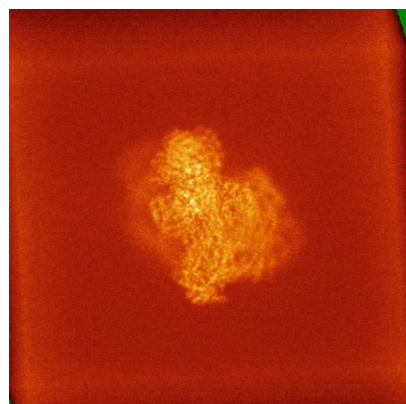


Y

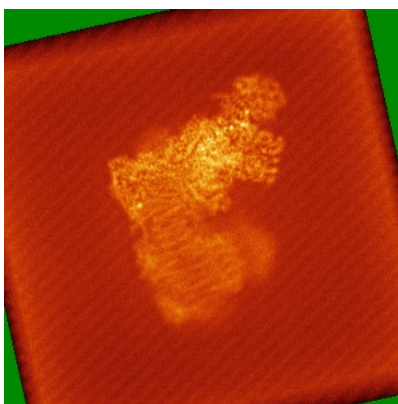


Z

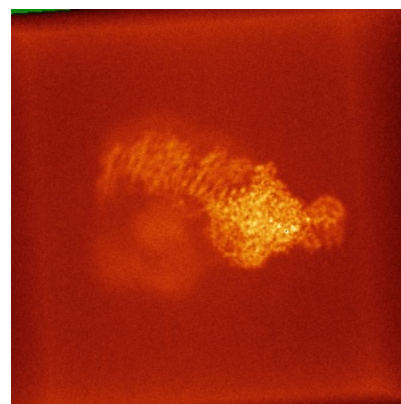
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

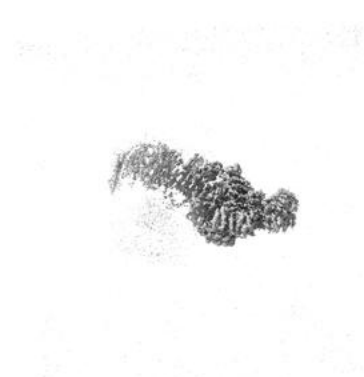
6.5.2 Raw map



X



Y



Z

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

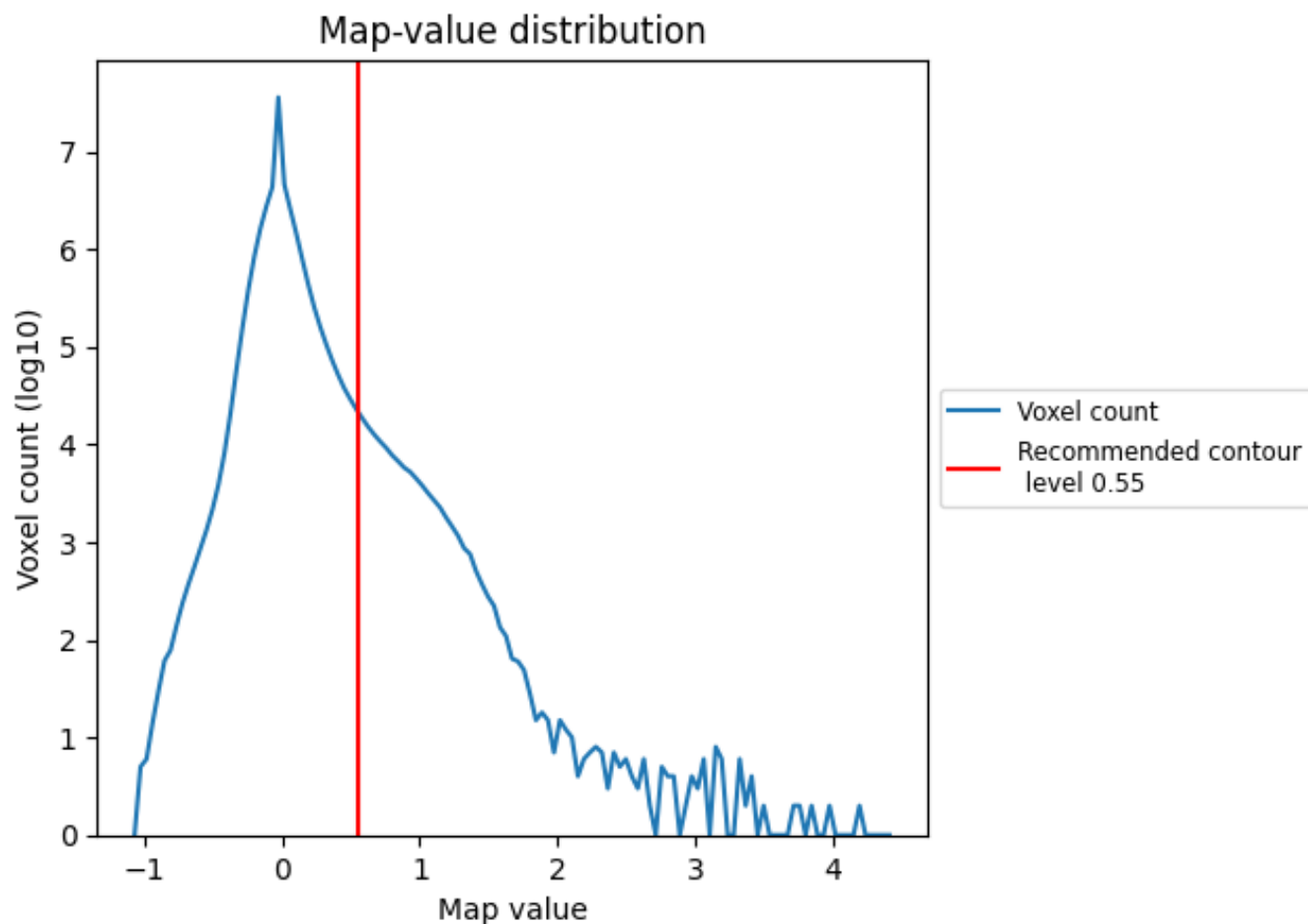
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

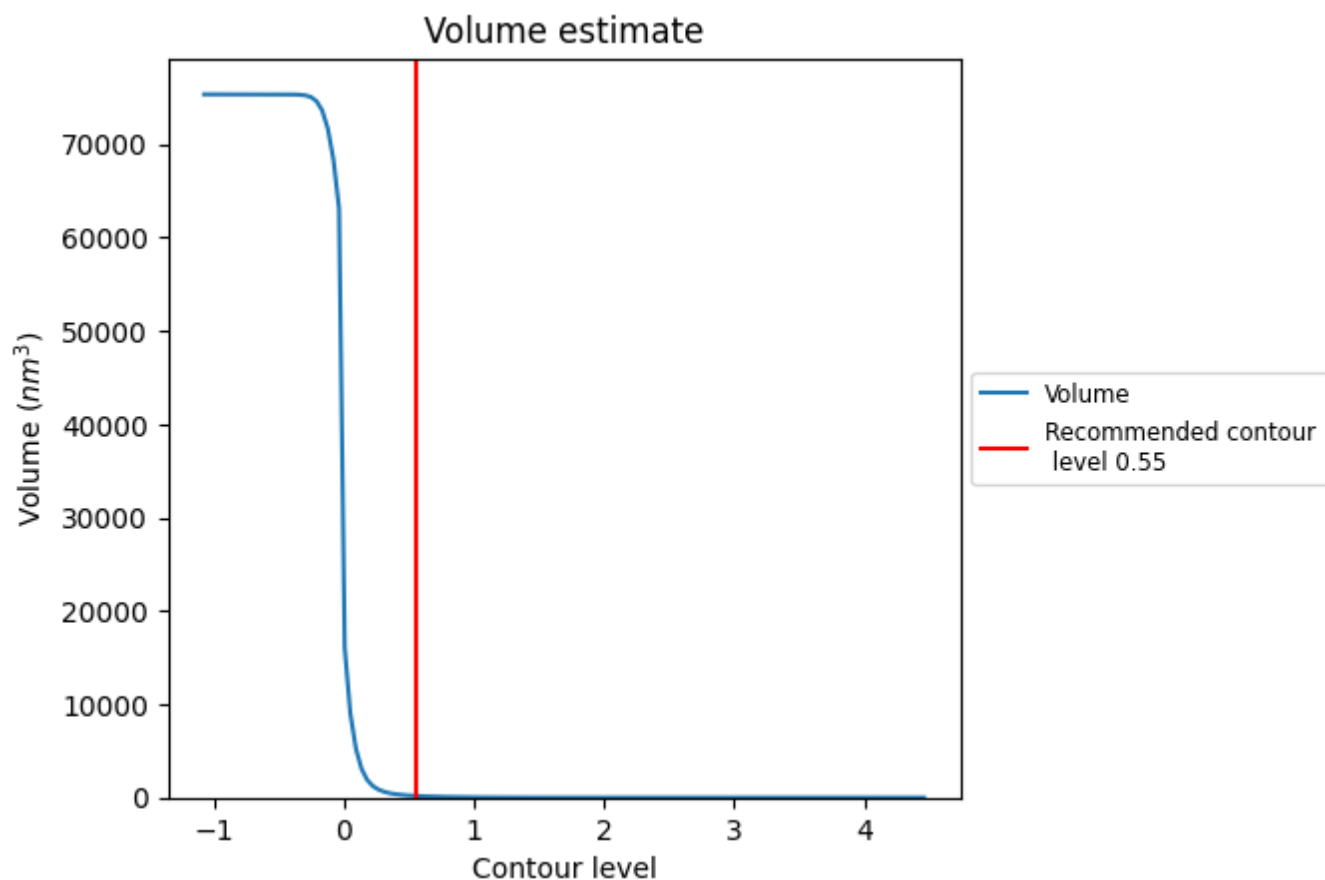
This section contains the results of statistical analysis of the map.

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.

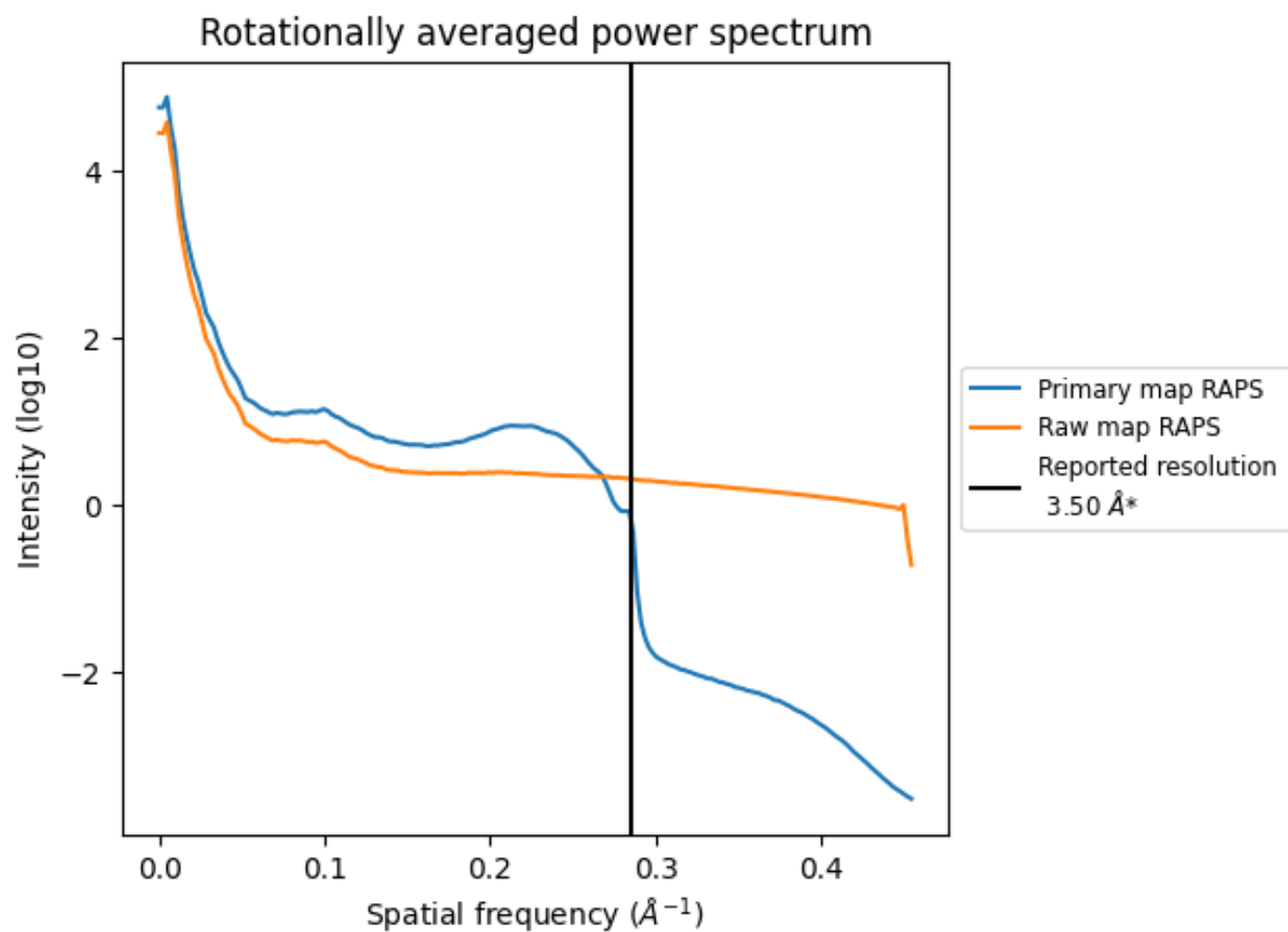
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

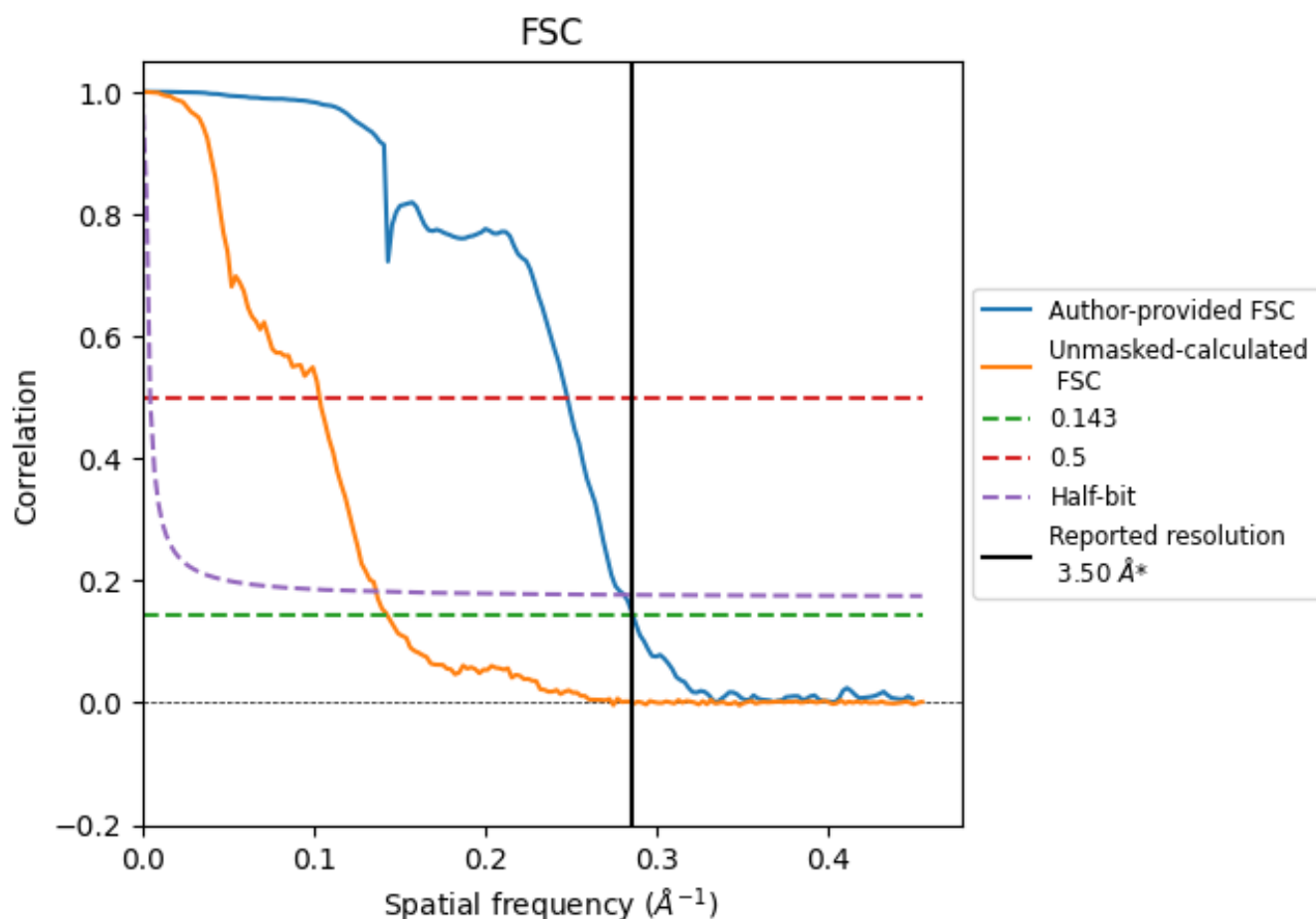


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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](#)

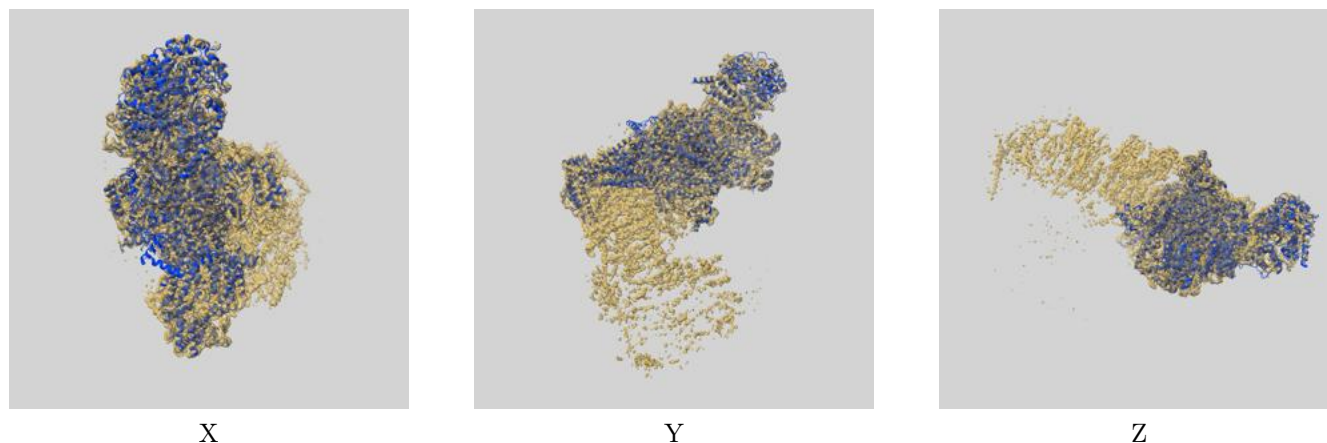
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.04	3.56
Unmasked-calculated*	7.00	9.68	7.34

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

9 Map-model fit [i](#)

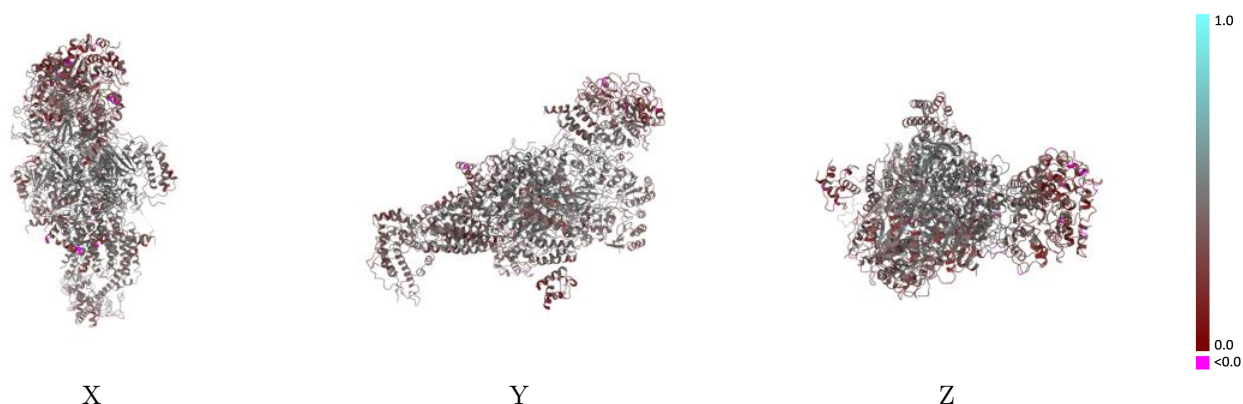
This section contains information regarding the fit between EMDB map EMD-38513 and PDB model 8XNS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



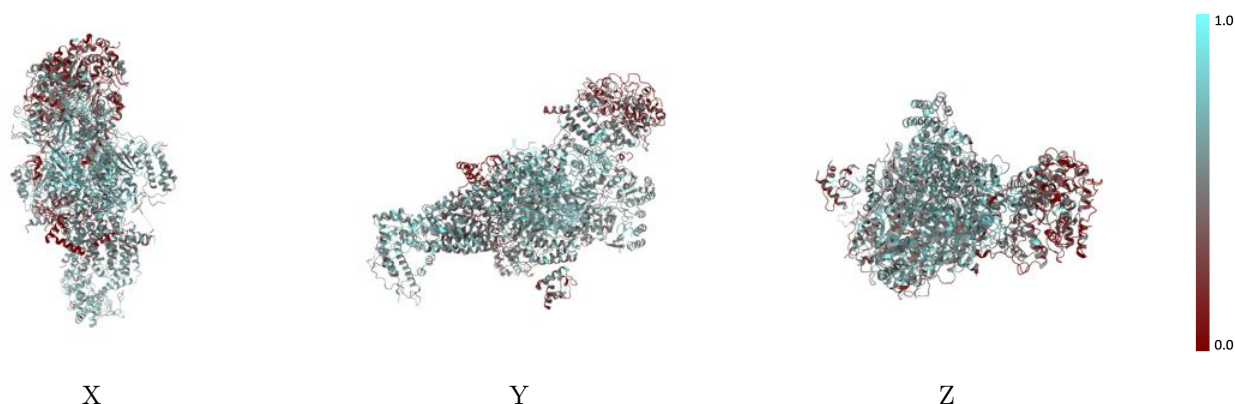
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



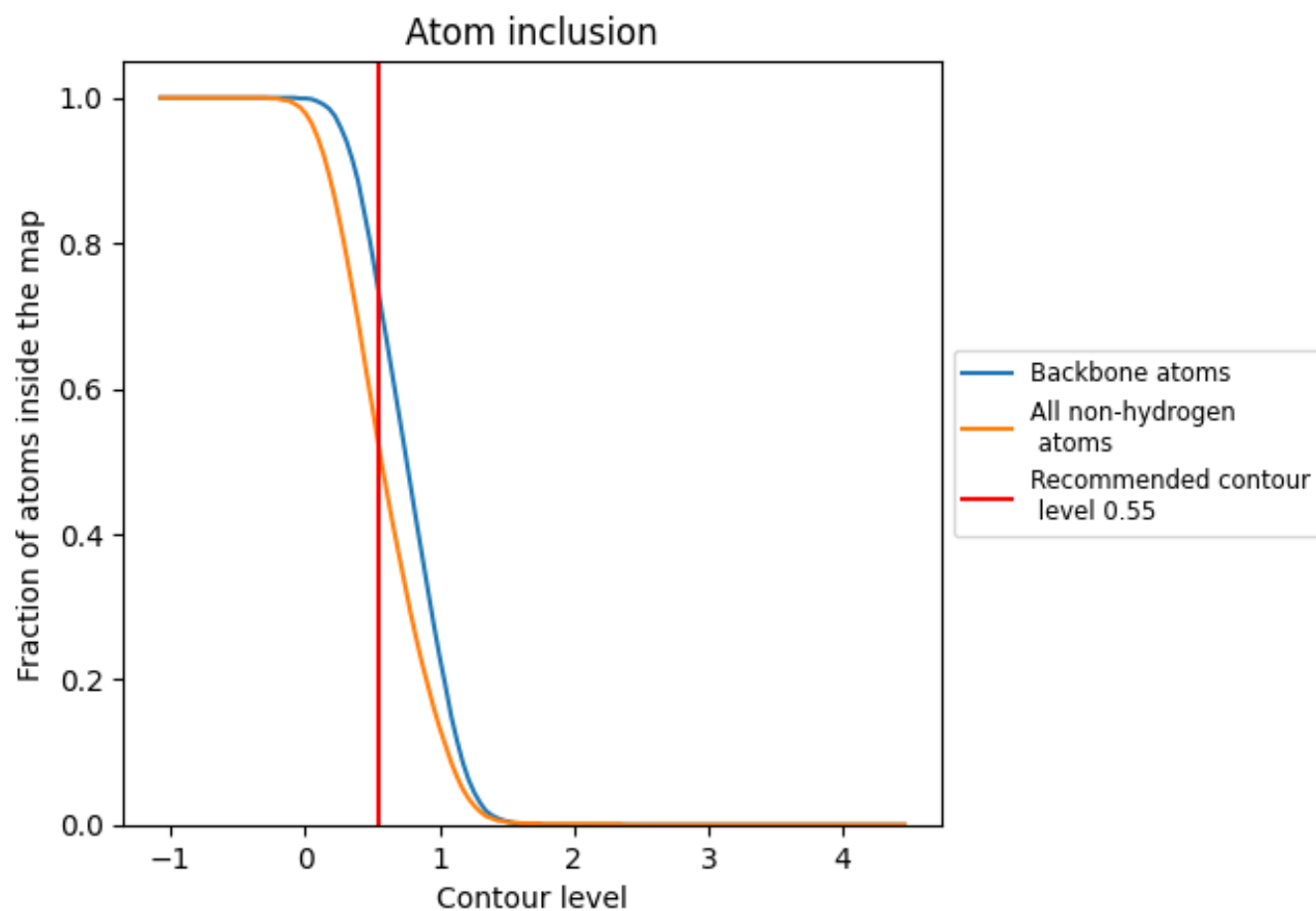
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 52% 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	 0.5210	 0.3890
A	 0.4950	 0.4110
B	 0.6280	 0.4500
C	 0.6460	 0.4660
D	 0.6540	 0.4590
E	 0.3250	 0.3020
F	 0.3740	 0.3230
G	 0.5850	 0.4080
H	 0.5420	 0.4030
I	 0.6740	 0.4500
P	 0.5190	 0.3650
Q	 0.5020	 0.4220
R	 0.2490	 0.3360
S	 0.5680	 0.3650
T	 0.3690	 0.2640
V	 0.5990	 0.3880
W	 0.5470	 0.4040
X	 0.5770	 0.3730
Z	 0.5630	 0.3780
a	 0.6280	 0.4230
b	 0.5650	 0.3790
q	 0.1610	 0.3140
r	 0.2620	 0.2990
s	 0.0540	 0.2700

