



Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 01:02 pm BST

PDB ID : 7A24 / pdb_00007a24
EMDB ID : EMD-11615
Title : Assembly intermediate of the plant mitochondrial complex I
Authors : Soufari, H.; Waltz, F.; Hashem, Y.
Deposited on : 2020-08-16
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

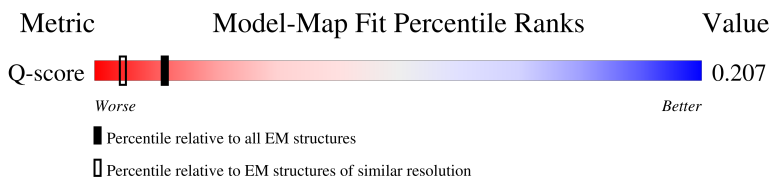
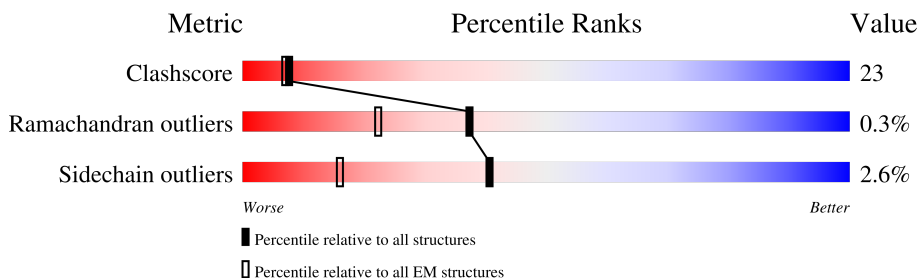
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

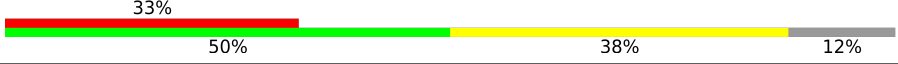
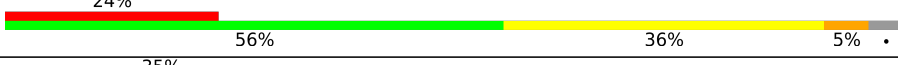
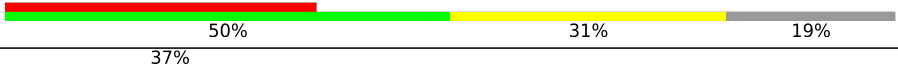
The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	
2	I	499	
3	J	119	
4	N	205	

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Mol	Chain	Length	Quality of chain
5	H	325	
6	K	100	
7	Y	106	
8	Z	143	
9	V	65	
10	W	65	
11	S	131	
12	i	81	
13	j	83	
14	G	394	
15	C	748	
16	T	402	
17	F	190	
18	B	255	
19	O	154	
20	P	110	
21	R	169	
22	U	159	
23	E	218	
24	D	222	
25	X	133	
26	c	106	
27	Q	97	
28	k	122	
29	r	24	

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Mol	Chain	Length	Quality of chain
30	n	113	
31	o	252	
32	p	275	
32	q	275	
33	z	610	

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
34	SF4	A	501	-	-	X	-
34	SF4	D	301	-	-	X	-
34	SF4	E	301	-	-	X	-
37	CDL	i	201	-	-	X	-
39	FES	B	301	-	-	X	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 49497 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 51kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3328	2100	593	610	25		

- Molecule 2 is a protein called Nad2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	481	Total	C	N	O	S	0	0
			3754	2525	569	633	27		

- Molecule 3 is a protein called Nad3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	96	Total	C	N	O	S	0	0
			800	559	112	126	3		

- Molecule 4 is a protein called Nad6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	149	Total	C	N	O	S	0	0
			1201	810	194	189	8		

- Molecule 5 is a protein called Nad1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	318	Total	C	N	O	S	0	0
			2493	1691	378	409	15		

- Molecule 6 is a protein called Nad4Lm.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	85	Total	C	N	O	S	0	0
			667	450	101	110	6		

- Molecule 7 is a protein called PGIV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	98	Total	C	N	O	S	0	0
			774	484	133	145	12		

- Molecule 8 is a protein called B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	140	Total	C	N	O	S	0	0
			1103	701	195	199	8		

- Molecule 9 is a protein called MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	57	Total	C	N	O	S	0	0
			461	296	82	78	5		

- Molecule 10 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	37	Total	C	N	O	S	0	0
			273	179	45	46	3		

- Molecule 11 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	101	Total	C	N	O	S	0	0
			821	513	143	161	4		

- Molecule 12 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	63	Total	C	N	O	S	0	0
			492	319	87	81	5		

- Molecule 13 is a protein called 15kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	j	68	Total	C	N	O	S	0	0
			582	359	113	103	7		

- Molecule 14 is a protein called Nad7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	382	Total	C	N	O	S	0	0
			3049	1939	535	551	24		

- Molecule 15 is a protein called 75kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	693	Total	C	N	O	S	0	0
			5288	3315	926	1008	39		

- Molecule 16 is a protein called 39kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	328	Total	C	N	O	S	0	0
			2535	1628	433	459	15		

- Molecule 17 is a protein called Nad9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	178	Total	C	N	O	S	0	0
			1518	979	262	272	5		

- Molecule 18 is a protein called 24kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	219	Total	C	N	O	S	0	0
			1702	1081	286	323	12		

- Molecule 19 is a protein called 18kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	111	Total	C	N	O	S	0	0
			874	561	150	162	1		

- Molecule 20 is a protein called 13kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	71	Total	C	N	O	S	0	0
			554	348	97	103	6		

- Molecule 21 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	121	Total	C	N	O	S	0	0
			977	614	165	193	5		

- Molecule 22 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	122	Total	C	N	O	S	0	0
			1011	643	184	183	1		

- Molecule 23 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	153	Total	C	N	O	S	0	0
			1215	779	212	210	14		

- Molecule 24 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	177	Total	C	N	O	S	0	0
			1438	901	239	287	11		

- Molecule 25 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	103	Total	C	N	O	S	0	0
			843	537	151	152	3		

- Molecule 26 is a protein called MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	99	Total	C	N	O	S	0	0
			744	479	121	140	4		

- Molecule 27 is a protein called B8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	92	Total	C	N	O	S	0	0
			722	456	128	132	6		

- Molecule 28 is a protein called ACPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	78	Total	C	N	O	S	0	0
			614	390	94	127	3		

- Molecule 29 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	r	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 30 is a protein called P2.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	n	27	Total	C	N	O	0	0
			205	133	35	37		

- Molecule 31 is a protein called CAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	202	Total	C	N	O	S	0	0
			1568	1006	270	287	5		

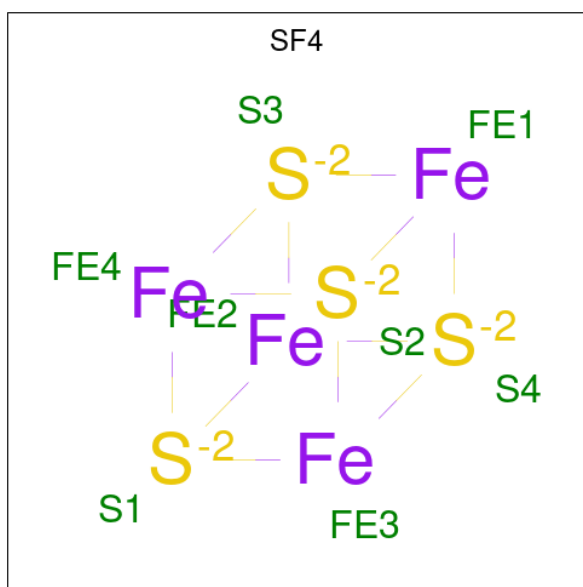
- Molecule 32 is a protein called CA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	228	Total	C	N	O	S	0	0
			1736	1088	318	324	6		
32	p	224	Total	C	N	O	S	0	0
			1705	1068	311	320	6		

- Molecule 33 is a protein called GLDH.

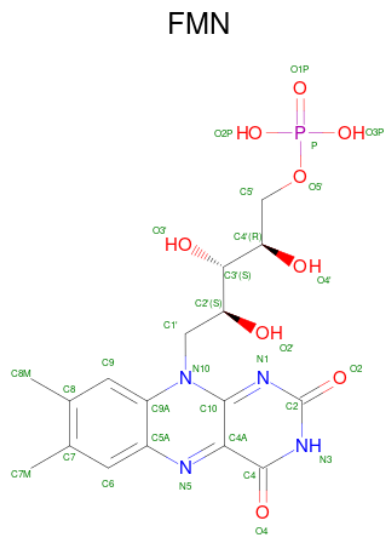
Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	499	Total	C	N	O	S	0	0
			3992	2527	700	754	11		

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



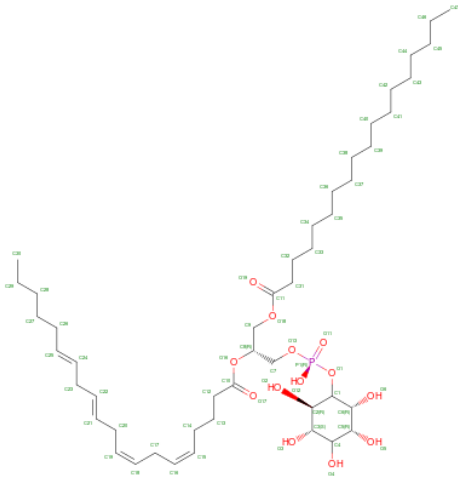
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	C	1	Total	Fe	S	0
			8	4	4	
34	E	1	Total	Fe	S	0
			8	4	4	
34	D	1	Total	Fe	S	0
			8	4	4	
34	D	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



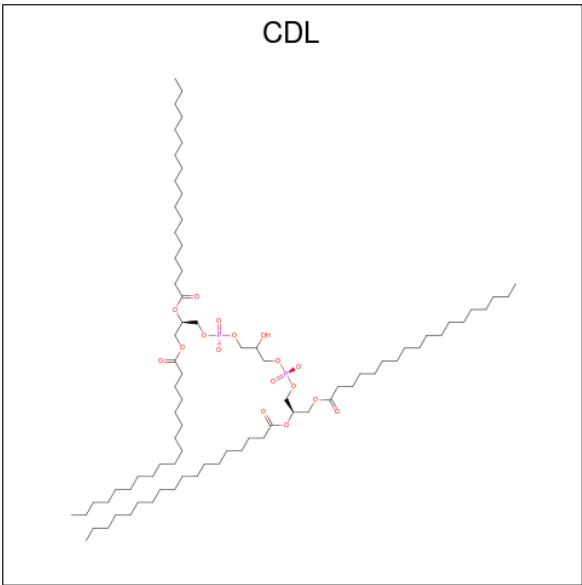
Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 36 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



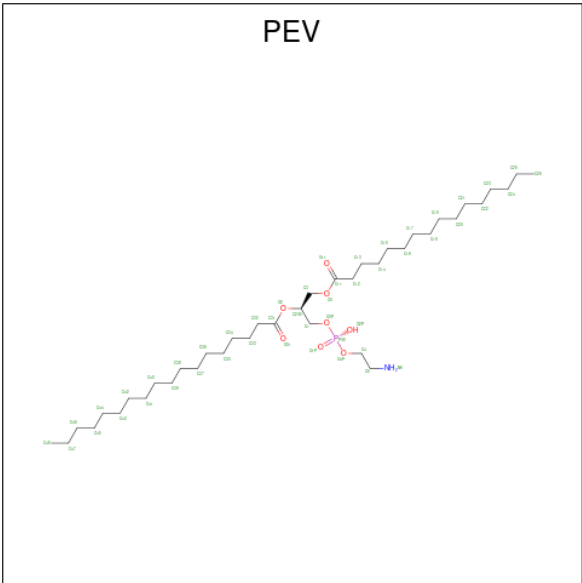
Mol	Chain	Residues	Atoms				AltConf
36	I	1	Total 42	C 28	O 13	P 1	0
36	c	1	Total 37	C 23	O 13	P 1	0

- Molecule 37 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



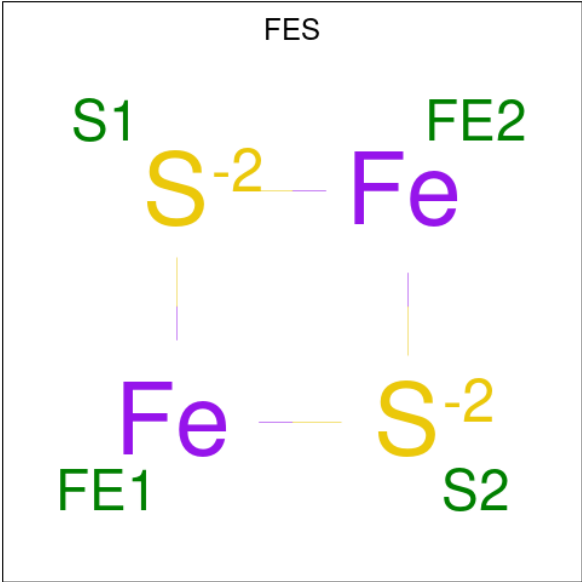
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
37	i	1	90	71	17	2	0

- Molecule 38 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



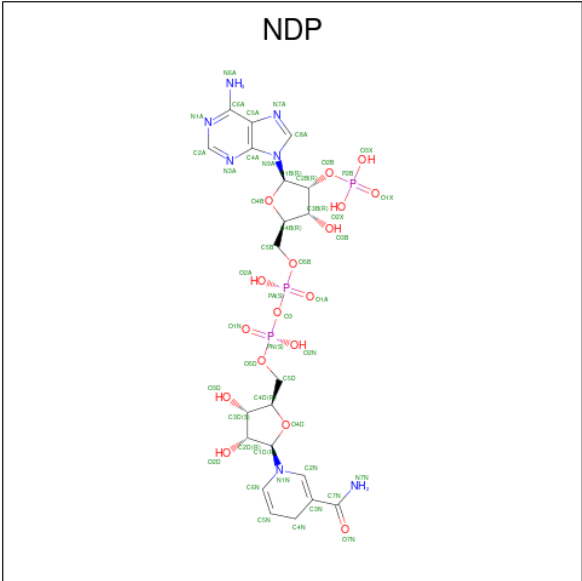
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	G	1	28	18	1	8	1	0

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
39	C	1	Total	Fe	S	0
			4	2	2	
39	B	1	Total	Fe	S	0
			4	2	2	

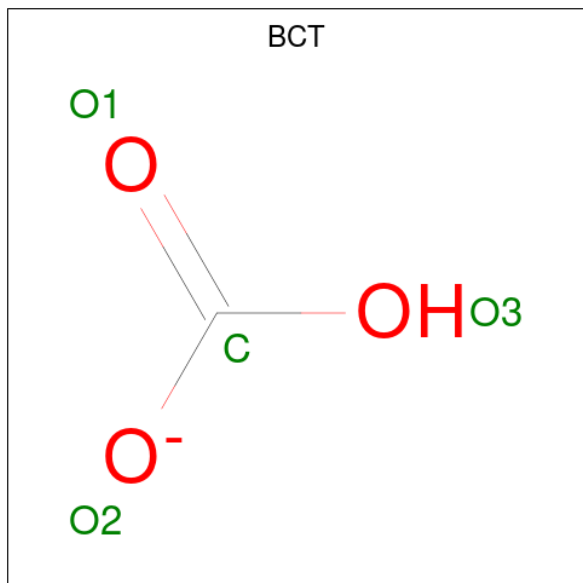
- Molecule 40 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



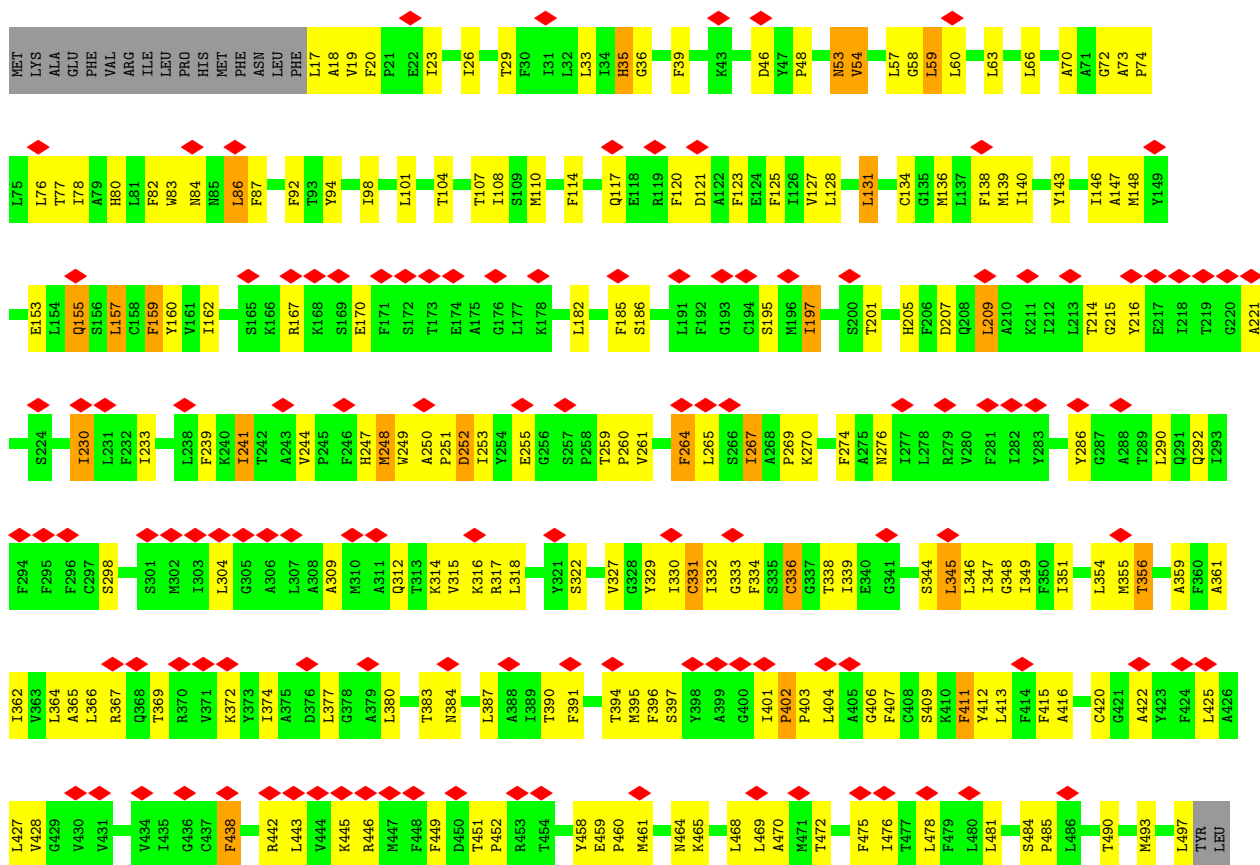
- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	P	1	Total	Zn	0
			1	1	
41	q	1	Total	Zn	0
			1	1	

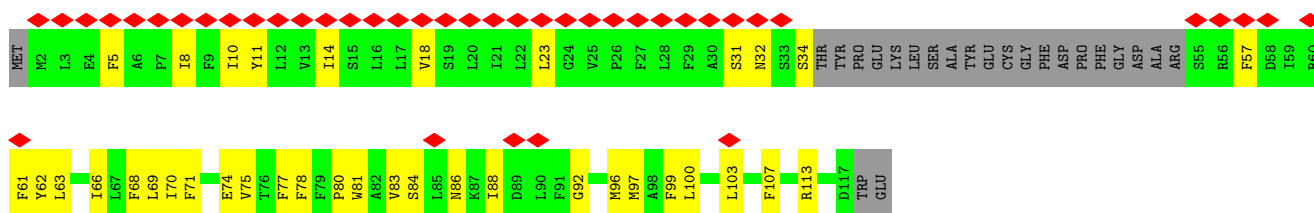
- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



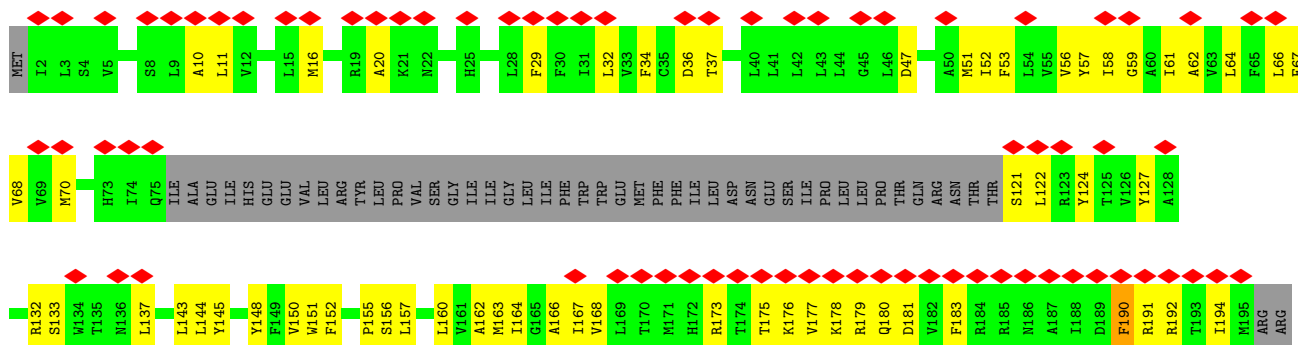
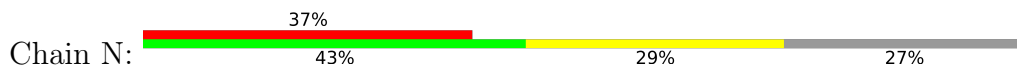
Mol	Chain	Residues	Atoms			AltConf
42	q	1	Total	C	O	0
			4	1	3	



• Molecule 3: Nad3m



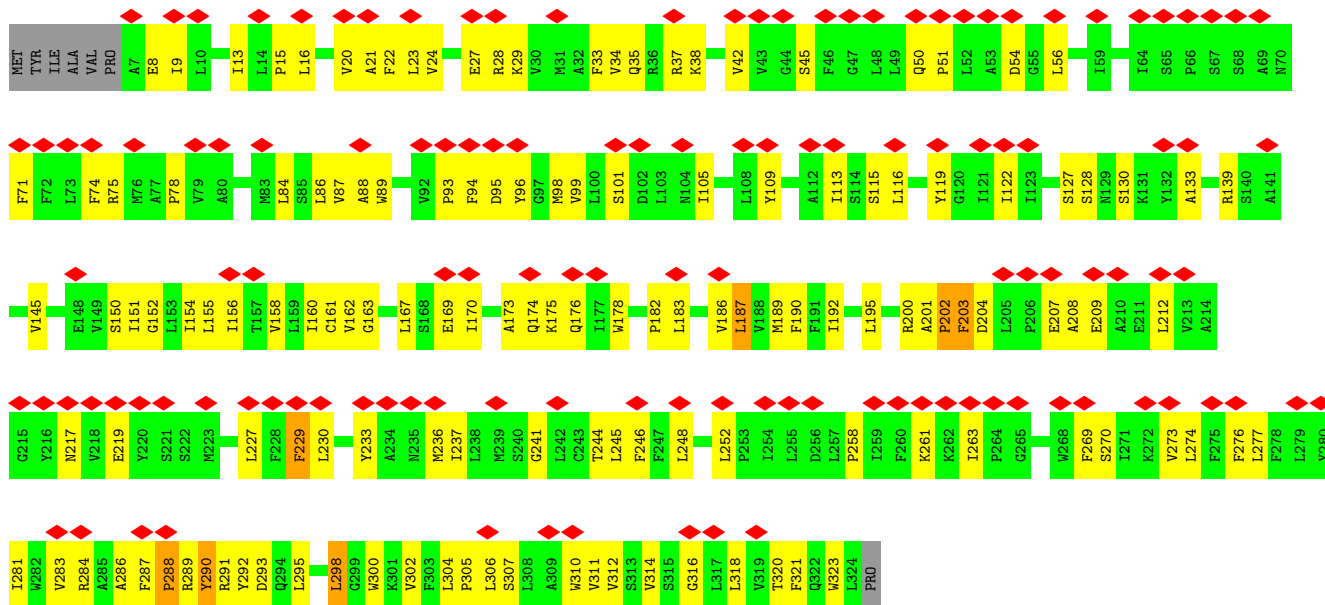
• Molecule 4: Nad6m



THR
THR
ASP
PRO
LEU
THR
ILE
TYR

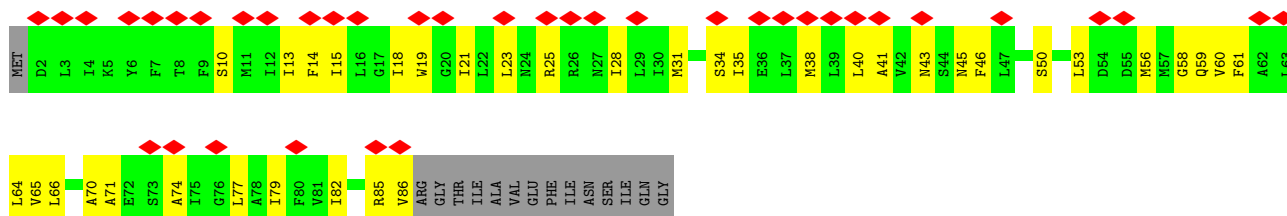
• Molecule 5: Nad1m

Chain H: 



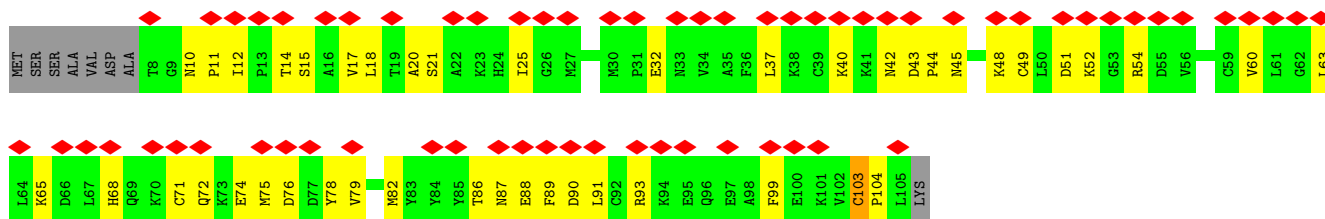
• Molecule 6: Nad4Lm

Chain K: 



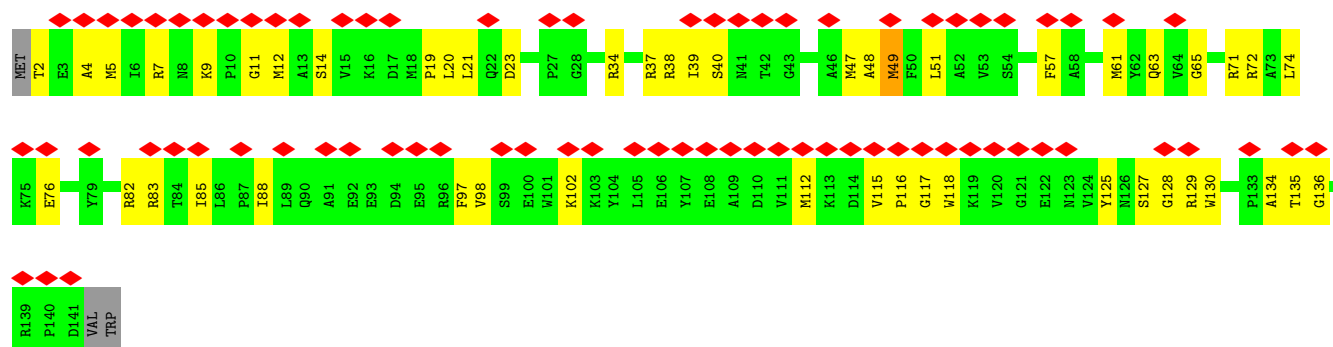
• Molecule 7: PGIV

Chain Y: 

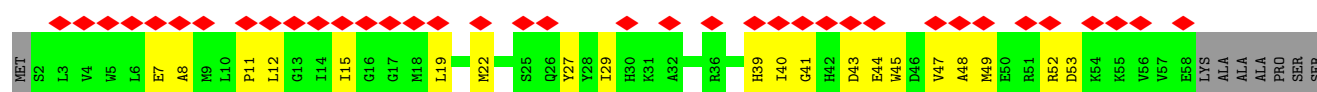


• Molecule 8: B16.6

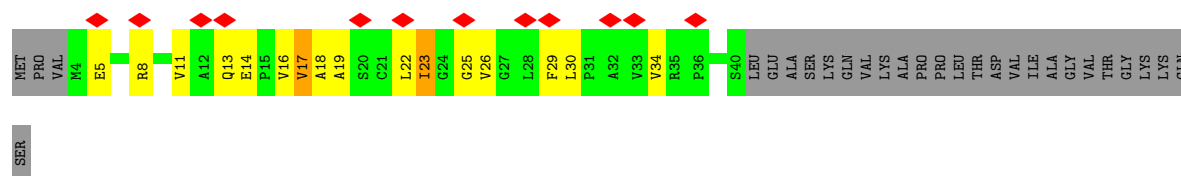
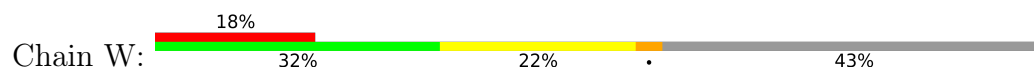
Chain Z: 



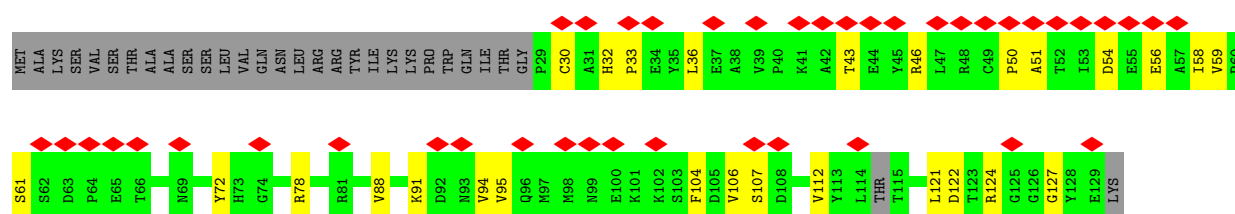
• Molecule 9: MWFE



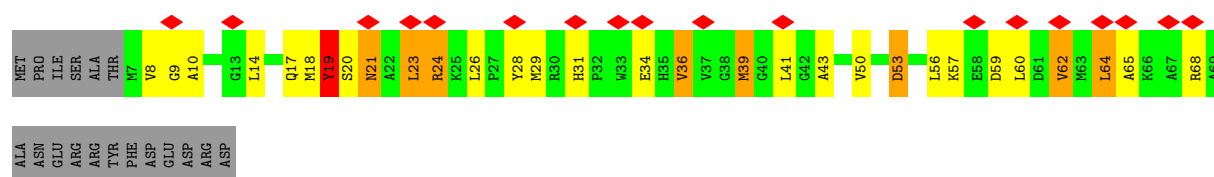
• Molecule 10: B9



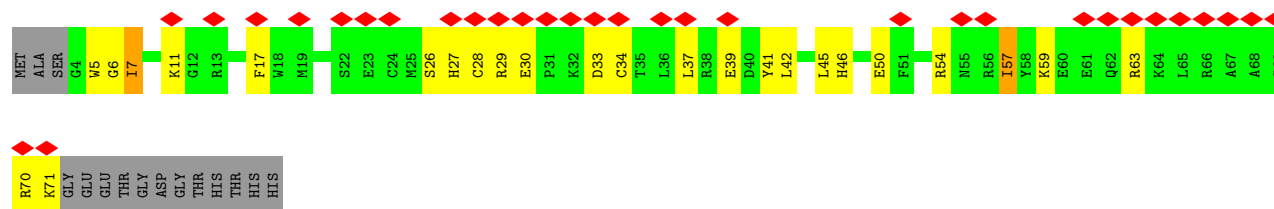
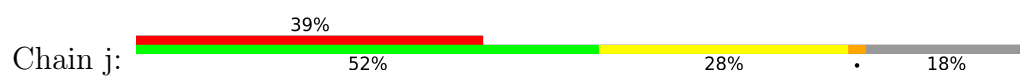
• Molecule 11: B14.5a



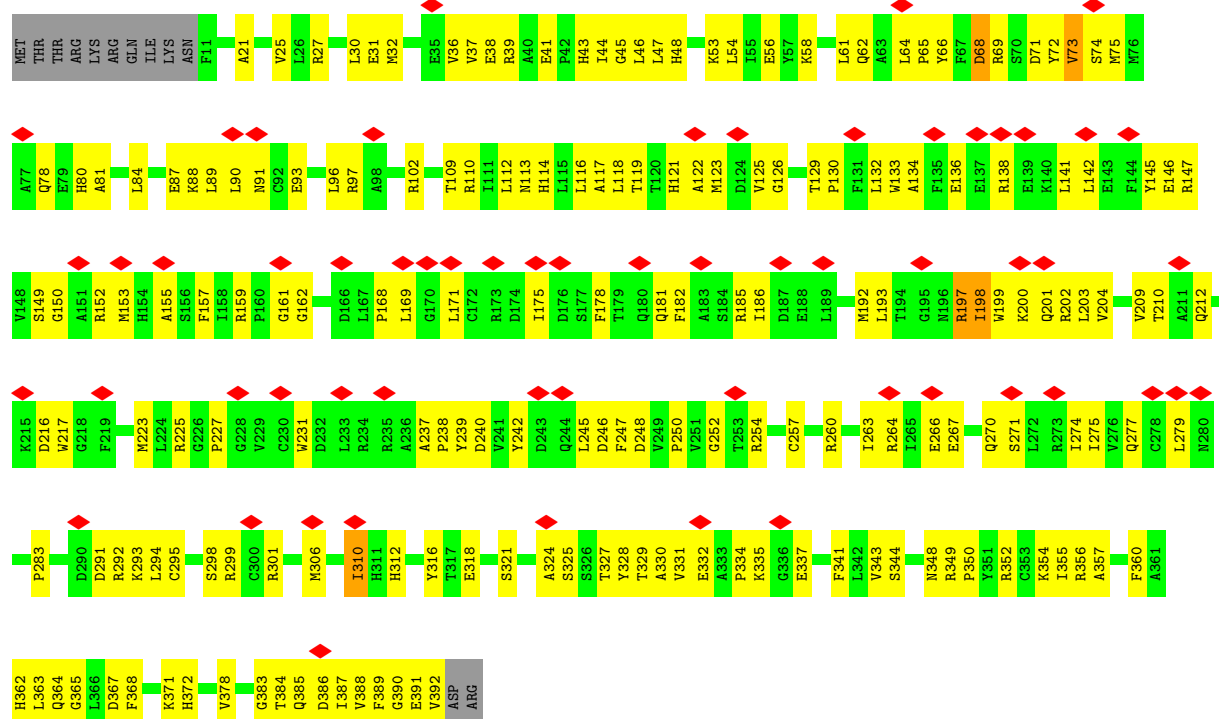
• Molecule 12: B14.5b



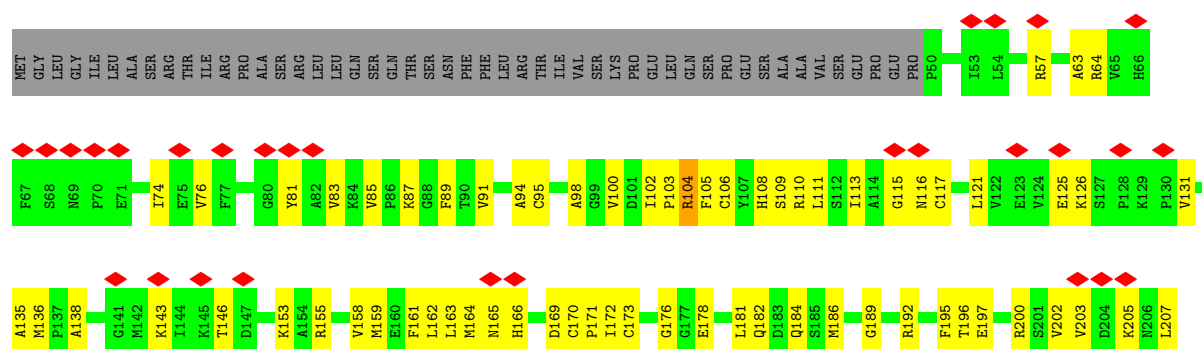
• Molecule 13: 15kDa

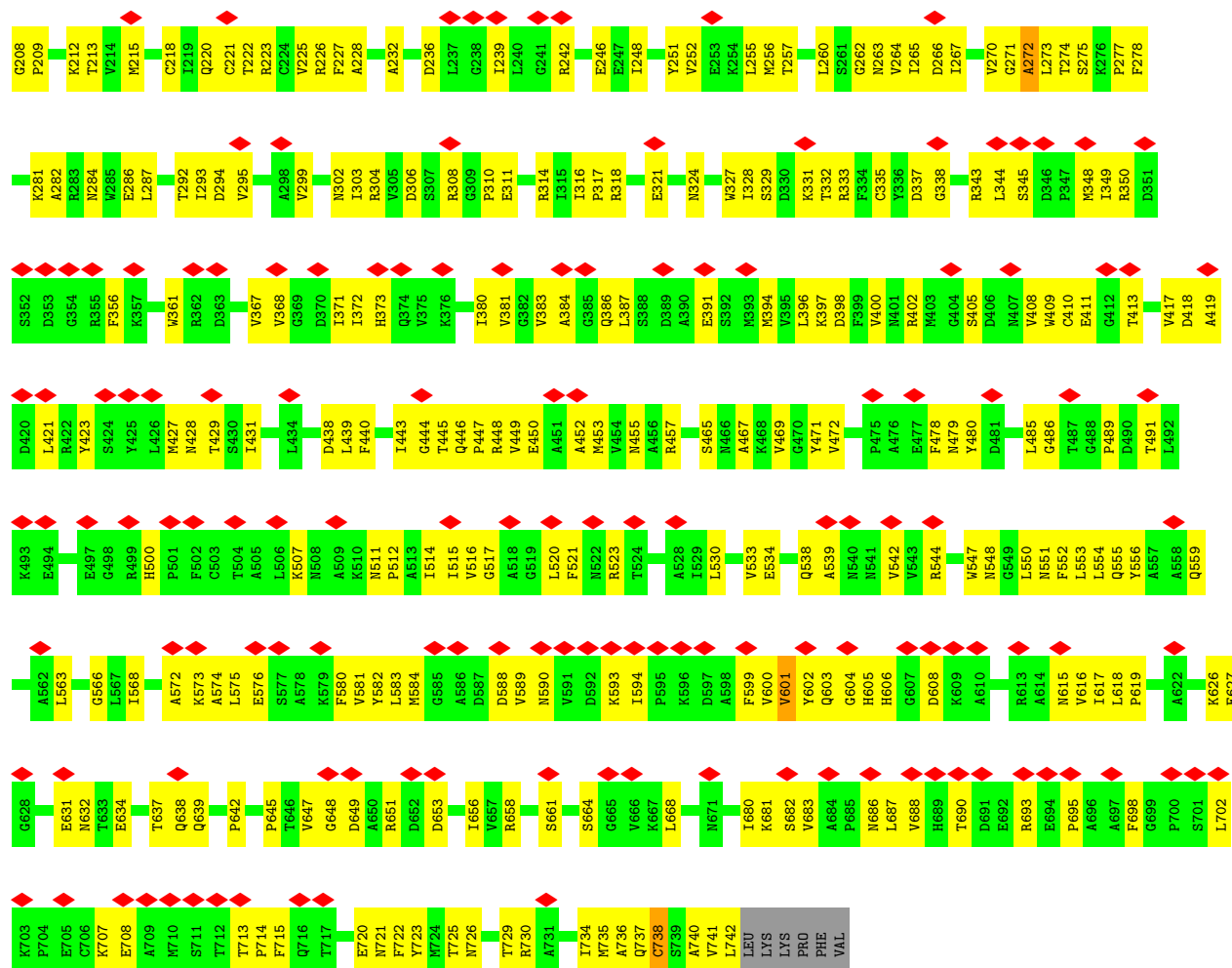


• Molecule 14: Nad7m

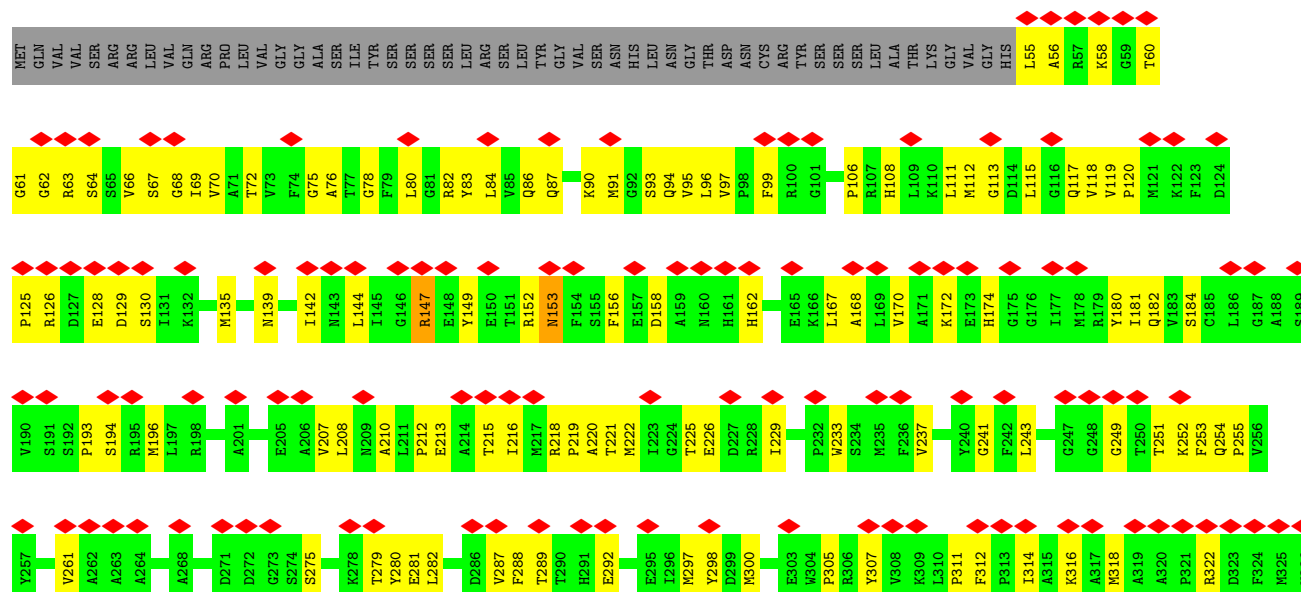
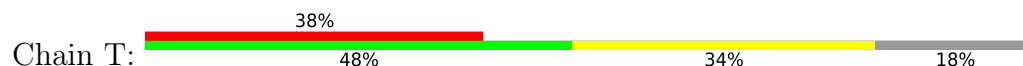


• Molecule 15: 75kDa

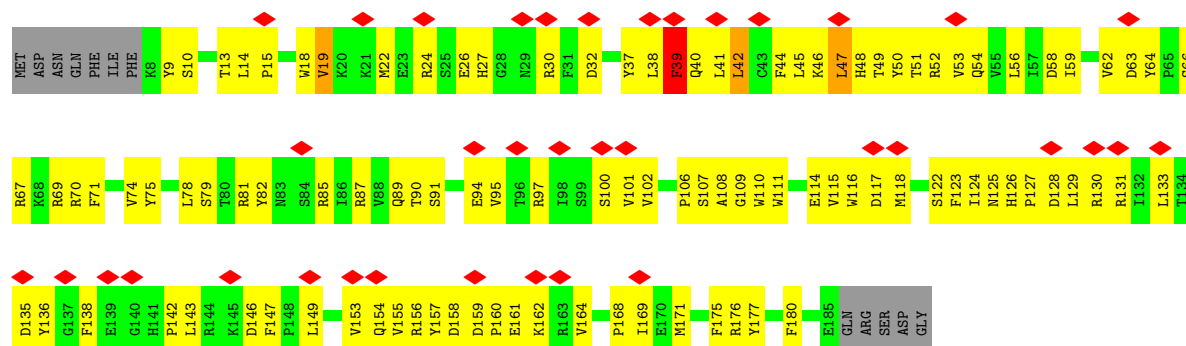




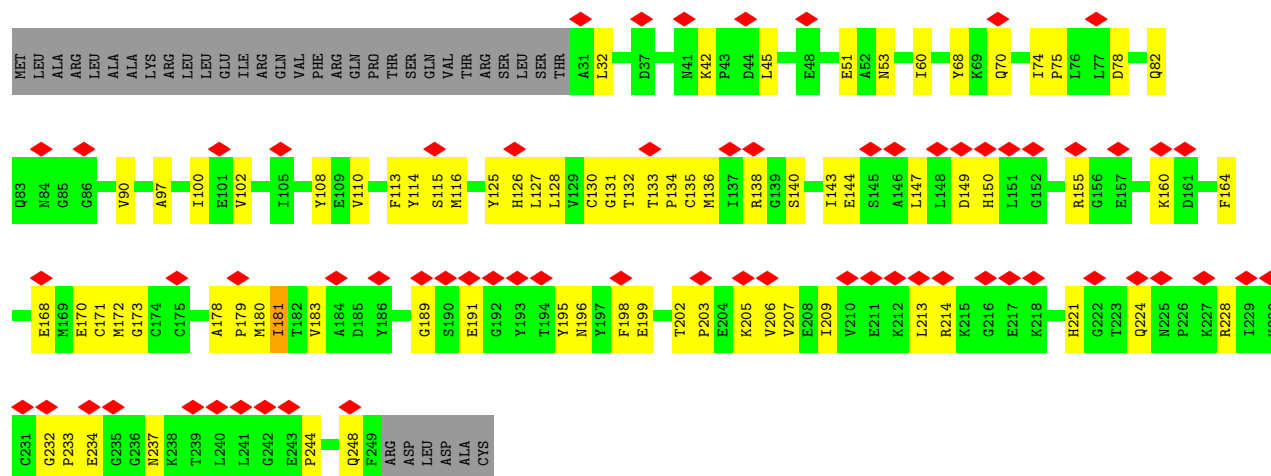
Molecule 16: 39kDa



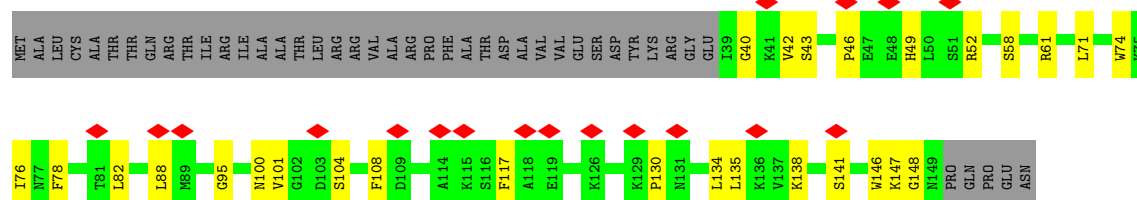
- Molecule 17: Nad9m



- Molecule 18: 24kDa



- Molecule 19: 18kDa



Chain P:

277

50%

15%

35%

MET ALA SER ASN LEU LEU LYS ALA LEU ILE ARG SER GLN LEU PRO SER SER ARG ARG ARG PHE SER VAL ALA THR THR LEU LEU GLY ILE PRO THR ASP ASP LEU VAL G39 T41 Q46 D47 R48 S49 K50 K51 S52 L56 I57 S58 E59 V60 K64 V65 D66 G67 S68

Chain R:

28% 40% 29% 28%

Chain R: MET PHE LEU ARG ALA ILE GLY ARG PRO LEU LEU ALA LYS V14 K15 Q16 T17 T18 G19 I20 V21 G22 L23 D24 V25 V26 P27 N28 A29 R30 V31 V32 L33 I34 D35 L36 Y37 K38 K39 T40 L41 K42 E43 I44 V47 P48 E49 D50 E51 R54 K55 A56 V57 E58 S59 F60 T61 R62 Q63 R64 L65 M66 V67 C68 K69 E70 E71 E72 D73 W74 W75 M76 I77 E78 K79 R80 L81 G82 C83 V86 E87 E88 L89 I90 E91 E92 A93 R94 D95 L99 K102 M103 W109 G110 D114 Y115 E116 C117 E118 V119 I120 E121 N122 P125 I126 P127 K128 H129 P130 P131 Q132 H133

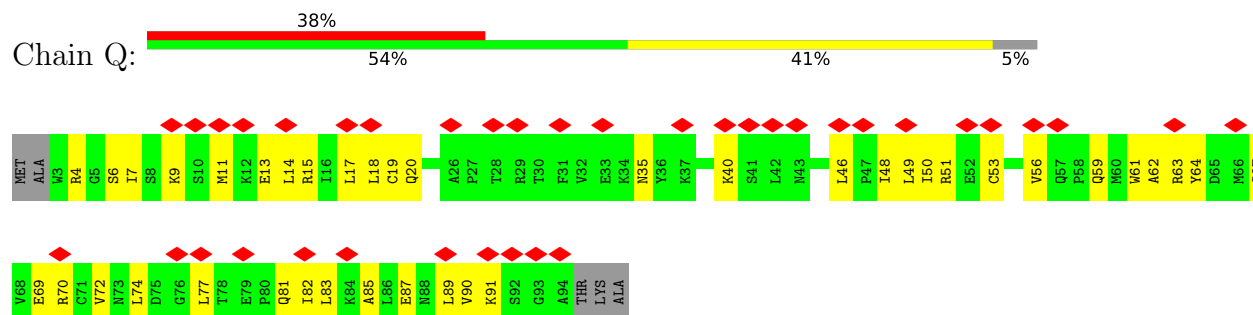
Chain U:

Amino Acid	Count	Category
MET	1	Grey
ALA	1	Grey
LEU	1	Grey
THR	1	Grey
VAL	1	Grey
ALA	1	Grey
LYS	1	Green
SER	1	Green
ALA	1	Green
LEU	1	Green
GLU	1	Green
ALA	1	Green
ILE	1	Green
ARG	1	Green
GLU	1	Green
LYS	1	Green
GLY	1	Green
LEU	1	Green
GLY	1	Green
GLY	1	Green
PHE	1	Green
MET	1	Green
R32	1	Red
C33	1	Red
L34	1	Red
P35	1	Red
D36	1	Red
G37	1	Red
N38	1	Red
L39	1	Red
L40	1	Red
Q41	1	Red
T42	1	Red
K43	1	Red
T44	1	Red
H45	1	Red
N46	1	Red
I47	1	Red
G48	1	Red
A49	1	Red
T50	1	Red
L51	1	Red
V52	1	Red
G53	1	Red
V54	1	Red
D55	1	Red
K56	1	Red
F57	1	Red
G58	1	Red
N59	1	Red
K60	1	Red
V61	1	Green
V62	1	Green
Q63	1	Green
K64	1	Green
L65	1	Green
D66	1	Green
D67	1	Green
T68	1	Green
Q69	1	Green
Y70	1	Green
G71	1	Green
R72	1	Green
H73	1	Green
R74	1	Green
W75	1	Green
V76	1	Green
E77	1	Green
E78	1	Green
A79	1	Green
S80	1	Green
K81	1	Green
D82	1	Green
R83	1	Green
Y84	1	Green
N85	1	Green
A86	1	Green
S87	1	Green
Q88	1	Green
W89	1	Green
P90	1	Green
A91	1	Green
E92	1	Green
W93	1	Green
H94	1	Green
H98	1	Green
F99	1	Green
I100	1	Green
D102	1	Green
H103	1	Green
T104	1	Green
G105	1	Green
D106	1	Green
E107	1	Green
L108	1	Green
L109	1	Green
S110	1	Green
L111	1	Green
K112	1	Green
P113	1	Green
K114	1	Green
R115	1	Green
Y116	1	Green
G117	1	Green
L118	1	Green
E119	1	Green
H120	1	Green
K121	1	Green
F122	1	Green
M123	1	Green
F124	1	Green
S125	1	Green
G126	1	Green
E127	1	Green
G128	1	Green
D129	1	Green
A130	1	Green
Y131	1	Green
I132	1	Green
Y133	1	Green
S135	1	Green
K136	1	Green
G137	1	Green
H138	1	Green
T139	1	Green
L140	1	Green
M141	1	Green
P142	1	Green
G143	1	Green
Q144	1	Green
K145	1	Green
N146	1	Green
W147	1	Green
T148	1	Green
R149	1	Green
Y150	1	Green
Q151	1	Green
S152	1	Green
W153	1	Green
VAL	1	Grey
PRO	1	Grey
THR	1	Grey
LYS	1	Grey
THR	1	Grey
GLN	1	Grey

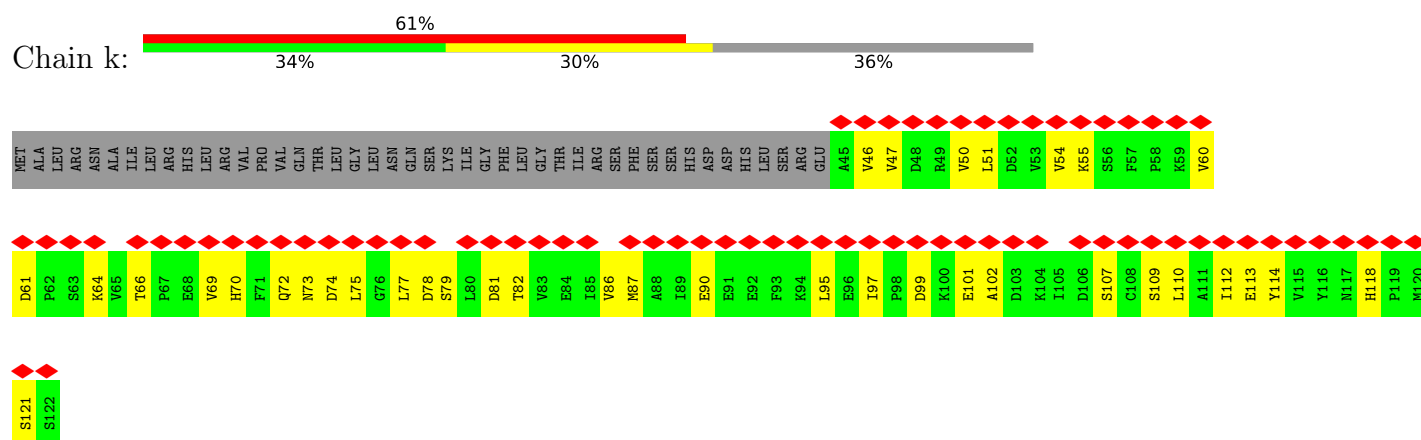
Chain E:

LEU SER MET ILE THR ARG ASN THR ALA MET LYS S70 S76 S77 S78 S79 S80 S81 S82 S83 S84 S85 S86 S87 S88 S89 S90 S91 S92 S93 S94 S95 S96 S97 S98 S99 G102 G103 G104 D107 L108 D109 R110 F111 G112 I113 I114 F115 R116 P119 R120

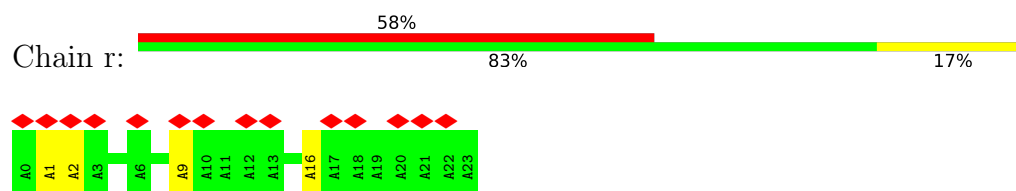
- Molecule 27: B8



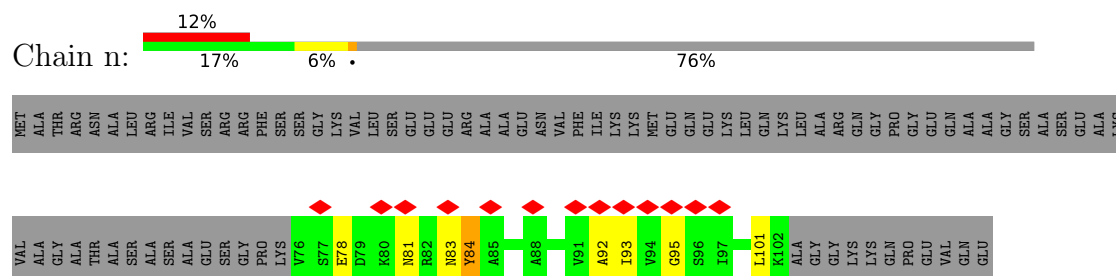
- Molecule 28: ACPM1



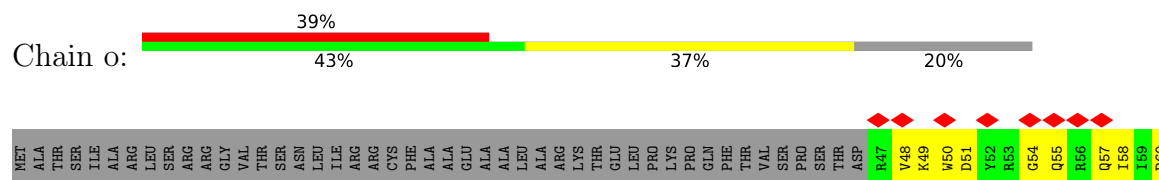
- Molecule 29: Unk1

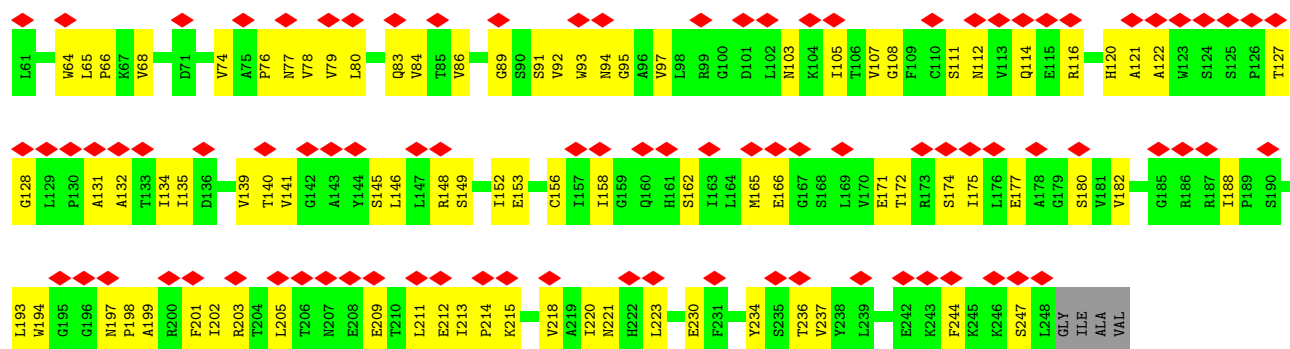


- Molecule 30: P2

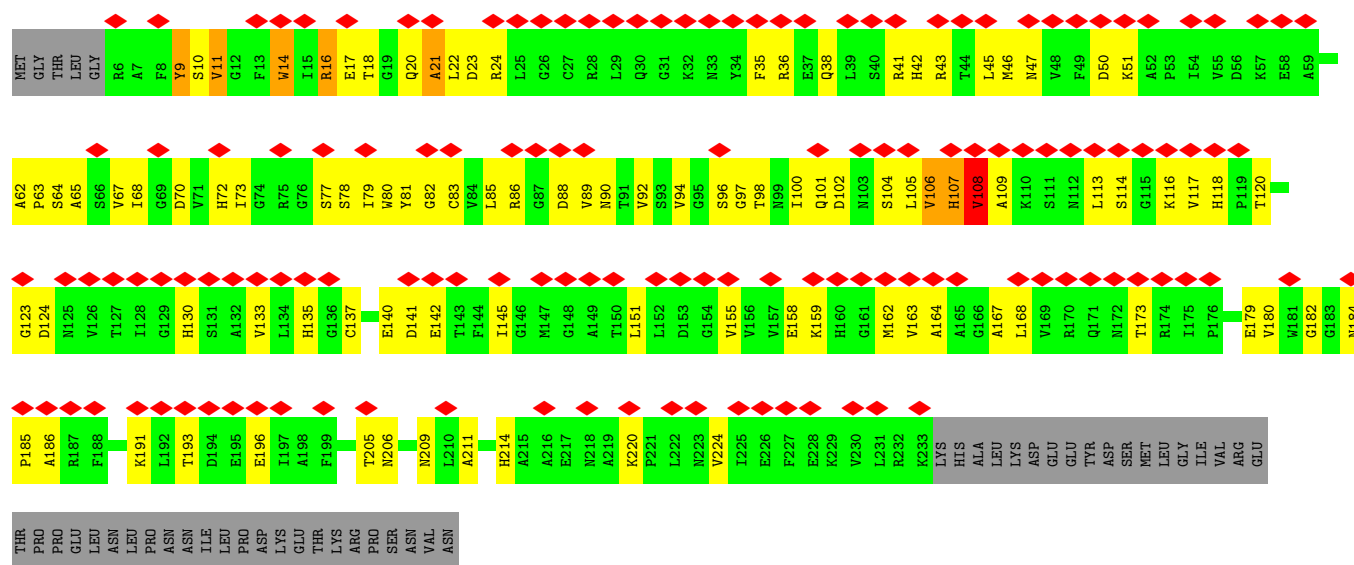


- Molecule 31: CAL1

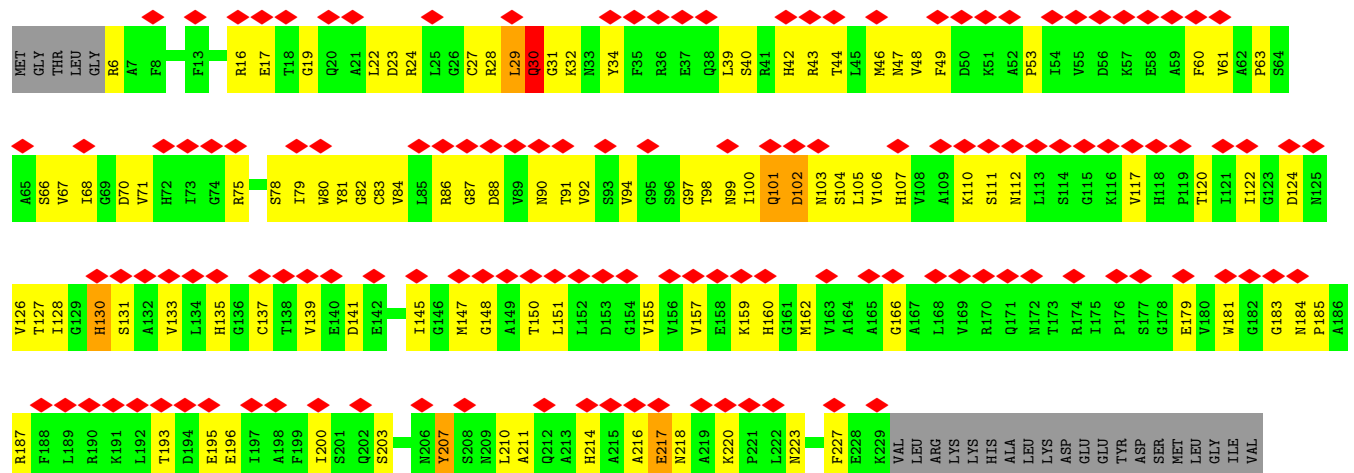
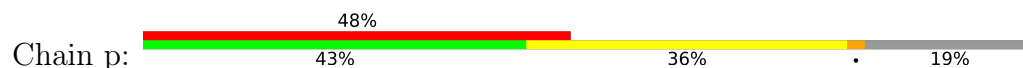




• Molecule 32: CA1



• Molecule 32: CA1



ARG
GLU
THR
SER
PRO
PHE
GLU
LEU
LEU
ASN
ARG
GLU
LEU
VAL
ASN
PRO
GLY
SER
ASN
TLE
LEU
PRO
ASP
LYS
THR
GLU
THR
LYS
ARG
SER
PRO
SER
SER
ASN
VAL
ASN

• Molecule 33: GLDH

Chain z: 

MET
LEU
ARG
SER
GLN
PHE
LEU
LEU
LEU
ARG
ARG
SER
GLY
VAL
TLE
GLY
SER
SER
ASN
TLE
LEU
PRO
ASP
LYS
THR
GLU
THR
LYS
ARG
SER
PRO
SER
SER
ASN
VAL
ASN

SER
GLU
ALA
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CYS
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ARG
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PRO
PRO
PRO
PRO
ALA
ALA
THR

R124
N125
F126
N127
P128
Q129
E130
N131
A132
A133
D134
L135
Y136
A137
L138
V139
K140
E141
S142
H143
K144
K145
K146
L147
I148
I149
R150
P151
V152
G153
S154
G155
L156
S157
P158
N159
G160
I161
G162
L163
S164
R165
S166
G167
M168
V169
N170
L171
A172
L173
M174
D175
K176
L177
L178
E179
V180
Q181
K182
E183

K184
K185
R186
V187
T188
V189
Q190
A191
G192
I193
R194
V195
Q196
Q197
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V199
D200
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I202
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H204
Y205
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Q210
N211
F212
A213
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R216
E217
Q218
Q219
I220
G221
G222
I223
I224
Q225
V226
G227
A228
H229
G230
T231
G232
R234
L235
P236
V237
T238
D239
E240
Q241
V242
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S244
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V248
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S258
R259
E260
D262
K261
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A269
R270
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G275
L276
G277
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Q285
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L301
Q302
E303

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L321
Y322
I323
P324
Y325
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V330
V331
V332
T333
C334
N335
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P482
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Q541
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Q543

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N583
K584
A585
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M599
V600
E601
K602
L603

F604
P605
VAL
SER
THR
THR
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.065	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.11, 1.11, 1.11	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NDP, FES, T7X, ZN, BCT, CDL, FMN, PEV

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	0.40	0/3401	0.59	0/4588
2	I	0.89	0/3855	1.34	8/5234 (0.2%)
3	J	0.31	0/826	0.41	0/1120
4	N	0.41	0/1227	0.58	1/1664 (0.1%)
5	H	0.57	2/2565 (0.1%)	0.81	9/3492 (0.3%)
6	K	0.40	0/677	0.55	0/916
7	Y	0.45	0/788	0.63	0/1059
8	Z	0.38	0/1132	0.65	1/1530 (0.1%)
9	V	0.26	0/473	0.39	0/636
10	W	0.71	0/277	1.00	2/375 (0.5%)
11	S	0.25	0/840	0.47	0/1141
12	i	0.88	0/502	1.41	3/676 (0.4%)
13	j	0.87	0/595	1.27	0/791
14	G	0.52	0/3120	0.69	2/4221 (0.0%)
15	C	0.48	0/5386	0.69	5/7299 (0.1%)
16	T	0.44	0/2591	0.64	0/3509
17	F	0.47	0/1564	0.71	2/2120 (0.1%)
18	B	0.31	0/1743	0.48	0/2364
19	O	0.41	0/899	0.46	0/1215
20	P	0.46	0/567	0.64	0/768
21	R	0.50	0/995	0.82	4/1349 (0.3%)
22	U	0.40	0/1044	0.52	0/1413
23	E	0.67	1/1250 (0.1%)	0.97	4/1697 (0.2%)
24	D	0.70	0/1467	1.04	3/1981 (0.2%)
25	X	0.19	0/861	0.35	0/1166
26	c	0.48	1/760 (0.1%)	0.61	0/1028
27	Q	0.23	0/734	0.37	0/989
28	k	0.13	0/625	0.33	0/848
29	r	0.16	0/119	0.31	0/165
30	n	0.95	0/208	1.32	0/282
31	o	0.25	0/1606	0.46	0/2192
32	p	0.44	0/1737	0.75	4/2353 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	q	0.35	0/1768	0.70	4/2395 (0.2%)
33	z	0.98	0/4078	1.20	2/5520 (0.0%)
All	All	0.57	4/50280 (0.0%)	0.81	54/68096 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
32	q	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	E	186	PRO	N-CD	-10.09	1.33	1.47
5	H	288	PRO	C-O	-6.28	1.16	1.23
26	c	44	SER	CA-CB	-5.83	1.44	1.53
5	H	307	SER	CA-CB	-5.06	1.45	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	202	PRO	N-CA-C	-11.73	98.59	113.84
23	E	189	PRO	N-CA-C	-10.56	97.81	110.70
2	I	53	ASN	N-CA-C	-9.88	100.78	113.12
32	q	9	TYR	N-CA-C	-9.18	102.09	113.38
5	H	229	PHE	CB-CA-C	8.60	125.46	110.85
2	I	402	PRO	N-CA-C	8.52	121.10	110.70
10	W	23	ILE	N-CA-C	-8.41	101.55	113.07
2	I	54	VAL	N-CA-C	-8.24	102.40	110.72
21	R	129	HIS	N-CA-C	-7.88	103.23	112.92
15	C	737	GLN	CB-CA-C	7.75	117.50	109.83
15	C	738	CYS	N-CA-C	-7.67	103.65	113.16
2	I	57	LEU	N-CA-C	-7.39	103.23	111.28
14	G	198	ILE	N-CA-C	-7.16	102.49	113.16
4	N	192	ARG	CB-CA-C	7.14	116.90	109.83
21	R	128	LYS	CB-CA-C	6.89	119.98	110.06
21	R	122	ASN	CB-CA-C	-6.86	96.11	109.76
32	p	185	PRO	N-CA-C	-6.81	98.45	112.47
2	I	121	ASP	N-CA-C	-6.80	104.55	112.92
21	R	131	PRO	N-CA-C	6.71	123.06	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	z	524	ARG	CB-CA-C	6.62	116.39	109.83
5	H	202	PRO	CB-CA-C	-6.53	102.58	111.85
10	W	17	VAL	N-CA-C	-6.51	106.34	113.43
23	E	94	CYS	CB-CA-C	6.21	123.80	110.21
14	G	197	ARG	N-CA-C	-6.00	105.96	113.28
5	H	286	ALA	N-CA-C	5.92	120.37	113.20
5	H	229	PHE	CA-CB-CG	-5.89	107.91	113.80
32	q	10	SER	N-CA-C	-5.84	106.20	113.15
2	I	60	LEU	N-CA-C	-5.72	105.41	112.90
5	H	298	LEU	N-CA-C	-5.69	106.21	114.12
2	I	248	MET	CB-CA-C	-5.61	110.09	116.54
2	I	159	PHE	CB-CA-C	5.58	120.05	110.79
17	F	50	TYR	CB-CA-C	5.52	120.77	109.55
15	C	736	ALA	N-CA-C	-5.52	102.11	110.28
12	i	23	LEU	N-CA-C	-5.46	105.33	111.28
33	z	122	GLN	CB-CA-C	5.45	116.19	109.16
15	C	236	ASP	N-CA-C	-5.42	106.60	113.43
17	F	39	PHE	N-CA-C	-5.38	105.52	111.71
12	i	24	ARG	N-CA-C	-5.38	106.69	113.20
23	E	99	MET	N-CA-C	-5.36	105.52	111.36
8	Z	49	MET	N-CA-C	-5.32	105.61	112.68
12	i	23	LEU	N-CA-CB	-5.29	102.35	110.12
5	H	203	PHE	CB-CA-C	-5.27	104.21	112.12
5	H	187	LEU	N-CA-C	-5.24	105.56	111.28
5	H	284	ARG	N-CA-C	-5.21	105.21	112.45
24	D	124	ILE	N-CA-C	-5.17	102.91	109.58
32	p	130	HIS	CB-CA-C	-5.17	100.03	109.54
23	E	156	GLY	CA-C-O	-5.13	118.13	122.29
15	C	736	ALA	CA-C-O	-5.11	115.44	121.16
24	D	130	GLU	N-CA-C	-5.09	105.73	111.28
32	q	11	VAL	N-CA-C	-5.09	106.29	112.76
24	D	201	LEU	N-CA-C	-5.06	106.93	113.01
32	p	22	LEU	N-CA-C	-5.06	106.61	112.89
32	q	21	ALA	N-CA-C	-5.01	106.86	112.87
32	p	101	GLN	CA-C-O	-5.01	113.99	119.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	q	109	ALA	Peptide

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	3328	0	3314	166	0
2	I	3754	0	3862	245	0
3	J	800	0	816	42	0
4	N	1201	0	1284	57	0
5	H	2493	0	2590	146	0
6	K	667	0	719	44	0
7	Y	774	0	767	37	0
8	Z	1103	0	1093	52	0
9	V	461	0	459	22	0
10	W	273	0	294	13	0
11	S	821	0	795	31	0
12	i	492	0	513	23	0
13	j	582	0	556	25	0
14	G	3049	0	3016	193	0
15	C	5288	0	5278	277	0
16	T	2535	0	2583	104	0
17	F	1518	0	1470	103	0
18	B	1702	0	1685	65	0
19	O	874	0	865	28	0
20	P	554	0	544	12	0
21	R	977	0	960	59	0
22	U	1011	0	952	42	0
23	E	1215	0	1195	87	0
24	D	1438	0	1368	97	0
25	X	843	0	834	24	0
26	c	744	0	742	35	0
27	Q	722	0	752	28	0
28	k	614	0	603	30	0
29	r	120	0	122	4	0
30	n	205	0	209	8	0
31	o	1568	0	1579	83	0
32	p	1705	0	1688	101	0
32	q	1736	0	1723	121	0
33	z	3992	0	3996	208	0
34	A	8	0	0	3	0
34	C	16	0	0	1	0
34	D	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	E	8	0	0	6	0
35	A	31	0	19	3	0
36	I	42	0	0	2	0
36	c	37	0	0	0	0
37	i	90	0	130	34	0
38	G	28	0	29	6	0
39	B	4	0	0	2	0
39	C	4	0	0	0	0
40	T	48	0	26	4	0
41	P	1	0	0	0	0
41	q	1	0	0	0	0
42	q	4	0	1	1	0
All	All	49497	0	49431	2258	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 23.

All (2258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:461:MET:CE	2:I:465:LYS:HE3	1.34	1.55
33:z:122:GLN:CD	33:z:172:ALA:HB1	1.25	1.54
33:z:129:PRO:CB	33:z:170:ASN:HB2	1.04	1.51
33:z:129:PRO:CA	33:z:170:ASN:HB2	1.40	1.47
33:z:129:PRO:HB3	33:z:170:ASN:CB	1.48	1.43
33:z:129:PRO:CB	33:z:170:ASN:CB	1.97	1.38
2:I:18:ALA:HB2	2:I:78:ILE:CG2	1.54	1.38
33:z:122:GLN:HG3	33:z:172:ALA:CB	1.56	1.33
21:R:115:TYR:CZ	21:R:117:CYS:SG	2.22	1.31
2:I:94:TYR:CE1	2:I:98:ILE:HD11	1.67	1.30
21:R:115:TYR:CE1	21:R:117:CYS:SG	2.25	1.28
33:z:122:GLN:OE1	33:z:172:ALA:HB1	1.34	1.27
33:z:122:GLN:CG	33:z:172:ALA:CB	2.10	1.27
14:G:47:LEU:HD23	14:G:389:PHE:C	1.59	1.26
2:I:354:LEU:CG	2:I:472:THR:HG23	1.64	1.25
33:z:231:THR:CG2	33:z:488:ARG:HD2	1.66	1.24
2:I:18:ALA:CB	2:I:78:ILE:HG22	1.68	1.23
13:j:29:ARG:HA	33:z:121:VAL:CG2	1.72	1.20
33:z:122:GLN:CG	33:z:172:ALA:HB1	1.72	1.16
33:z:122:GLN:CD	33:z:172:ALA:CB	2.18	1.16
2:I:110:MET:SD	2:I:468:LEU:CD2	2.34	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:111:LEU:HD11	15:C:267:ILE:HD11	1.21	1.15
33:z:129:PRO:HB3	33:z:170:ASN:C	1.71	1.14
2:I:354:LEU:HG	2:I:472:THR:CG2	1.78	1.12
2:I:461:MET:HE2	2:I:465:LYS:HE3	1.18	1.11
33:z:129:PRO:HB3	33:z:170:ASN:CA	1.79	1.10
33:z:124:ARG:HH11	33:z:154:SER:HB2	1.03	1.10
2:I:461:MET:CE	2:I:465:LYS:CE	2.30	1.10
15:C:264:VAL:HA	15:C:267:ILE:CG2	1.83	1.08
33:z:122:GLN:HG3	33:z:172:ALA:HB2	1.10	1.08
13:j:29:ARG:CA	33:z:121:VAL:HG23	1.83	1.07
23:E:129:GLY:HA2	34:E:301:SF4:S4	1.94	1.07
2:I:354:LEU:CD2	2:I:475:PHE:CD2	2.37	1.06
2:I:354:LEU:HG	2:I:472:THR:HG23	1.06	1.05
14:G:306:MET:HE1	15:C:170:CYS:SG	1.96	1.05
1:A:228:ILE:HD13	1:A:402:CYS:HB3	1.38	1.05
32:q:17:GLU:HG3	32:p:23:ASP:HB2	1.37	1.05
2:I:461:MET:HE3	2:I:465:LYS:HE3	1.13	1.04
12:i:64:LEU:O	12:i:68:ARG:HG3	1.57	1.04
5:H:204:ASP:HB2	5:H:207:GLU:HB3	1.37	1.04
15:C:111:LEU:HD11	15:C:267:ILE:CD1	1.88	1.03
15:C:227:PHE:HB2	15:C:267:ILE:CD1	1.89	1.02
2:I:396:PHE:HB3	2:I:404:LEU:CD1	1.90	1.02
2:I:396:PHE:HB3	2:I:404:LEU:HD12	1.41	1.01
2:I:461:MET:HE3	2:I:465:LYS:CE	1.91	1.01
15:C:264:VAL:HA	15:C:267:ILE:HG22	1.40	1.01
15:C:264:VAL:CA	15:C:267:ILE:HG22	1.90	1.01
15:C:264:VAL:C	15:C:267:ILE:HG22	1.86	1.01
2:I:366:LEU:CD1	2:I:377:LEU:CD1	2.38	1.00
33:z:129:PRO:CG	33:z:170:ASN:HB2	1.92	1.00
33:z:124:ARG:HH11	33:z:154:SER:CB	1.75	1.00
32:q:18:THR:O	32:q:22:LEU:HD13	1.62	0.99
15:C:212:LYS:HZ1	15:C:274:THR:HG21	1.27	0.99
33:z:231:THR:HG22	33:z:488:ARG:CD	1.91	0.99
33:z:124:ARG:NH1	33:z:154:SER:HB2	1.79	0.98
2:I:110:MET:CG	2:I:468:LEU:HD22	1.94	0.97
2:I:366:LEU:HD11	2:I:377:LEU:CD1	1.95	0.97
3:J:97:MET:SD	5:H:312:VAL:HG12	2.04	0.97
33:z:129:PRO:CA	33:z:170:ASN:CB	2.06	0.97
15:C:111:LEU:CD1	15:C:267:ILE:HD11	1.94	0.97
2:I:110:MET:SD	2:I:468:LEU:HD21	2.04	0.96
33:z:231:THR:HG22	33:z:488:ARG:HD2	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:159:PHE:CD2	2:I:162:ILE:HD11	2.01	0.95
2:I:380:LEU:HD21	2:I:384:ASN:HB3	1.48	0.94
33:z:122:GLN:OE1	33:z:172:ALA:CB	2.13	0.93
37:i:201:CDL:H761	37:i:201:CDL:H221	1.51	0.93
2:I:332:ILE:HG22	2:I:425:LEU:HD21	1.50	0.93
15:C:212:LYS:NZ	15:C:274:THR:HG21	1.83	0.93
2:I:329:TYR:O	2:I:332:ILE:HG12	1.70	0.92
2:I:438:PHE:HE1	2:I:442:ARG:HH21	1.16	0.92
2:I:53:ASN:ND2	26:c:52:GLY:HA2	1.85	0.92
33:z:182:LYS:H	33:z:182:LYS:HD3	1.33	0.91
14:G:47:LEU:HD23	14:G:389:PHE:O	1.68	0.91
33:z:319:LYS:HE3	33:z:488:ARG:HH11	1.36	0.90
15:C:264:VAL:O	15:C:267:ILE:HG22	1.72	0.90
1:A:182:ARG:NH1	18:B:171:CYS:O	2.05	0.90
1:A:228:ILE:HD11	18:B:113:PHE:CZ	2.07	0.90
5:H:154:ILE:HD12	5:H:186:VAL:HG13	1.53	0.89
1:A:125:MET:SD	1:A:264:THR:HG23	2.13	0.89
2:I:354:LEU:CD2	2:I:475:PHE:HD2	1.84	0.89
33:z:129:PRO:HB3	33:z:170:ASN:HB2	0.97	0.88
37:i:201:CDL:H372	37:i:201:CDL:H162	1.55	0.87
2:I:461:MET:HE2	2:I:465:LYS:CE	1.96	0.87
14:G:47:LEU:CD2	14:G:389:PHE:C	2.47	0.87
37:i:201:CDL:HB32	37:i:201:CDL:H512	1.55	0.87
14:G:69:ARG:HD3	34:E:301:SF4:S2	2.13	0.87
18:B:228:ARG:HB3	18:B:234:GLU:HA	1.55	0.87
2:I:354:LEU:HD21	2:I:475:PHE:HD2	1.39	0.86
2:I:396:PHE:CB	2:I:404:LEU:CD1	2.53	0.86
33:z:110:HIS:H	33:z:121:VAL:HG11	1.40	0.86
1:A:228:ILE:HD11	18:B:113:PHE:HZ	1.38	0.86
2:I:94:TYR:CE1	2:I:98:ILE:CD1	2.58	0.86
2:I:380:LEU:HD23	2:I:383:THR:O	1.76	0.86
15:C:264:VAL:O	15:C:267:ILE:CG2	2.23	0.86
17:F:118:MET:HB3	17:F:143:LEU:HB2	1.59	0.85
14:G:110:ARG:NH2	14:G:332:GLU:O	2.10	0.85
4:N:64:LEU:HB3	6:K:77:LEU:HD12	1.57	0.84
13:j:29:ARG:HA	33:z:121:VAL:HG23	0.86	0.83
2:I:366:LEU:HD11	2:I:377:LEU:HD11	1.60	0.83
15:C:264:VAL:HA	15:C:267:ILE:HG21	1.60	0.83
2:I:365:ALA:HA	2:I:461:MET:HG3	1.60	0.83
2:I:92:PHE:CD2	2:I:497:LEU:HD21	2.13	0.83
17:F:41:LEU:HD12	17:F:41:LEU:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:212:LYS:NZ	15:C:274:THR:CG2	2.42	0.82
1:A:228:ILE:HG22	1:A:450:LEU:HD13	1.60	0.82
2:I:366:LEU:HD12	2:I:377:LEU:HD13	1.60	0.82
1:A:228:ILE:HG22	1:A:450:LEU:CD1	2.09	0.82
2:I:354:LEU:CD2	2:I:475:PHE:CE2	2.62	0.82
2:I:244:VAL:HG23	2:I:304:LEU:HD22	1.61	0.81
4:N:61:ILE:HD11	6:K:70:ALA:HA	1.60	0.81
10:W:19:ALA:O	10:W:23:ILE:HG12	1.81	0.81
2:I:110:MET:CG	2:I:468:LEU:CD2	2.57	0.81
2:I:17:LEU:HD22	2:I:20:PHE:CZ	2.16	0.80
37:i:201:CDL:H212	37:i:201:CDL:H381	1.62	0.80
8:Z:129:ARG:HE	8:Z:130:TRP:H	1.29	0.80
2:I:366:LEU:CD1	2:I:377:LEU:HD13	2.12	0.79
14:G:152:ARG:HH12	23:E:192:ALA:CB	1.94	0.79
6:K:43:ASN:HD21	6:K:66:LEU:HG	1.46	0.79
6:K:59:GLN:HE22	13:j:7:ILE:HG23	1.45	0.79
32:q:81:TYR:HH	32:q:214:HIS:HD1	1.30	0.79
33:z:107:GLU:OE1	33:z:176:LYS:HA	1.81	0.79
2:I:396:PHE:CB	2:I:404:LEU:HD11	2.12	0.79
10:W:22:LEU:O	10:W:22:LEU:HD23	1.82	0.78
2:I:82:PHE:HA	2:I:86:LEU:HD12	1.64	0.78
15:C:299:VAL:HG21	15:C:453:MET:HB2	1.65	0.78
2:I:94:TYR:CZ	2:I:98:ILE:HD11	2.19	0.78
31:o:48:VAL:HB	32:p:223:ASN:HD22	1.48	0.78
15:C:173:CYS:SG	15:C:271:GLY:HA3	2.24	0.78
5:H:88:ALA:HB2	5:H:113:ILE:HG21	1.66	0.78
17:F:97:ARG:HH22	25:X:76:ASP:HB3	1.48	0.78
37:i:201:CDL:H152	37:i:201:CDL:H351	1.66	0.78
33:z:450:CYS:HG	33:z:511:TRP:HE3	1.28	0.77
2:I:78:ILE:HD11	26:c:5:ILE:HD11	1.64	0.77
2:I:354:LEU:CD1	2:I:472:THR:HG23	2.15	0.77
15:C:159:MET:HG2	15:C:189:GLY:HA3	1.67	0.77
32:q:18:THR:O	32:q:22:LEU:CD1	2.32	0.77
14:G:74:SER:HB3	14:G:113:ASN:HD22	1.48	0.77
15:C:264:VAL:CA	15:C:267:ILE:CG2	2.56	0.77
2:I:354:LEU:HD21	2:I:475:PHE:CD2	2.15	0.77
2:I:354:LEU:HD11	2:I:472:THR:OG1	1.84	0.77
1:A:181:ILE:HG21	1:A:189:ARG:HB3	1.66	0.76
33:z:533:PHE:HA	33:z:537:ARG:HG2	1.67	0.76
32:p:16:ARG:HH21	32:p:16:ARG:HG2	1.49	0.76
33:z:182:LYS:H	33:z:182:LYS:CD	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:53:ASN:HD22	26:c:55:PRO:CG	1.98	0.76
2:I:361:ALA:HB2	2:I:468:LEU:HD23	1.68	0.76
15:C:316:ILE:HG13	15:C:317:PRO:HD2	1.68	0.76
17:F:128:ASP:OD1	17:F:130:ARG:NH1	2.19	0.76
31:o:112:ASN:HD21	31:o:140:THR:HG23	1.51	0.76
33:z:231:THR:CG2	33:z:488:ARG:CD	2.59	0.76
16:T:72:THR:HG22	16:T:96:LEU:HB2	1.67	0.76
33:z:321:LEU:CD2	33:z:486:GLU:HG2	2.17	0.75
2:I:17:LEU:CD2	2:I:20:PHE:CZ	2.70	0.75
37:i:201:CDL:H241	37:i:201:CDL:C77	2.15	0.75
14:G:47:LEU:HD23	14:G:390:GLY:N	2.01	0.75
14:G:152:ARG:HH12	23:E:192:ALA:HB3	1.49	0.75
1:A:166:LEU:HD12	1:A:205:LEU:HD23	1.68	0.74
33:z:129:PRO:CB	33:z:170:ASN:O	2.35	0.74
17:F:135:ASP:OD1	17:F:136:TYR:N	2.21	0.74
21:R:49:GLU:HA	21:R:54:ARG:HD3	1.68	0.74
33:z:129:PRO:HB3	33:z:170:ASN:O	1.86	0.74
28:k:61:ASP:HB3	28:k:64:LYS:HE3	1.68	0.74
5:H:320:THR:HG21	10:W:30:LEU:HB3	1.68	0.74
2:I:159:PHE:CE2	2:I:162:ILE:HD11	2.23	0.74
14:G:352:ARG:HH22	14:G:354:LYS:HD3	1.53	0.74
2:I:438:PHE:HE1	2:I:442:ARG:NH2	1.86	0.73
16:T:75:GLY:HA3	16:T:144:LEU:HB2	1.68	0.73
17:F:30:ARG:NH2	17:F:89:GLN:OE1	2.21	0.73
18:B:144:GLU:OE2	18:B:155:ARG:NH2	2.21	0.73
1:A:185:TYR:HB3	1:A:188:GLU:HB2	1.69	0.73
32:p:99:ASN:HD22	32:p:207:TYR:HB2	1.51	0.73
27:Q:50:ILE:O	27:Q:51:ARG:NH1	2.21	0.73
15:C:205:LYS:O	15:C:213:THR:OG1	2.06	0.73
2:I:19:VAL:HG22	2:I:87:PHE:CZ	2.23	0.73
2:I:244:VAL:HA	2:I:247:HIS:HB3	1.71	0.73
16:T:76:ALA:HB3	16:T:97:VAL:HG13	1.70	0.73
14:G:152:ARG:NH1	23:E:192:ALA:H	1.87	0.72
15:C:227:PHE:HB2	15:C:267:ILE:HD13	1.69	0.72
20:P:74:GLY:HA3	20:P:81:GLY:HA3	1.71	0.72
33:z:319:LYS:HE3	33:z:488:ARG:NH1	2.03	0.72
21:R:64:ARG:NH2	21:R:83:CYS:SG	2.62	0.72
21:R:67:VAL:HG11	21:R:81:LEU:HB2	1.71	0.72
5:H:273:VAL:HG11	9:V:19:LEU:HD22	1.71	0.72
15:C:260:LEU:HD13	15:C:453:MET:HE1	1.69	0.72
33:z:178:LEU:O	33:z:178:LEU:HD12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HD11	1:A:192:LEU:HD23	1.72	0.72
2:I:244:VAL:CG2	2:I:304:LEU:HD22	2.18	0.72
33:z:347:LYS:H	33:z:347:LYS:HD2	1.53	0.72
14:G:310:ILE:HD13	15:C:182:GLN:HA	1.72	0.72
23:E:191:THR:HG22	23:E:193:GLU:CG	2.20	0.72
24:D:154:ARG:HG2	24:D:197:LYS:HE3	1.71	0.72
1:A:228:ILE:CD1	18:B:113:PHE:HZ	2.01	0.72
14:G:47:LEU:CD2	14:G:390:GLY:N	2.53	0.72
33:z:582:TYR:HD1	33:z:582:TYR:H	1.38	0.72
37:i:201:CDL:H112	37:i:201:CDL:OA8	1.90	0.72
2:I:18:ALA:CB	2:I:78:ILE:CG2	2.45	0.71
5:H:15:PRO:HB2	9:V:22:MET:HG3	1.71	0.71
11:S:94:VAL:HG11	21:R:115:TYR:HE2	1.53	0.71
33:z:553:HIS:HB3	33:z:556:LYS:HG2	1.71	0.71
15:C:106:CYS:HB3	15:C:221:CYS:HB2	1.71	0.71
8:Z:118:TRP:HE1	13:j:57:ILE:HG12	1.53	0.71
15:C:534:GLU:O	15:C:538:GLN:NE2	2.23	0.71
1:A:337:LEU:HB3	1:A:352:LYS:HG3	1.72	0.71
14:G:197:ARG:HH12	24:D:73:LEU:HA	1.55	0.71
23:E:154:SER:OG	23:E:175:CYS:SG	2.49	0.71
23:E:119:PRO:HB3	23:E:142:VAL:HG13	1.71	0.71
2:I:148:MET:HG3	2:I:276:ASN:HD21	1.54	0.71
31:o:49:LYS:HG3	32:q:45:LEU:HG	1.72	0.71
15:C:400:VAL:HG21	15:C:408:VAL:HB	1.73	0.70
2:I:390:THR:HG21	2:I:469:LEU:HD23	1.71	0.70
7:Y:51:ASP:HA	7:Y:54:ARG:HD2	1.72	0.70
15:C:523:ARG:NH2	15:C:713:THR:O	2.24	0.70
7:Y:71:CYS:SG	7:Y:71:CYS:O	2.49	0.70
33:z:276:LEU:HB3	33:z:589:LEU:HD12	1.72	0.70
14:G:102:ARG:NH2	14:G:162:GLY:O	2.23	0.70
17:F:117:ASP:OD1	17:F:131:ARG:NH1	2.24	0.70
1:A:293:ASN:ND2	1:A:315:MET:SD	2.64	0.70
2:I:53:ASN:HD22	26:c:55:PRO:HG3	1.57	0.70
2:I:354:LEU:CD2	2:I:472:THR:HG23	2.21	0.70
21:R:126:ILE:HD12	21:R:132:GLN:HG3	1.74	0.70
1:A:288:PHE:HB3	1:A:314:GLU:HG3	1.73	0.69
2:I:396:PHE:HB2	2:I:404:LEU:HD11	1.74	0.69
37:i:201:CDL:H452	37:i:201:CDL:H402	1.74	0.69
17:F:124:ILE:HG22	17:F:125:ASN:HD22	1.55	0.69
2:I:108:ILE:HG12	2:I:264:PHE:HZ	1.56	0.69
18:B:172:MET:N	39:B:301:FES:S1	2.62	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:o:223:LEU:HD22	32:p:110:LYS:HB3	1.73	0.69
22:U:43:LYS:NZ	22:U:77:GLU:OE2	2.22	0.69
2:I:354:LEU:HD22	2:I:475:PHE:CE2	2.26	0.69
2:I:17:LEU:HB2	2:I:78:ILE:HD13	1.73	0.69
4:N:124:TYR:OH	7:Y:40:LYS:NZ	2.25	0.69
22:U:75:TRP:HB3	24:D:99:GLU:HB3	1.73	0.69
33:z:120:GLU:H	33:z:120:GLU:CD	2.00	0.69
5:H:200:ARG:HH22	5:H:281:ILE:HA	1.57	0.69
12:i:65:ALA:HA	12:i:68:ARG:HD3	1.74	0.69
14:G:152:ARG:HH11	23:E:192:ALA:H	1.39	0.69
15:C:302:ASN:OD1	15:C:318:ARG:NH1	2.26	0.69
2:I:345:LEU:HD21	2:I:349:ILE:HD11	1.74	0.69
32:p:16:ARG:HG2	32:p:16:ARG:NH2	2.04	0.69
33:z:242:VAL:HG12	33:z:284:LEU:HG	1.74	0.68
2:I:312:GLN:HA	2:I:312:GLN:NE2	2.08	0.68
14:G:91:ASN:ND2	21:R:125:PRO:HB2	2.07	0.68
2:I:110:MET:SD	2:I:468:LEU:HD22	2.27	0.68
17:F:47:LEU:HA	21:R:95:ASP:HB3	1.75	0.68
33:z:450:CYS:SG	33:z:511:TRP:HA	2.33	0.68
15:C:225:VAL:CG2	15:C:248:ILE:HG23	2.24	0.68
21:R:126:ILE:CD1	21:R:132:GLN:HG3	2.24	0.68
31:o:230:GLU:O	32:q:36:ARG:NH1	2.27	0.68
3:J:11:TYR:HA	5:H:9:ILE:HD13	1.74	0.68
15:C:76:VAL:HG11	15:C:138:ALA:HB1	1.75	0.68
1:A:163:GLU:OE2	1:A:279:ARG:NH1	2.27	0.68
2:I:354:LEU:HD22	2:I:475:PHE:CD2	2.26	0.68
22:U:92:GLU:HG3	24:D:209:THR:HG21	1.76	0.68
20:P:65:VAL:HG21	20:P:70:VAL:HG12	1.76	0.68
17:F:81:ARG:NH2	21:R:83:CYS:SG	2.67	0.67
1:A:228:ILE:CD1	1:A:402:CYS:HB3	2.21	0.67
2:I:387:LEU:HD13	12:i:23:LEU:CD2	2.24	0.67
23:E:191:THR:HG22	23:E:193:GLU:HG2	1.76	0.67
2:I:19:VAL:O	2:I:19:VAL:HG12	1.94	0.67
2:I:365:ALA:HA	2:I:461:MET:CG	2.25	0.67
33:z:129:PRO:CB	33:z:170:ASN:C	2.59	0.67
2:I:110:MET:HG3	2:I:468:LEU:HD22	1.75	0.67
3:J:34:SER:OG	23:E:148:GLU:OE2	2.12	0.67
7:Y:25:ILE:HD13	7:Y:63:LEU:HD23	1.75	0.67
12:i:18:MET:C	12:i:20:SER:H	2.02	0.67
14:G:125:VAL:HG13	14:G:202:ARG:HG2	1.77	0.67
33:z:597:ASN:N	33:z:597:ASN:OD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:LEU:HD11	2:I:98:ILE:HG23	1.77	0.67
2:I:380:LEU:CD2	2:I:384:ASN:HB3	2.24	0.67
14:G:109:THR:OG1	14:G:145:TYR:OH	2.11	0.67
33:z:304:ILE:HG12	33:z:331:VAL:HG11	1.74	0.67
1:A:304:HIS:H	18:B:138:ARG:HD3	1.60	0.67
2:I:197:ILE:HD11	2:I:230:ILE:HG12	1.77	0.67
14:G:47:LEU:HD21	14:G:390:GLY:HA2	1.77	0.67
16:T:359:LYS:HG2	16:T:360:PHE:H	1.60	0.67
33:z:569:LEU:N	33:z:569:LEU:HD23	2.09	0.67
24:D:172:CYS:SG	24:D:176:ALA:N	2.64	0.67
7:Y:43:ASP:HB2	8:Z:129:ARG:HH22	1.59	0.67
14:G:68:ASP:OD1	14:G:68:ASP:N	2.28	0.67
15:C:449:VAL:HG13	15:C:722:PHE:HB2	1.76	0.67
2:I:29:THR:HG21	2:I:131:LEU:HG	1.76	0.66
3:J:99:PHE:CD2	4:N:156:SER:HB2	2.30	0.66
14:G:225:ARG:NH1	14:G:267:GLU:OE2	2.29	0.66
22:U:88:GLN:HG2	22:U:122:GLU:HG2	1.76	0.66
30:n:78:GLU:OE1	30:n:78:GLU:N	2.28	0.66
33:z:489:TRP:CE3	33:z:508:ILE:HG21	2.30	0.66
5:H:128:SER:HB2	5:H:217:ASN:HA	1.77	0.66
33:z:247:LEU:HD23	33:z:247:LEU:H	1.59	0.66
15:C:380:ILE:HG23	15:C:580:PHE:HD2	1.60	0.66
15:C:486:GLY:HA3	15:C:491:THR:HG21	1.78	0.66
16:T:225:THR:HG21	17:F:162:LYS:HD3	1.77	0.66
32:q:98:THR:OG1	32:q:123:GLY:O	2.12	0.66
2:I:396:PHE:HB3	2:I:404:LEU:HD11	1.72	0.66
33:z:599:MET:H	33:z:599:MET:HE2	1.59	0.66
15:C:207:LEU:HD12	15:C:213:THR:HG21	1.76	0.66
15:C:583:LEU:HD22	15:C:589:VAL:HG11	1.76	0.66
16:T:221:THR:HA	40:T:501:NDP:H42N	1.78	0.66
4:N:10:ALA:HB2	4:N:36:ASP:HB2	1.77	0.66
7:Y:60:VAL:HG11	8:Z:88:ILE:HG12	1.77	0.66
15:C:594:ILE:HD12	15:C:600:VAL:HG21	1.77	0.66
14:G:36:VAL:HG13	14:G:372:HIS:HA	1.76	0.66
17:F:81:ARG:NH2	21:R:83:CYS:O	2.25	0.65
23:E:146:MET:HE2	23:E:150:ARG:HB2	1.77	0.65
2:I:354:LEU:HD23	2:I:475:PHE:CE2	2.31	0.65
4:N:155:PRO:HG2	6:K:64:LEU:HD22	1.77	0.65
7:Y:11:PRO:HG3	7:Y:65:LYS:HD3	1.76	0.65
14:G:357:ALA:HB1	14:G:391:GLU:HB3	1.79	0.65
17:F:26:GLU:OE2	21:R:126:ILE:HG21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:o:131:ALA:HB1	31:o:149:SER:HB3	1.78	0.65
33:z:559:ILE:HG22	33:z:559:ILE:O	1.96	0.65
17:F:22:MET:HB2	17:F:32:ASP:HB3	1.78	0.65
17:F:81:ARG:NE	21:R:92:GLU:OE2	2.29	0.65
23:E:191:THR:CG2	23:E:193:GLU:HG3	2.27	0.65
14:G:298:SER:HB2	14:G:301:ARG:HD3	1.78	0.65
17:F:100:SER:HB2	17:F:123:PHE:HB3	1.77	0.65
32:p:159:LYS:HB3	32:p:160:HIS:HD2	1.61	0.65
15:C:64:ARG:HH21	19:O:134:LEU:HG	1.61	0.65
15:C:512:PRO:O	15:C:547:TRP:NE1	2.19	0.65
1:A:330:VAL:HG21	1:A:337:LEU:HD12	1.78	0.65
5:H:290:TYR:HE2	38:G:601:PEV:H331	1.62	0.65
15:C:85:VAL:HG11	15:C:94:ALA:HA	1.78	0.65
26:c:14:PRO:O	26:c:91:ASN:ND2	2.30	0.65
32:q:35:PHE:H	32:p:48:VAL:HG21	1.60	0.65
14:G:88:LYS:HD2	21:R:130:VAL:HG21	1.78	0.65
21:R:115:TYR:OH	21:R:117:CYS:SG	2.53	0.65
31:o:77:ASN:ND2	32:p:66:SER:OG	2.29	0.65
1:A:441:GLN:O	1:A:445:HIS:ND1	2.30	0.64
37:i:201:CDL:HB32	37:i:201:CDL:C51	2.27	0.64
37:i:201:CDL:H241	37:i:201:CDL:H772	1.78	0.64
14:G:31:GLU:HB3	14:G:39:ARG:HG2	1.79	0.64
23:E:186:PRO:HD3	24:D:186:ALA:HA	1.78	0.64
2:I:366:LEU:CD1	2:I:377:LEU:HD12	2.28	0.64
14:G:47:LEU:HG	14:G:47:LEU:O	1.97	0.64
14:G:56:GLU:HG2	14:G:352:ARG:H	1.62	0.64
33:z:446:VAL:HG22	33:z:515:ILE:HG23	1.79	0.64
1:A:125:MET:HG3	1:A:172:MET:HB2	1.79	0.64
15:C:212:LYS:HZ2	15:C:274:THR:CG2	2.10	0.64
33:z:489:TRP:HE3	33:z:508:ILE:HG21	1.62	0.64
32:q:43:ARG:HD2	32:p:216:ALA:HA	1.79	0.64
2:I:387:LEU:HD13	12:i:23:LEU:HD21	1.79	0.64
4:N:53:PHE:O	4:N:57:TYR:HB2	1.97	0.64
5:H:302:VAL:HG22	10:W:16:VAL:HG21	1.80	0.64
6:K:50:SER:HB2	6:K:58:GLY:HA3	1.79	0.64
16:T:182:GLN:HB3	16:T:216:ILE:HG12	1.80	0.64
31:o:223:LEU:HB2	32:p:110:LYS:HD3	1.79	0.64
12:i:59:ASP:HA	12:i:62:VAL:HG22	1.78	0.64
28:k:64:LYS:HZ2	28:k:75:LEU:HD23	1.63	0.64
2:I:110:MET:SD	2:I:468:LEU:HD23	2.35	0.64
5:H:291:ARG:HG2	5:H:291:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:47:GLN:NE2	25:X:48:ASP:OD1	2.31	0.64
32:q:105:LEU:HG	32:p:130:HIS:HB3	1.80	0.64
2:I:470:ALA:HA	12:i:19:TYR:HE1	1.62	0.63
33:z:302:GLN:H	33:z:302:GLN:CD	2.05	0.63
1:A:224:ALA:HB1	18:B:116:MET:HB2	1.78	0.63
15:C:125:GLU:HB2	15:C:143:LYS:HB2	1.80	0.63
15:C:469:VAL:HG21	15:C:480:TYR:HE1	1.63	0.63
23:E:164:TYR:CG	24:D:163:ILE:HG21	2.32	0.63
33:z:319:LYS:HD2	33:z:488:ARG:HD3	1.80	0.63
14:G:318:GLU:HA	17:F:180:PHE:HB3	1.79	0.63
15:C:264:VAL:O	15:C:267:ILE:HG23	1.99	0.63
15:C:321:GLU:O	15:C:457:ARG:NH2	2.31	0.63
15:C:165:ASN:HB3	15:C:200:ARG:HG3	1.81	0.63
15:C:387:LEU:HD11	15:C:726:ASN:HD22	1.62	0.63
1:A:138:VAL:HG21	1:A:165:CYS:SG	2.37	0.63
1:A:309:CYS:HB3	18:B:233:PRO:HA	1.81	0.63
3:J:23:LEU:HD11	5:H:75:ARG:HG2	1.81	0.63
15:C:111:LEU:O	19:O:138:LYS:NZ	2.30	0.63
15:C:207:LEU:HD22	15:C:256:MET:HG3	1.81	0.63
15:C:443:ILE:HA	15:C:472:VAL:HG23	1.80	0.63
24:D:156:ASP:N	24:D:156:ASP:OD1	2.30	0.63
32:p:30:GLN:OE1	32:p:30:GLN:N	2.31	0.63
5:H:155:LEU:HA	5:H:158:VAL:HG12	1.81	0.63
21:R:67:VAL:HG23	21:R:80:ARG:HD2	1.79	0.63
23:E:124:CYS:SG	23:E:125:MET:N	2.72	0.63
5:H:204:ASP:HB2	5:H:207:GLU:CB	2.24	0.63
17:F:52:ARG:HD2	21:R:92:GLU:HG2	1.80	0.63
25:X:23:ARG:NH1	28:k:79:SER:OG	2.31	0.63
28:k:95:LEU:HD21	28:k:121:SER:HA	1.79	0.63
28:k:110:LEU:HA	28:k:113:GLU:HG3	1.80	0.63
32:p:130:HIS:N	32:p:130:HIS:CD2	2.62	0.63
33:z:347:LYS:HD2	33:z:347:LYS:N	2.13	0.63
1:A:63:ARG:NH1	1:A:312:GLU:O	2.31	0.63
2:I:94:TYR:HE1	2:I:98:ILE:HD11	1.54	0.63
7:Y:45:ASN:HB3	7:Y:48:LYS:HG2	1.80	0.63
32:q:35:PHE:N	32:p:48:VAL:HG21	2.14	0.63
2:I:445:LYS:HG3	2:I:449:PHE:HB2	1.81	0.63
6:K:79:ILE:HA	6:K:82:ILE:HG22	1.81	0.63
37:i:201:CDL:HB62	37:i:201:CDL:H511	1.79	0.63
17:F:74:VAL:HG13	17:F:89:GLN:HG2	1.79	0.63
1:A:449:ALA:HB3	35:A:502:FMN:HM82	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:11:GLY:O	8:Z:12:MET:HG2	1.98	0.62
24:D:154:ARG:HA	24:D:197:LYS:HB3	1.81	0.62
32:q:68:ILE:HB	32:q:86:ARG:HA	1.80	0.62
1:A:182:ARG:NE	1:A:184:GLU:OE1	2.31	0.62
10:W:13:GLN:HG2	24:D:54:LYS:HG3	1.81	0.62
15:C:227:PHE:CB	15:C:267:ILE:HD13	2.29	0.62
17:F:156:ARG:NH1	23:E:133:ASN:O	2.33	0.62
17:F:159:ASP:OD1	17:F:159:ASP:N	2.32	0.62
26:c:45:VAL:HG13	26:c:62:MET:HG3	1.81	0.62
1:A:337:LEU:HD22	1:A:352:LYS:HB2	1.81	0.62
1:A:248:LEU:HD22	15:C:135:ALA:HB3	1.81	0.62
2:I:54:VAL:HG21	2:I:123:PHE:HB2	1.80	0.62
24:D:94:ILE:HG23	24:D:99:GLU:HG3	1.80	0.62
32:q:86:ARG:HB2	32:q:107:HIS:HB2	1.82	0.62
33:z:275:GLY:HA3	33:z:600:VAL:HG11	1.82	0.62
32:q:85:LEU:HG	32:q:106:VAL:HB	1.81	0.62
32:p:162:MET:HE1	32:p:196:GLU:HB3	1.80	0.62
1:A:228:ILE:CD1	1:A:244:GLY:O	2.48	0.62
3:J:31:SER:OG	3:J:32:ASN:N	2.32	0.62
5:H:50:GLN:NE2	5:H:54:ASP:OD1	2.32	0.62
31:o:103:ASN:ND2	31:o:131:ALA:O	2.33	0.62
32:q:113:LEU:HD11	32:p:195:GLU:HG3	1.82	0.62
2:I:459:GLU:CG	2:I:460:PRO:HD2	2.30	0.62
5:H:277:LEU:O	5:H:281:ILE:HG12	2.00	0.62
5:H:320:THR:OG1	5:H:321:PHE:N	2.30	0.62
14:G:47:LEU:HD21	14:G:390:GLY:CA	2.29	0.62
17:F:154:GLN:OE1	23:E:133:ASN:ND2	2.33	0.62
18:B:78:ASP:OD1	18:B:82:GLN:NE2	2.31	0.62
33:z:302:GLN:H	33:z:302:GLN:NE2	1.97	0.62
5:H:291:ARG:HD3	14:G:202:ARG:HE	1.64	0.62
8:Z:57:PHE:CD2	8:Z:57:PHE:O	2.53	0.62
32:p:70:ASP:HB3	32:p:91:THR:HA	1.82	0.62
32:p:99:ASN:ND2	32:p:207:TYR:HB2	2.15	0.62
2:I:39:PHE:HB3	26:c:57:ILE:CD1	2.30	0.61
24:D:161:LYS:HG2	24:D:161:LYS:O	1.99	0.61
31:o:237:VAL:HG21	32:p:39:LEU:HB2	1.82	0.61
31:o:202:ILE:HG22	31:o:203:ARG:HG3	1.82	0.61
3:J:97:MET:SD	5:H:312:VAL:CG1	2.84	0.61
5:H:154:ILE:HG23	5:H:186:VAL:CG1	2.30	0.61
1:A:445:HIS:HB3	15:C:121:LEU:HD11	1.82	0.61
2:I:459:GLU:HG2	2:I:460:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:66:ILE:HG23	6:K:74:ALA:HB1	1.83	0.61
14:G:47:LEU:CD2	14:G:390:GLY:HA2	2.31	0.61
24:D:72:PHE:O	24:D:73:LEU:C	2.43	0.61
28:k:72:GLN:NE2	28:k:77:LEU:O	2.34	0.61
32:q:18:THR:C	32:q:22:LEU:HD13	2.26	0.61
23:E:191:THR:CG2	23:E:193:GLU:CG	2.79	0.61
24:D:191:GLU:OE1	24:D:191:GLU:N	2.27	0.61
31:o:74:VAL:HG12	31:o:78:VAL:HG21	1.80	0.61
33:z:129:PRO:CD	33:z:170:ASN:CB	2.66	0.61
33:z:449:SER:HA	33:z:552:GLU:HA	1.83	0.61
15:C:368:VAL:O	15:C:372:ILE:HG23	2.00	0.61
32:p:86:ARG:NH2	32:p:88:ASP:H	1.99	0.61
33:z:189:VAL:HG11	33:z:198:LEU:HD13	1.82	0.61
1:A:228:ILE:HD13	1:A:402:CYS:CB	2.24	0.61
22:U:133:TYR:HB3	24:D:192:GLU:HG3	1.82	0.61
14:G:80:HIS:CD2	14:G:102:ARG:HD3	2.36	0.61
7:Y:42:ASN:ND2	7:Y:43:ASP:OD1	2.33	0.61
31:o:237:VAL:HG23	32:p:39:LEU:HD12	1.83	0.61
14:G:41:GLU:OE2	14:G:43:HIS:NE2	2.34	0.60
31:o:66:PRO:HB2	31:o:80:LEU:HD23	1.83	0.60
33:z:321:LEU:HD22	33:z:486:GLU:HG2	1.83	0.60
2:I:351:ILE:HG21	2:I:406:GLY:HA2	1.83	0.60
5:H:151:ILE:HG23	5:H:190:PHE:HE1	1.66	0.60
14:G:72:TYR:CZ	14:G:388:VAL:HG13	2.35	0.60
3:J:88:ILE:HD12	3:J:92:GLY:HA3	1.82	0.60
15:C:100:VAL:HG11	15:C:146:THR:HG21	1.83	0.60
15:C:626:LYS:NZ	15:C:653:ASP:OD2	2.26	0.60
26:c:39:THR:HB	30:n:95:GLY:HA3	1.81	0.60
14:G:337:GLU:OE2	17:F:85:ARG:NH2	2.34	0.60
23:E:202:LEU:O	23:E:206:ILE:HG12	2.01	0.60
1:A:251:PRO:HB3	19:O:141:SER:HB3	1.83	0.60
2:I:18:ALA:HB2	2:I:78:ILE:HG22	0.71	0.60
2:I:345:LEU:HD23	2:I:345:LEU:C	2.27	0.60
15:C:286:GLU:OE2	15:C:308:ARG:NH2	2.34	0.60
5:H:23:LEU:HD11	5:H:236:MET:HE2	1.82	0.60
5:H:207:GLU:HA	5:H:212:LEU:HB2	1.84	0.60
13:j:11:LYS:HG2	13:j:11:LYS:O	2.01	0.60
16:T:168:ALA:HB2	16:T:207:VAL:HG23	1.84	0.60
2:I:359:ALA:HA	2:I:394:THR:HG21	1.84	0.60
14:G:61:LEU:HD21	14:G:316:TYR:CE1	2.37	0.60
15:C:507:LYS:NZ	15:C:539:ALA:O	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:193:THR:HG23	32:q:196:GLU:H	1.66	0.60
33:z:485:ILE:HG13	33:z:514:ILE:HA	1.84	0.60
22:U:98:HIS:CE1	24:D:100:LYS:HD2	2.37	0.60
28:k:70:HIS:HB3	28:k:73:ASN:HB2	1.83	0.60
31:o:86:VAL:HA	31:o:107:VAL:HG22	1.82	0.60
33:z:243:ILE:HG13	33:z:285:GLN:HB3	1.83	0.60
1:A:380:MET:HB3	1:A:384:THR:HG21	1.84	0.60
15:C:521:PHE:HE1	15:C:530:LEU:HD21	1.67	0.60
15:C:631:GLU:OE2	15:C:686:ASN:ND2	2.30	0.60
33:z:198:LEU:HD22	33:z:220:ILE:HG21	1.84	0.60
2:I:396:PHE:CB	2:I:404:LEU:HD12	2.24	0.59
15:C:172:ILE:HG13	24:D:150:ARG:HD2	1.84	0.59
15:C:227:PHE:CB	15:C:267:ILE:CD1	2.73	0.59
23:E:157:SER:H	23:E:188:CYS:HA	1.67	0.59
33:z:187:VAL:HG21	33:z:198:LEU:HD11	1.83	0.59
2:I:354:LEU:HD23	2:I:475:PHE:CD2	2.33	0.59
2:I:481:LEU:HD22	2:I:481:LEU:H	1.65	0.59
24:D:129:CYS:HA	24:D:132:VAL:HG12	1.85	0.59
32:q:17:GLU:CG	32:p:23:ASP:HB2	2.21	0.59
2:I:252:ASP:HA	2:I:317:ARG:HH22	1.67	0.59
6:K:53:LEU:HD22	13:j:45:LEU:HD22	1.83	0.59
14:G:216:ASP:HB3	17:F:106:PRO:HD2	1.84	0.59
14:G:352:ARG:NH2	14:G:354:LYS:HD3	2.17	0.59
37:i:201:CDL:H402	37:i:201:CDL:C45	2.33	0.59
24:D:96:TYR:OH	24:D:184:GLU:OE2	2.19	0.59
33:z:272:GLY:HA3	33:z:276:LEU:HD13	1.84	0.59
2:I:26:ILE:CG1	2:I:134:CYS:SG	2.91	0.59
5:H:212:LEU:HD21	5:H:229:PHE:CE1	2.37	0.59
8:Z:57:PHE:O	8:Z:57:PHE:CG	2.51	0.59
16:T:64:SER:OG	17:F:171:MET:HB3	2.03	0.59
27:Q:53:CYS:SG	27:Q:56:VAL:HB	2.42	0.59
33:z:558:GLU:H	33:z:558:GLU:CD	2.10	0.59
33:z:582:TYR:N	33:z:582:TYR:CD1	2.70	0.59
15:C:445:THR:HG21	15:C:515:ILE:HG22	1.85	0.59
17:F:53:VAL:HA	17:F:79:SER:HA	1.85	0.59
31:o:165:MET:HE3	31:o:166:GLU:H	1.68	0.59
33:z:262:ASP:HB3	33:z:265:LEU:HB3	1.83	0.59
8:Z:40:SER:HB3	11:S:33:PRO:HB3	1.83	0.59
18:B:126:HIS:CE1	18:B:128:LEU:HD21	2.38	0.59
23:E:94:CYS:SG	23:E:190:PRO:HD3	2.42	0.59
32:q:80:TRP:HD1	32:q:101:GLN:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:12:LEU:HA	9:V:15:ILE:HG22	1.85	0.59
1:A:140:ALA:HA	1:A:268:VAL:HG13	1.83	0.59
4:N:179:ARG:HD2	29:r:1:ALA:HB2	1.84	0.59
5:H:38:LYS:HE2	24:D:93:THR:HG21	1.85	0.59
14:G:25:VAL:HG12	23:E:135:MET:HE2	1.84	0.59
33:z:191:ALA:HB1	33:z:221:GLY:HA3	1.83	0.59
5:H:203:PHE:HD1	5:H:295:LEU:HG	1.68	0.59
5:H:291:ARG:HG2	5:H:291:ARG:NH1	2.18	0.59
14:G:90:LEU:HD13	14:G:294:LEU:HD13	1.85	0.59
16:T:60:THR:HB	19:O:82:LEU:HD21	1.85	0.59
32:p:27:CYS:O	32:p:27:CYS:SG	2.61	0.59
2:I:92:PHE:HD1	2:I:493:MET:HB3	1.67	0.58
5:H:20:VAL:HG11	5:H:230:LEU:HA	1.84	0.58
37:i:201:CDL:H372	37:i:201:CDL:C16	2.30	0.58
32:q:100:ILE:HD13	32:q:106:VAL:HG21	1.84	0.58
8:Z:21:LEU:H	11:S:58:ILE:HB	1.68	0.58
9:V:40:ILE:HG13	9:V:41:GLY:H	1.68	0.58
11:S:46:ARG:HD3	11:S:50:PRO:HD3	1.85	0.58
32:p:67:VAL:HG12	32:p:71:VAL:HG21	1.86	0.58
1:A:236:LEU:HD11	1:A:253:PRO:HB3	1.85	0.58
17:F:38:LEU:HD22	17:F:90:THR:HG21	1.84	0.58
18:B:143:ILE:HG23	18:B:206:VAL:HG21	1.84	0.58
28:k:86:VAL:HG11	28:k:102:ALA:HB1	1.84	0.58
1:A:409:ARG:HE	1:A:410:GLU:HG2	1.67	0.58
2:I:125:PHE:CE1	2:I:162:ILE:HB	2.39	0.58
16:T:249:GLY:O	16:T:289:THR:OG1	2.21	0.58
33:z:196:GLN:HB2	33:z:216:ARG:HB3	1.84	0.58
11:S:43:THR:HG22	22:U:69:GLN:H	1.67	0.58
14:G:328:TYR:CE2	14:G:330:ALA:HB2	2.39	0.58
2:I:139:MET:HE3	2:I:276:ASN:HD22	1.68	0.58
14:G:264:ARG:NH2	14:G:384:THR:O	2.34	0.58
31:o:58:ILE:HG23	31:o:66:PRO:HG2	1.84	0.58
32:p:83:CYS:SG	32:p:100:ILE:HG21	2.43	0.58
15:C:293:ILE:HG13	15:C:638:GLN:HB3	1.85	0.58
15:C:603:GLN:HG3	15:C:656:ILE:HG21	1.85	0.58
16:T:80:LEU:HB2	16:T:222:MET:HE1	1.85	0.58
25:X:34:CYS:HB3	28:k:87:MET:HE2	1.85	0.58
5:H:23:LEU:HD22	5:H:233:TYR:HB3	1.84	0.58
15:C:277:PRO:HB3	15:C:734:ILE:HD13	1.86	0.58
32:q:105:LEU:O	32:q:107:HIS:N	2.33	0.58
33:z:365:GLU:HB3	33:z:386:ASP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLU:OE1	1:A:471:ARG:NH2	2.37	0.57
2:I:380:LEU:CD2	2:I:384:ASN:O	2.52	0.57
5:H:42:VAL:HG23	22:U:38:ASN:H	1.68	0.57
14:G:250:PRO:HB3	14:G:266:GLU:HG2	1.87	0.57
14:G:328:TYR:HD1	14:G:341:PHE:HB2	1.67	0.57
19:O:76:ILE:HG13	19:O:108:PHE:HE2	1.69	0.57
20:P:65:VAL:HG22	20:P:66:ASP:H	1.68	0.57
31:o:145:SER:OG	31:o:162:SER:O	2.21	0.57
18:B:132:THR:HG22	18:B:133:THR:H	1.68	0.57
18:B:233:PRO:HD2	18:B:237:ASN:HA	1.85	0.57
22:U:46:ASN:HD21	22:U:75:TRP:HE1	1.51	0.57
7:Y:89:PHE:HB3	7:Y:93:ARG:HH12	1.68	0.57
8:Z:82:ARG:NH1	9:V:43:ASP:OD2	2.33	0.57
14:G:91:ASN:HA	21:R:127:PRO:HD3	1.86	0.57
15:C:227:PHE:HB2	15:C:267:ILE:HD12	1.80	0.57
27:Q:74:LEU:HD13	27:Q:82:ILE:HG12	1.86	0.57
33:z:129:PRO:HA	33:z:170:ASN:CB	2.15	0.57
33:z:135:LEU:HD22	33:z:169:VAL:HG13	1.86	0.57
5:H:56:LEU:HD23	23:E:79:ALA:HB2	1.86	0.57
11:S:88:VAL:HG22	21:R:118:GLU:HG2	1.86	0.57
37:i:201:CDL:H212	37:i:201:CDL:H411	1.86	0.57
15:C:418:ASP:OD2	27:Q:40:LYS:NZ	2.29	0.57
17:F:59:ILE:HG22	17:F:115:VAL:HG21	1.86	0.57
21:R:120:ILE:HG22	21:R:120:ILE:O	2.04	0.57
27:Q:20:GLN:NE2	27:Q:53:CYS:O	2.37	0.57
32:p:151:LEU:HD23	32:p:155:VAL:HG11	1.86	0.57
3:J:78:PHE:CE1	5:H:311:VAL:HG11	2.39	0.57
4:N:175:THR:HG22	4:N:176:LYS:H	1.70	0.57
32:p:46:MET:HB3	32:p:53:PRO:HG2	1.86	0.57
2:I:39:PHE:HB3	26:c:57:ILE:HD13	1.85	0.57
5:H:318:LEU:HD22	5:H:323:TRP:HB2	1.85	0.57
37:i:201:CDL:H151	26:c:50:LEU:HD13	1.86	0.57
33:z:129:PRO:HB2	33:z:170:ASN:O	2.02	0.57
2:I:461:MET:HE2	2:I:465:LYS:CD	2.35	0.57
14:G:74:SER:OG	14:G:74:SER:O	2.21	0.57
17:F:97:ARG:HG2	17:F:122:SER:HB2	1.87	0.57
17:F:157:TYR:HE1	17:F:168:PRO:HG3	1.70	0.57
32:q:36:ARG:HB2	32:p:44:THR:HB	1.86	0.57
32:p:135:HIS:N	32:p:137:CYS:SG	2.76	0.57
2:I:354:LEU:CD1	2:I:472:THR:CG2	2.82	0.57
16:T:193:PRO:HB2	16:T:345:ASN:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HD12	1:A:244:GLY:O	2.04	0.57
8:Z:34:ARG:HD2	8:Z:38:ARG:HG2	1.87	0.57
14:G:217:TRP:HA	17:F:107:SER:HB3	1.87	0.57
17:F:153:VAL:HG12	17:F:169:ILE:HA	1.87	0.57
26:c:5:ILE:HG21	26:c:19:ASN:HB2	1.87	0.57
32:p:28:ARG:HA	32:p:28:ARG:NE	2.19	0.57
32:p:105:LEU:HB3	32:p:107:HIS:NE2	2.19	0.57
33:z:110:HIS:HB3	33:z:121:VAL:HG21	1.86	0.57
14:G:306:MET:HG3	15:C:163:LEU:HD22	1.87	0.57
23:E:158:CYS:N	34:E:301:SF4:S3	2.64	0.57
27:Q:14:LEU:HD23	27:Q:48:ILE:HG23	1.87	0.57
33:z:474:ILE:HA	33:z:539:LEU:HD11	1.86	0.57
1:A:148:CYS:HB3	18:B:173:GLY:O	2.05	0.56
21:R:26:VAL:HG22	21:R:87:GLU:HG3	1.85	0.56
15:C:161:PHE:HA	15:C:164:MET:HE3	1.87	0.56
24:D:174:VAL:HG23	24:D:174:VAL:O	2.04	0.56
32:q:80:TRP:CD1	32:q:101:GLN:HA	2.40	0.56
2:I:104:THR:O	2:I:108:ILE:HG13	2.05	0.56
2:I:470:ALA:HA	12:i:19:TYR:CE1	2.40	0.56
2:I:478:LEU:HG	2:I:478:LEU:O	2.04	0.56
5:H:292:TYR:HA	5:H:295:LEU:HB3	1.86	0.56
37:i:201:CDL:H761	37:i:201:CDL:C22	2.31	0.56
17:F:175:PHE:HB3	19:O:100:ASN:HD22	1.69	0.56
23:E:191:THR:HG22	23:E:193:GLU:HG3	1.87	0.56
31:o:65:LEU:HD12	31:o:66:PRO:HD2	1.87	0.56
32:q:14:TRP:CD1	32:q:14:TRP:C	2.83	0.56
32:q:17:GLU:HG2	32:p:19:GLY:O	2.04	0.56
33:z:446:VAL:HG13	33:z:515:ILE:HG12	1.87	0.56
1:A:92:VAL:HG13	1:A:170:VAL:HG21	1.88	0.56
14:G:168:PRO:HG2	14:G:171:LEU:HB2	1.87	0.56
24:D:73:LEU:N	24:D:73:LEU:HD12	2.20	0.56
28:k:109:SER:HA	28:k:112:ILE:HD12	1.87	0.56
33:z:582:TYR:HD1	33:z:582:TYR:N	2.04	0.56
33:z:599:MET:HA	33:z:602:LYS:HD2	1.86	0.56
1:A:435:LEU:HB3	1:A:462:ILE:HD11	1.88	0.56
2:I:26:ILE:HD11	2:I:134:CYS:SG	2.46	0.56
2:I:338:THR:OG1	2:I:420:CYS:SG	2.63	0.56
2:I:459:GLU:CG	2:I:460:PRO:CD	2.84	0.56
4:N:160:LEU:HA	4:N:163:MET:HE3	1.88	0.56
15:C:103:PRO:HG3	15:C:155:ARG:HD3	1.86	0.56
15:C:225:VAL:HG23	15:C:248:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:627:GLU:HB2	15:C:642:PRO:HD3	1.86	0.56
14:G:318:GLU:O	14:G:348:ASN:ND2	2.31	0.56
14:G:385:GLN:HB2	14:G:387:ILE:HG12	1.88	0.56
21:R:14:VAL:HG12	21:R:74:TRP:HE1	1.70	0.56
32:q:117:VAL:HG13	32:q:118:HIS:H	1.69	0.56
3:J:77:PHE:O	4:N:145:TYR:OH	2.12	0.56
10:W:14:GLU:HB3	10:W:17:VAL:HG12	1.86	0.56
16:T:328:LYS:HE2	16:T:331:PHE:HB3	1.87	0.56
15:C:720:GLU:N	15:C:720:GLU:OE2	2.39	0.56
32:p:75:ARG:O	32:p:97:GLY:N	2.36	0.56
33:z:224:ILE:HA	33:z:228:ALA:HB2	1.88	0.56
2:I:170:GLU:H	2:I:170:GLU:CD	2.13	0.56
15:C:427:MET:HA	15:C:551:ASN:HB2	1.87	0.56
18:B:138:ARG:HG3	18:B:178:ALA:HB1	1.88	0.56
23:E:130:THR:HG22	23:E:130:THR:O	2.05	0.56
32:q:73:ILE:HG12	32:q:79:ILE:HD11	1.88	0.56
33:z:568:ALA:HA	33:z:572:ARG:HB2	1.87	0.56
2:I:159:PHE:HA	2:I:162:ILE:HG12	1.87	0.56
5:H:96:TYR:CZ	7:Y:91:LEU:HD21	2.41	0.56
33:z:187:VAL:HG21	33:z:198:LEU:CD1	2.36	0.56
33:z:223:ILE:HA	33:z:226:VAL:HG22	1.88	0.56
1:A:178:TYR:HB3	1:A:239:LEU:HD11	1.88	0.55
5:H:20:VAL:HG13	5:H:233:TYR:HB2	1.89	0.55
14:G:47:LEU:CD2	14:G:390:GLY:CA	2.84	0.55
15:C:131:VAL:HB	15:C:136:MET:HE3	1.87	0.55
15:C:292:THR:HG22	15:C:293:ILE:H	1.70	0.55
23:E:97:GLU:HG2	23:E:190:PRO:O	2.06	0.55
1:A:64:ILE:O	1:A:160:LYS:NZ	2.35	0.55
12:i:18:MET:C	12:i:20:SER:N	2.64	0.55
22:U:46:ASN:HA	22:U:49:ALA:HB3	1.88	0.55
32:p:131:SER:HB2	32:p:148:GLY:HA2	1.88	0.55
3:J:10:ILE:O	3:J:14:ILE:HG12	2.07	0.55
37:i:201:CDL:H511	37:i:201:CDL:CB6	2.36	0.55
14:G:209:VAL:HG23	14:G:227:PRO:HG3	1.89	0.55
15:C:741:VAL:O	15:C:741:VAL:HG12	2.06	0.55
18:B:196:ASN:HB3	18:B:221:HIS:HB3	1.88	0.55
1:A:180:TYR:CG	1:A:235:LEU:HD11	2.42	0.55
2:I:17:LEU:CD2	2:I:20:PHE:CE1	2.89	0.55
2:I:404:LEU:HD22	2:I:476:ILE:CG2	2.37	0.55
5:H:174:GLN:NE2	5:H:246:PHE:O	2.39	0.55
15:C:608:ASP:OD2	15:C:730:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:505:GLU:H	33:z:505:GLU:CD	2.13	0.55
14:G:250:PRO:HG2	14:G:263:ILE:HG23	1.87	0.55
38:G:601:PEV:O2P	38:G:601:PEV:H2	2.06	0.55
24:D:145:ARG:CZ	24:D:151:ARG:HG3	2.36	0.55
31:o:182:VAL:HA	31:o:199:ALA:HB2	1.88	0.55
33:z:276:LEU:HG	33:z:586:ARG:HA	1.89	0.55
16:T:83:TYR:CE2	17:F:160:PRO:HB3	2.41	0.55
33:z:387:ILE:HD11	33:z:392:PHE:HB3	1.87	0.55
13:j:28:CYS:O	13:j:28:CYS:SG	2.65	0.55
15:C:257:THR:HA	15:C:741:VAL:HG13	1.87	0.55
16:T:128:GLU:C	16:T:130:SER:H	2.13	0.55
32:q:90:ASN:ND2	32:q:117:VAL:O	2.39	0.55
14:G:72:TYR:CE2	23:E:92:ALA:HA	2.41	0.55
23:E:131:LEU:HD23	23:E:172:VAL:HG21	1.88	0.55
32:q:107:HIS:HD2	32:p:130:HIS:CE1	2.25	0.55
33:z:215:ILE:HB	33:z:439:ASP:HB3	1.89	0.55
2:I:53:ASN:ND2	26:c:52:GLY:CA	2.67	0.55
2:I:110:MET:HG2	2:I:468:LEU:CD2	2.36	0.55
14:G:146:GLU:OE1	24:D:104:SER:OG	2.19	0.55
15:C:271:GLY:O	15:C:272:ALA:C	2.50	0.55
17:F:48:HIS:HD2	17:F:51:THR:H	1.53	0.55
32:q:167:ALA:HB1	32:q:182:GLY:HA2	1.89	0.55
1:A:74:PRO:HB3	1:A:157:ASP:H	1.72	0.55
1:A:301:ILE:HA	1:A:377:VAL:HG13	1.88	0.55
2:I:354:LEU:CD1	2:I:472:THR:OG1	2.52	0.55
5:H:35:GLN:HG2	14:G:129:THR:HA	1.88	0.55
1:A:145:PRO:HD2	1:A:345:SER:HB3	1.89	0.54
2:I:354:LEU:CG	2:I:472:THR:CG2	2.54	0.54
3:J:83:VAL:HG21	4:N:137:LEU:HB3	1.89	0.54
5:H:34:VAL:HG13	24:D:83:THR:HG23	1.89	0.54
5:H:93:PRO:HB3	5:H:99:VAL:HB	1.88	0.54
14:G:56:GLU:O	14:G:349:ARG:NH1	2.39	0.54
2:I:110:MET:HG2	2:I:468:LEU:HD22	1.88	0.54
2:I:362:ILE:HD13	2:I:391:PHE:HA	1.89	0.54
14:G:239:TYR:HB3	21:R:131:PRO:HA	1.89	0.54
15:C:651:ARG:NE	25:X:130:SER:O	2.41	0.54
15:C:681:LYS:HB2	15:C:688:VAL:HG21	1.88	0.54
20:P:58:SER:HA	20:P:103:ARG:HH22	1.72	0.54
5:H:21:ALA:O	5:H:24:VAL:HG22	2.07	0.54
5:H:283:VAL:O	5:H:283:VAL:HG12	2.06	0.54
6:K:79:ILE:O	6:K:82:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:104:ARG:HG2	15:C:104:ARG:O	2.08	0.54
15:C:207:LEU:HD12	15:C:213:THR:CG2	2.37	0.54
16:T:219:PRO:HG2	40:T:501:NDP:H6N	1.89	0.54
31:o:146:LEU:HD11	32:q:130:HIS:HB2	1.89	0.54
32:q:47:ASN:ND2	32:p:81:TYR:OH	2.41	0.54
1:A:78:GLY:O	1:A:82:ARG:NH1	2.41	0.54
1:A:158:PRO:HB2	1:A:192:LEU:HD13	1.88	0.54
5:H:270:SER:O	5:H:274:LEU:HG	2.06	0.54
14:G:329:THR:HG23	21:R:131:PRO:CD	2.38	0.54
14:G:329:THR:HG23	21:R:131:PRO:HD2	1.89	0.54
14:G:360:PHE:CE1	17:F:110:TRP:HB3	2.42	0.54
31:o:91:SER:OG	31:o:93:TRP:NE1	2.39	0.54
33:z:125:ASN:CG	33:z:152:VAL:HG21	2.33	0.54
2:I:26:ILE:HG13	2:I:134:CYS:SG	2.48	0.54
4:N:144:LEU:HD11	6:K:64:LEU:HD21	1.90	0.54
11:S:61:SER:OG	14:G:292:ARG:NH1	2.31	0.54
14:G:130:PRO:HG2	14:G:193:LEU:HD21	1.88	0.54
33:z:226:VAL:HG23	33:z:226:VAL:O	2.08	0.54
2:I:17:LEU:HD22	2:I:20:PHE:CE1	2.42	0.54
3:J:81:TRP:CD2	3:J:96:MET:HG2	2.42	0.54
4:N:162:ALA:HB2	6:K:71:ALA:HB1	1.88	0.54
16:T:322:ARG:HD3	16:T:336:PRO:HB3	1.90	0.54
17:F:102:VAL:HG11	17:F:127:PRO:HD2	1.90	0.54
22:U:38:ASN:HD22	23:E:110:ARG:HH22	1.54	0.54
22:U:126:GLY:HA3	24:D:188:GLU:HG3	1.89	0.54
31:o:108:GLY:N	31:o:135:ILE:O	2.41	0.54
1:A:138:VAL:HG11	1:A:161:LEU:HD11	1.90	0.54
2:I:364:LEU:O	2:I:367:ARG:HG2	2.08	0.54
32:q:140:GLU:HG3	32:q:158:GLU:HA	1.89	0.54
14:G:48:HIS:CG	14:G:48:HIS:O	2.61	0.54
14:G:110:ARG:HA	14:G:334:PRO:HG3	1.89	0.54
31:o:171:GLU:O	31:o:174:SER:OG	2.19	0.54
32:q:50:ASP:OD1	32:q:51:LYS:NZ	2.31	0.54
32:q:163:VAL:HG12	32:q:167:ALA:HB3	1.89	0.54
33:z:152:VAL:HG12	33:z:168:MET:HB3	1.89	0.54
1:A:446:THR:HB	34:A:501:SF4:S3	2.48	0.54
8:Z:20:LEU:H	11:S:58:ILE:HG21	1.73	0.54
14:G:81:ALA:HB2	14:G:331:VAL:HG22	1.90	0.54
18:B:178:ALA:HB3	18:B:179:PRO:HD3	1.90	0.54
19:O:46:PRO:HG2	19:O:49:HIS:HD2	1.72	0.54
26:c:49:TYR:CD1	26:c:49:TYR:C	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:42:HIS:CD2	32:p:43:ARG:HH11	2.26	0.54
33:z:107:GLU:CD	33:z:176:LYS:O	2.51	0.54
33:z:174:MET:HB3	33:z:190:GLN:HB2	1.89	0.54
33:z:291:GLU:HB2	33:z:337:VAL:HG22	1.88	0.54
1:A:141:ASP:HA	1:A:182:ARG:HB2	1.89	0.54
2:I:252:ASP:N	2:I:252:ASP:OD1	2.40	0.54
5:H:84:LEU:HA	5:H:87:VAL:HG12	1.90	0.54
5:H:167:LEU:HD23	5:H:245:LEU:HD13	1.90	0.54
8:Z:9:LYS:HB2	8:Z:19:PRO:HG3	1.90	0.54
14:G:310:ILE:HD12	15:C:163:LEU:HD11	1.89	0.54
15:C:110:ARG:HB2	15:C:327:TRP:HZ2	1.73	0.54
16:T:311:PRO:HD2	16:T:314:ILE:HD12	1.90	0.54
22:U:115:ARG:HD3	24:D:118:THR:HA	1.90	0.54
1:A:228:ILE:HG23	1:A:400:GLU:O	2.08	0.53
2:I:170:GLU:OE1	2:I:170:GLU:N	2.37	0.53
15:C:398:ASP:HB3	15:C:668:LEU:HD11	1.89	0.53
15:C:581:VAL:HB	15:C:600:VAL:HG22	1.89	0.53
18:B:228:ARG:NH1	18:B:232:GLY:O	2.41	0.53
1:A:172:MET:SD	1:A:264:THR:OG1	2.65	0.53
4:N:16:MET:HE3	4:N:20:ALA:HB2	1.88	0.53
5:H:42:VAL:HG11	23:E:111:PHE:HA	1.90	0.53
17:F:38:LEU:HD21	17:F:75:TYR:CZ	2.42	0.53
32:p:126:VAL:HG12	32:p:128:ILE:HG13	1.89	0.53
32:p:130:HIS:CD2	32:p:130:HIS:H	2.26	0.53
1:A:122:TRP:N	1:A:122:TRP:CD1	2.75	0.53
12:i:14:LEU:HD23	12:i:14:LEU:C	2.32	0.53
23:E:89:PHE:CE2	23:E:135:MET:HE3	2.43	0.53
31:o:108:GLY:N	31:o:111:SER:OG	2.42	0.53
1:A:289:GLY:HA2	1:A:316:SER:HB2	1.90	0.53
2:I:53:ASN:HD21	26:c:52:GLY:HA2	1.70	0.53
2:I:401:ILE:HG22	2:I:403:PRO:HD2	1.89	0.53
5:H:24:VAL:HG12	5:H:233:TYR:CD2	2.44	0.53
5:H:130:SER:HB2	5:H:133:ALA:HB3	1.90	0.53
6:K:53:LEU:HD22	13:j:45:LEU:HB3	1.89	0.53
10:W:5:GLU:HA	10:W:8:ARG:HH11	1.73	0.53
13:j:17:PHE:HB3	13:j:41:TYR:HA	1.90	0.53
15:C:317:PRO:HB3	15:C:328:ILE:HG12	1.89	0.53
2:I:354:LEU:HD11	2:I:472:THR:CB	2.38	0.53
31:o:64:TRP:HB3	31:o:83:GLN:HG3	1.89	0.53
33:z:190:GLN:HA	33:z:281:GLU:HA	1.91	0.53
1:A:301:ILE:HG21	1:A:327:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:332:ILE:HD11	2:I:413:LEU:HB3	1.89	0.53
5:H:170:ILE:O	5:H:174:GLN:NE2	2.41	0.53
15:C:605:HIS:CD2	15:C:606:HIS:HD2	2.26	0.53
17:F:135:ASP:OD2	17:F:156:ARG:NH1	2.42	0.53
24:D:111:HIS:H	24:D:159:MET:HE1	1.74	0.53
32:q:22:LEU:C	32:q:24:ARG:N	2.67	0.53
2:I:215:GLY:HA2	2:I:286:TYR:HD2	1.73	0.53
14:G:299:ARG:NH2	24:D:172:CYS:O	2.42	0.53
18:B:155:ARG:NH2	18:B:168:GLU:HB2	2.24	0.53
24:D:178:VAL:HG21	24:D:211:ILE:HG21	1.90	0.53
31:o:112:ASN:CG	31:o:220:ILE:HG21	2.33	0.53
31:o:152:ILE:HD13	31:o:158:ILE:HG13	1.91	0.53
32:q:135:HIS:CG	32:p:147:MET:HE3	2.43	0.53
33:z:248:VAL:HA	33:z:254:THR:HG22	1.90	0.53
33:z:392:PHE:O	33:z:392:PHE:HD1	1.91	0.53
1:A:248:LEU:HD11	15:C:115:GLY:HA3	1.91	0.53
5:H:42:VAL:CG1	23:E:111:PHE:HA	2.38	0.53
15:C:83:VAL:HG11	15:C:98:ALA:HB2	1.90	0.53
24:D:140:ILE:HA	24:D:154:ARG:O	2.08	0.53
26:c:43:ILE:HG22	26:c:43:ILE:O	2.08	0.53
32:q:43:ARG:O	32:q:47:ASN:ND2	2.38	0.53
32:p:92:VAL:HG12	32:p:94:VAL:HG23	1.90	0.53
2:I:195:SER:HA	6:K:46:PHE:CE1	2.44	0.53
2:I:267:ILE:HB	2:I:356:THR:HG21	1.91	0.53
9:V:44:GLU:HA	9:V:47:VAL:HG22	1.91	0.53
14:G:75:MET:N	14:G:75:MET:SD	2.82	0.53
22:U:75:TRP:CB	24:D:99:GLU:HB3	2.39	0.53
31:o:78:VAL:HG11	31:o:92:VAL:HG12	1.90	0.53
32:q:18:THR:HG22	32:q:22:LEU:CD1	2.38	0.53
33:z:450:CYS:SG	33:z:511:TRP:CE3	2.98	0.53
5:H:306:LEU:O	5:H:310:TRP:HD1	1.91	0.53
17:F:24:ARG:NH1	17:F:87:ARG:HH21	2.07	0.53
18:B:135:CYS:HB3	18:B:140:SER:HB2	1.90	0.53
27:Q:72:VAL:HG11	27:Q:85:ALA:HB1	1.91	0.53
31:o:89:GLY:O	31:o:221:ASN:ND2	2.42	0.53
32:q:105:LEU:HD23	32:q:133:VAL:HG22	1.91	0.53
1:A:323:ILE:HA	1:A:327:CYS:SG	2.49	0.52
2:I:19:VAL:HG22	2:I:87:PHE:CE1	2.43	0.52
2:I:309:ALA:HA	2:I:318:LEU:CD1	2.39	0.52
3:J:71:PHE:CE1	5:H:304:LEU:HD21	2.43	0.52
15:C:397:LYS:NZ	27:Q:13:GLU:OE2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:95:VAL:HG11	25:X:74:VAL:HG22	1.92	0.52
2:I:94:TYR:CZ	2:I:98:ILE:CD1	2.90	0.52
2:I:459:GLU:HG2	2:I:460:PRO:CD	2.39	0.52
5:H:316:GLY:O	5:H:320:THR:HG23	2.08	0.52
18:B:209:ILE:HD11	18:B:224:GLN:HG3	1.92	0.52
23:E:130:THR:HA	23:E:158:CYS:HB3	1.91	0.52
2:I:336:CYS:SG	2:I:338:THR:OG1	2.64	0.52
8:Z:47:MET:C	8:Z:49:MET:H	2.17	0.52
37:i:201:CDL:H211	30:n:93:ILE:HD11	1.90	0.52
15:C:602:TYR:CZ	15:C:604:GLY:HA3	2.45	0.52
16:T:62:GLY:HA3	16:T:90:LYS:O	2.10	0.52
24:D:152:THR:OG1	24:D:152:THR:O	2.27	0.52
28:k:101:GLU:HG2	28:k:114:TYR:CZ	2.44	0.52
2:I:107:THR:HA	2:I:110:MET:HE2	1.89	0.52
8:Z:115:VAL:CG1	8:Z:116:PRO:HD3	2.40	0.52
14:G:69:ARG:CD	34:E:301:SF4:S2	2.92	0.52
16:T:95:VAL:N	16:T:117:GLN:O	2.43	0.52
18:B:202:THR:H	18:B:205:LYS:HB2	1.74	0.52
32:p:207:TYR:HA	32:p:210:LEU:HB3	1.91	0.52
1:A:370:SER:OG	1:A:371:GLY:N	2.41	0.52
2:I:78:ILE:CD1	26:c:5:ILE:HD11	2.37	0.52
5:H:192:ILE:HG22	5:H:192:ILE:O	2.10	0.52
14:G:25:VAL:HG21	14:G:47:LEU:HB2	1.91	0.52
14:G:93:GLU:HA	21:R:129:HIS:NE2	2.25	0.52
15:C:338:GLY:O	15:C:606:HIS:HE1	1.93	0.52
16:T:113:GLY:HA3	16:T:118:VAL:HG23	1.92	0.52
16:T:149:TYR:HB3	16:T:340:ASN:HD21	1.74	0.52
19:O:42:VAL:HB	25:X:77:LEU:HD23	1.91	0.52
22:U:137:GLY:HA2	22:U:144:GLN:HG3	1.92	0.52
23:E:185:VAL:HG22	23:E:198:GLY:HA3	1.92	0.52
27:Q:15:ARG:NH1	27:Q:69:GLU:OE1	2.37	0.52
32:q:135:HIS:HB2	32:p:147:MET:HG2	1.92	0.52
32:q:184:ASN:HD21	32:p:183:GLY:HA2	1.74	0.52
33:z:284:LEU:HD12	33:z:284:LEU:N	2.25	0.52
5:H:233:TYR:O	5:H:237:ILE:HG13	2.09	0.52
14:G:58:LYS:O	14:G:350:PRO:HD2	2.09	0.52
15:C:368:VAL:HG22	15:C:616:VAL:HG11	1.90	0.52
16:T:83:TYR:O	16:T:87:GLN:HG2	2.09	0.52
23:E:157:SER:N	34:E:301:SF4:S3	2.82	0.52
33:z:144:GLU:O	33:z:145:LYS:N	2.42	0.52
13:j:27:HIS:CE1	33:z:128:GLN:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:245:LEU:HD13	14:G:274:ILE:HG23	1.91	0.52
32:q:68:ILE:HG21	32:p:214:HIS:HE1	1.74	0.52
33:z:319:LYS:HE2	33:z:321:LEU:HD21	1.91	0.52
2:I:205:HIS:HD2	2:I:207:ASP:HB3	1.75	0.52
3:J:99:PHE:HD2	4:N:156:SER:HB2	1.75	0.52
7:Y:86:THR:O	7:Y:86:THR:OG1	2.28	0.52
14:G:212:GLN:NE2	14:G:216:ASP:OD1	2.43	0.52
15:C:146:THR:O	15:C:155:ARG:NH2	2.43	0.52
25:X:40:ILE:HD12	25:X:89:ILE:HG22	1.92	0.52
32:q:64:SER:OG	32:q:82:GLY:N	2.41	0.52
32:q:94:VAL:HG13	32:q:98:THR:HB	1.91	0.52
33:z:120:GLU:CD	33:z:120:GLU:N	2.67	0.52
2:I:334:PHE:C	2:I:334:PHE:CD1	2.88	0.52
7:Y:90:ASP:OD2	8:Z:74:LEU:HD21	2.09	0.52
15:C:109:SER:O	19:O:138:LYS:NZ	2.41	0.52
32:q:77:SER:HB2	32:q:97:GLY:H	1.74	0.52
33:z:182:LYS:HG3	33:z:205:TYR:HD2	1.74	0.52
2:I:53:ASN:HD22	26:c:55:PRO:HG2	1.75	0.52
5:H:28:ARG:CZ	23:E:114:ILE:HD11	2.40	0.52
15:C:554:LEU:HD23	15:C:559:GLN:HB3	1.91	0.52
17:F:9:TYR:CZ	17:F:13:THR:HG21	2.45	0.52
21:R:66:ASN:O	21:R:70:GLU:HG2	2.09	0.52
32:q:22:LEU:C	32:q:24:ARG:H	2.17	0.52
1:A:221:HIS:CD2	1:A:239:LEU:HG	2.45	0.51
2:I:19:VAL:HG12	2:I:23:ILE:HG13	1.91	0.51
2:I:125:PHE:CE1	2:I:162:ILE:HG22	2.44	0.51
5:H:29:LYS:NZ	9:V:7:GLU:OE2	2.42	0.51
5:H:95:ASP:OD1	5:H:96:TYR:N	2.42	0.51
16:T:225:THR:O	16:T:226:GLU:HG2	2.10	0.51
16:T:237:VAL:HG13	16:T:241:GLY:HA2	1.92	0.51
15:C:402:ARG:NH2	27:Q:67:GLY:O	2.44	0.51
15:C:427:MET:HG3	15:C:551:ASN:HB2	1.93	0.51
21:R:30:ARG:O	21:R:34:ILE:HG12	2.11	0.51
28:k:50:VAL:O	28:k:54:VAL:HG23	2.10	0.51
32:q:184:ASN:ND2	32:p:184:ASN:H	2.08	0.51
8:Z:134:ALA:HB3	13:j:54:ARG:HH11	1.74	0.51
17:F:53:VAL:HG23	17:F:54:GLN:H	1.75	0.51
32:q:22:LEU:O	32:q:24:ARG:N	2.43	0.51
33:z:361:ASP:HB2	33:z:364:ARG:HB2	1.93	0.51
1:A:110:GLY:N	1:A:116:PHE:O	2.43	0.51
1:A:405:CYS:HB3	1:A:447:ILE:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:304:ARG:HB2	15:C:316:ILE:HG22	1.92	0.51
15:C:367:VAL:O	15:C:371:ILE:HG12	2.11	0.51
15:C:627:GLU:OE2	15:C:639:GLN:NE2	2.43	0.51
17:F:157:TYR:CE1	17:F:168:PRO:HG3	2.45	0.51
19:O:61:ARG:HB2	19:O:71:LEU:HD11	1.91	0.51
23:E:188:CYS:O	34:E:301:SF4:S1	2.69	0.51
24:D:124:ILE:O	24:D:124:ILE:HD12	2.10	0.51
1:A:471:ARG:NH1	1:A:475:GLU:OE1	2.43	0.51
9:V:43:ASP:N	9:V:43:ASP:OD1	2.43	0.51
16:T:68:GLY:O	16:T:139:ASN:ND2	2.42	0.51
20:P:65:VAL:O	20:P:107:ASP:HB3	2.11	0.51
33:z:239:ASP:HB2	33:z:270:ARG:HD3	1.92	0.51
33:z:599:MET:SD	33:z:599:MET:N	2.83	0.51
1:A:237:GLU:HG2	1:A:247:ARG:HH21	1.74	0.51
3:J:69:LEU:HD23	6:K:74:ALA:HB2	1.92	0.51
5:H:176:GLN:HE21	8:Z:63:GLN:HE22	1.57	0.51
12:i:21:ASN:HD22	12:i:21:ASN:N	2.08	0.51
37:i:201:CDL:H141	37:i:201:CDL:H731	1.93	0.51
14:G:27:ARG:NE	14:G:46:LEU:HD21	2.25	0.51
14:G:257:CYS:SG	14:G:260:ARG:NH2	2.84	0.51
15:C:176:GLY:HA2	34:C:801:SF4:S3	2.50	0.51
15:C:574:ALA:C	15:C:576:GLU:H	2.19	0.51
17:F:63:ASP:CG	17:F:70:ARG:HH21	2.18	0.51
23:E:84:ILE:HG23	23:E:113:ILE:HG13	1.92	0.51
26:c:49:TYR:HB2	26:c:62:MET:HB2	1.92	0.51
27:Q:59:GLN:OE1	27:Q:61:TRP:NE1	2.36	0.51
32:q:105:LEU:C	32:q:107:HIS:H	2.18	0.51
1:A:228:ILE:HD11	18:B:113:PHE:CE2	2.45	0.51
2:I:215:GLY:H	2:I:286:TYR:HB3	1.76	0.51
3:J:69:LEU:HD11	6:K:70:ALA:HB1	1.92	0.51
4:N:62:ALA:HB3	5:H:119:TYR:OH	2.10	0.51
37:i:201:CDL:H132	37:i:201:CDL:H712	1.91	0.51
15:C:239:ILE:HD11	15:C:246:GLU:CD	2.35	0.51
15:C:373:HIS:NE2	15:C:664:SER:O	2.36	0.51
15:C:443:ILE:HD12	15:C:533:VAL:HG22	1.92	0.51
22:U:115:ARG:NH2	22:U:115:ARG:HB3	2.26	0.51
23:E:173:ARG:N	23:E:173:ARG:HD2	2.26	0.51
24:D:77:VAL:O	24:D:77:VAL:HG12	2.10	0.51
26:c:36:ARG:NH1	26:c:80:ASN:OD1	2.44	0.51
30:n:84:TYR:H	30:n:84:TYR:HD1	1.57	0.51
1:A:231:GLU:N	1:A:231:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:HD12	1:A:355:CYS:SG	2.51	0.51
5:H:22:PHE:CD1	5:H:51:PRO:HG2	2.46	0.51
14:G:44:ILE:HD11	14:G:363:LEU:HD23	1.93	0.51
14:G:362:HIS:O	14:G:385:GLN:NE2	2.44	0.51
31:o:188:ILE:HG23	31:o:194:TRP:CD1	2.46	0.51
32:q:96:SER:N	32:q:124:ASP:OD1	2.44	0.51
1:A:180:TYR:CD1	1:A:235:LEU:HD11	2.45	0.51
3:J:84:SER:O	3:J:84:SER:OG	2.26	0.51
15:C:391:GLU:HA	15:C:680:ILE:HD11	1.92	0.51
33:z:121:VAL:O	33:z:121:VAL:HG13	2.10	0.51
33:z:129:PRO:CG	33:z:170:ASN:CB	2.70	0.51
20:P:70:VAL:HG13	20:P:89:LEU:HD11	1.92	0.51
31:o:177:GLU:O	31:o:180:SER:OG	2.21	0.51
32:q:72:HIS:O	32:q:94:VAL:N	2.43	0.51
32:q:168:LEU:HD22	32:p:166:GLY:HA3	1.92	0.51
1:A:154:MET:O	1:A:158:PRO:HB3	2.11	0.50
8:Z:7:ARG:HB3	8:Z:19:PRO:HD2	1.91	0.50
20:P:100:CYS:O	20:P:100:CYS:SG	2.69	0.50
31:o:50:TRP:CD1	32:q:43:ARG:HA	2.47	0.50
31:o:103:ASN:ND2	31:o:122:ALA:O	2.44	0.50
33:z:270:ARG:HD2	33:z:270:ARG:C	2.37	0.50
1:A:302:SER:OG	18:B:134:PRO:HB3	2.11	0.50
2:I:347:ILE:HG12	2:I:490:THR:HG21	1.93	0.50
5:H:283:VAL:O	5:H:283:VAL:CG1	2.59	0.50
5:H:323:TRP:HB3	8:Z:65:GLY:HA2	1.92	0.50
6:K:53:LEU:CD2	13:j:45:LEU:HB3	2.41	0.50
24:D:73:LEU:HD12	24:D:73:LEU:H	1.75	0.50
32:p:207:TYR:N	32:p:207:TYR:CD1	2.76	0.50
33:z:163:LEU:HD11	33:z:598:ASN:H	1.77	0.50
2:I:167:ARG:HB2	6:K:82:ILE:HD11	1.93	0.50
2:I:201:THR:HG21	2:I:209:LEU:HD12	1.93	0.50
14:G:136:GLU:HG2	24:D:92:VAL:HG21	1.92	0.50
15:C:284:ASN:ND2	15:C:284:ASN:O	2.45	0.50
17:F:44:PHE:O	17:F:45:LEU:HB2	2.10	0.50
26:c:4:ASP:OD1	26:c:4:ASP:N	2.45	0.50
27:Q:7:ILE:HG12	27:Q:90:VAL:HG21	1.94	0.50
32:q:68:ILE:HG21	32:p:214:HIS:CE1	2.46	0.50
2:I:54:VAL:O	2:I:58:GLY:N	2.41	0.50
5:H:207:GLU:HG3	5:H:212:LEU:HD13	1.93	0.50
16:T:261:VAL:HG13	16:T:282:LEU:HD12	1.93	0.50
16:T:300:MET:O	16:T:382:ARG:NE	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:312:PHE:CZ	16:T:348:THR:HA	2.47	0.50
16:T:355:ASP:OD1	16:T:355:ASP:N	2.42	0.50
25:X:95:GLN:OE1	25:X:97:HIS:N	2.45	0.50
31:o:79:VAL:HG11	32:q:81:TYR:CG	2.46	0.50
2:I:402:PRO:HA	2:I:407:PHE:CG	2.47	0.50
5:H:195:LEU:HD13	5:H:202:PRO:HD2	1.93	0.50
5:H:201:ALA:HB1	5:H:202:PRO:HD2	1.93	0.50
33:z:534:PHE:O	33:z:540:THR:HA	2.12	0.50
1:A:337:LEU:HD21	1:A:340:ILE:HG13	1.93	0.50
5:H:74:PHE:HB3	5:H:127:SER:CB	2.42	0.50
15:C:57:ARG:CZ	15:C:81:TYR:HB3	2.41	0.50
15:C:105:PHE:HZ	15:C:181:LEU:HA	1.76	0.50
15:C:348:MET:HB3	15:C:356:PHE:HB3	1.93	0.50
15:C:566:GLY:HA3	27:Q:49:LEU:HD21	1.94	0.50
17:F:48:HIS:O	17:F:52:ARG:HG2	2.12	0.50
17:F:58:ASP:OD1	17:F:59:ILE:N	2.45	0.50
31:o:79:VAL:HG11	32:q:81:TYR:CD1	2.46	0.50
32:p:60:PHE:HB3	32:p:211:ALA:HB1	1.94	0.50
2:I:138:PHE:HE1	2:I:147:ALA:HB1	1.77	0.50
10:W:11:VAL:HG22	10:W:18:ALA:HB1	1.92	0.50
14:G:21:ALA:HA	23:E:90:GLY:HA3	1.93	0.50
14:G:138:ARG:O	14:G:142:LEU:HG	2.11	0.50
15:C:281:LYS:HA	24:D:142:ALA:O	2.11	0.50
16:T:174:HIS:ND1	16:T:174:HIS:O	2.45	0.50
33:z:178:LEU:HA	33:z:189:VAL:HG23	1.93	0.50
1:A:248:LEU:HB3	1:A:250:PRO:HD2	1.93	0.50
2:I:250:ALA:HA	2:I:253:ILE:HG12	1.93	0.50
15:C:222:THR:O	15:C:226:ARG:HG3	2.12	0.50
30:n:101:LEU:O	30:n:101:LEU:HD23	2.12	0.50
33:z:107:GLU:OE1	33:z:176:LYS:CA	2.56	0.50
33:z:489:TRP:CE3	33:z:508:ILE:CG2	2.94	0.50
1:A:186:VAL:HB	18:B:195:TYR:HB3	1.94	0.50
1:A:381:ASP:O	1:A:384:THR:HG22	2.12	0.50
2:I:339:ILE:HD11	33:z:115:TRP:HB3	1.93	0.50
5:H:74:PHE:HE2	5:H:219:GLU:HB3	1.77	0.50
8:Z:135:THR:OG1	8:Z:136:GLY:N	2.45	0.50
15:C:293:ILE:HG22	15:C:294:ASP:H	1.77	0.50
31:o:209:GLU:O	31:o:213:ILE:HG13	2.12	0.50
33:z:436:LEU:C	33:z:436:LEU:HD12	2.37	0.50
2:I:66:LEU:HA	2:I:101:LEU:HD13	1.93	0.49
2:I:312:GLN:HA	2:I:312:GLN:HE21	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:355:MET:HG3	2:I:397:SER:HB3	1.92	0.49
3:J:80:PRO:HB2	4:N:145:TYR:HE2	1.77	0.49
11:S:50:PRO:HB2	24:D:105:PRO:HD2	1.94	0.49
27:Q:35:ASN:HD21	27:Q:83:LEU:HD13	1.76	0.49
32:q:42:HIS:CD2	32:p:43:ARG:HD3	2.47	0.49
32:q:179:GLU:HA	32:q:191:LYS:HD3	1.92	0.49
33:z:390:LEU:HD23	33:z:390:LEU:C	2.37	0.49
2:I:84:ASN:O	2:I:84:ASN:OD1	2.30	0.49
7:Y:10:ASN:O	7:Y:12:ILE:N	2.42	0.49
8:Z:112:MET:O	8:Z:116:PRO:HD2	2.12	0.49
16:T:97:VAL:O	16:T:120:PRO:HA	2.11	0.49
23:E:161:GLY:HA3	24:D:160:THR:HB	1.92	0.49
32:p:98:THR:HG22	32:p:126:VAL:H	1.77	0.49
32:p:179:GLU:HB3	32:p:181:TRP:HE1	1.77	0.49
1:A:227:TYR:HB3	1:A:400:GLU:HB3	1.93	0.49
4:N:132:ARG:HH21	8:Z:83:ARG:HH22	1.61	0.49
5:H:323:TRP:HB3	8:Z:65:GLY:CA	2.42	0.49
10:W:19:ALA:O	10:W:23:ILE:CG1	2.58	0.49
11:S:30:CYS:HB3	11:S:32:HIS:HD1	1.78	0.49
12:i:9:GLY:O	12:i:39:MET:HG3	2.12	0.49
14:G:197:ARG:HG3	24:D:76:MET:HE2	1.93	0.49
15:C:186:MET:HG3	15:C:186:MET:O	2.12	0.49
16:T:60:THR:HG23	16:T:61:GLY:H	1.77	0.49
31:o:60:PRO:HB3	31:o:65:LEU:HD13	1.94	0.49
1:A:480:GLU:O	1:A:481:LEU:HG	2.12	0.49
2:I:481:LEU:HD22	2:I:481:LEU:N	2.27	0.49
14:G:264:ARG:NE	14:G:386:ASP:OD2	2.45	0.49
16:T:78:GLY:HA3	40:T:501:NDP:H52A	1.95	0.49
5:H:154:ILE:HG23	5:H:186:VAL:HG12	1.94	0.49
6:K:79:ILE:O	6:K:82:ILE:CG2	2.61	0.49
14:G:53:LYS:HE2	17:F:147:PHE:HD2	1.77	0.49
15:C:349:ILE:HG22	15:C:616:VAL:HG23	1.94	0.49
22:U:94:HIS:ND1	22:U:94:HIS:O	2.45	0.49
1:A:343:GLY:H	1:A:347:VAL:HG21	1.77	0.49
15:C:239:ILE:HG23	15:C:239:ILE:O	2.13	0.49
15:C:465:SER:O	15:C:467:ALA:N	2.44	0.49
24:D:213:GLU:OE1	24:D:216:ARG:NH1	2.45	0.49
2:I:125:PHE:HA	2:I:128:LEU:HD12	1.94	0.49
2:I:361:ALA:CB	2:I:469:LEU:HD11	2.42	0.49
2:I:425:LEU:HD12	2:I:425:LEU:O	2.12	0.49
5:H:37:ARG:HD2	23:E:107:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:19:TRP:O	6:K:23:LEU:HG	2.12	0.49
13:j:28:CYS:HB2	13:j:34:CYS:SG	2.53	0.49
15:C:295:VAL:HG23	15:C:387:LEU:HD22	1.94	0.49
15:C:740:ALA:C	15:C:742:LEU:H	2.21	0.49
17:F:39:PHE:CD1	17:F:39:PHE:C	2.90	0.49
22:U:38:ASN:HD22	23:E:110:ARG:NH2	2.09	0.49
2:I:35:HIS:ND1	26:c:64:THR:HG21	2.28	0.49
2:I:465:LYS:O	2:I:469:LEU:HD13	2.13	0.49
8:Z:37:ARG:HD2	8:Z:39:ILE:HD12	1.94	0.49
15:C:103:PRO:HB2	15:C:184:GLN:HE21	1.77	0.49
15:C:213:THR:HG22	15:C:273:LEU:HD22	1.93	0.49
24:D:172:CYS:SG	24:D:175:ASP:N	2.85	0.49
31:o:120:HIS:CG	31:o:121:ALA:H	2.31	0.49
2:I:416:ALA:O	2:I:420:CYS:SG	2.71	0.49
4:N:67:PHE:HA	4:N:70:MET:HE2	1.95	0.49
15:C:409:TRP:HD1	15:C:410:CYS:O	1.95	0.49
16:T:111:LEU:O	16:T:112:MET:HG2	2.12	0.49
24:D:52:LEU:O	24:D:56:ILE:HG12	2.13	0.49
31:o:50:TRP:HZ2	32:q:41:ARG:HA	1.77	0.49
32:q:18:THR:HG22	32:q:22:LEU:HD13	1.94	0.49
32:p:124:ASP:H	32:p:141:ASP:HA	1.78	0.49
1:A:361:ASP:OD1	1:A:361:ASP:N	2.45	0.49
2:I:380:LEU:HD22	2:I:384:ASN:O	2.12	0.49
4:N:52:ILE:O	4:N:56:VAL:HG22	2.13	0.49
8:Z:98:VAL:O	8:Z:102:LYS:HG2	2.13	0.49
15:C:292:THR:HG22	15:C:293:ILE:N	2.27	0.49
15:C:383:VAL:HB	15:C:583:LEU:HD23	1.95	0.49
15:C:485:LEU:HD22	15:C:500:HIS:HE2	1.76	0.49
15:C:680:ILE:HA	15:C:683:VAL:HG12	1.94	0.49
16:T:152:ARG:HH11	16:T:332:PRO:HG3	1.78	0.49
28:k:97:ILE:HG23	28:k:114:TYR:HE2	1.77	0.49
32:p:187:ARG:HG3	32:p:187:ARG:O	2.12	0.49
1:A:57:GLY:HA2	1:A:325:ARG:HH12	1.77	0.48
2:I:404:LEU:HD22	2:I:476:ILE:HG22	1.95	0.48
5:H:37:ARG:HB2	23:E:107:ASP:OD2	2.13	0.48
5:H:248:LEU:HD22	5:H:276:PHE:HE2	1.77	0.48
14:G:352:ARG:HG2	17:F:62:VAL:HG22	1.95	0.48
17:F:175:PHE:HB3	19:O:100:ASN:ND2	2.28	0.48
31:o:50:TRP:H	32:q:45:LEU:HB3	1.78	0.48
31:o:135:ILE:HD13	31:o:141:VAL:HG21	1.94	0.48
32:q:18:THR:CG2	32:q:22:LEU:CD1	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:173:THR:HG21	32:q:186:ALA:HB1	1.95	0.48
32:p:94:VAL:HG22	32:p:122:ILE:HD12	1.95	0.48
33:z:599:MET:H	33:z:599:MET:CE	2.24	0.48
1:A:228:ILE:HG21	1:A:402:CYS:N	2.27	0.48
2:I:19:VAL:O	2:I:19:VAL:CG1	2.60	0.48
6:K:56:MET:HE2	13:j:6:GLY:O	2.13	0.48
14:G:53:LYS:HE3	17:F:149:LEU:HA	1.94	0.48
27:Q:14:LEU:O	27:Q:49:LEU:N	2.43	0.48
31:o:54:GLY:HA2	32:q:42:HIS:CE1	2.48	0.48
32:q:17:GLU:OE2	32:q:21:ALA:HB2	2.12	0.48
32:p:139:VAL:HG23	32:p:157:VAL:HB	1.95	0.48
33:z:110:HIS:N	33:z:121:VAL:HG11	2.21	0.48
1:A:85:TRP:CD2	1:A:204:LEU:HD13	2.49	0.48
1:A:228:ILE:HG21	1:A:402:CYS:H	1.77	0.48
1:A:245:LYS:HE3	15:C:239:ILE:HD13	1.95	0.48
1:A:408:CYS:HB3	34:A:501:SF4:S4	2.53	0.48
1:A:433:ASP:CG	1:A:466:ARG:HH22	2.19	0.48
2:I:345:LEU:HD21	2:I:349:ILE:CD1	2.43	0.48
2:I:380:LEU:HD23	2:I:380:LEU:O	2.14	0.48
14:G:181:GLN:OE1	14:G:185:ARG:NH2	2.45	0.48
14:G:365:GLY:HA2	14:G:368:PHE:CE2	2.48	0.48
15:C:196:THR:O	15:C:197:GLU:HG3	2.12	0.48
15:C:277:PRO:HB3	15:C:734:ILE:CD1	2.43	0.48
16:T:75:GLY:CA	16:T:144:LEU:HB2	2.42	0.48
16:T:172:LYS:HD2	16:T:210:ALA:O	2.14	0.48
17:F:42:LEU:HD12	17:F:101:VAL:HG11	1.96	0.48
33:z:178:LEU:HD12	33:z:178:LEU:C	2.38	0.48
33:z:542:LYS:HZ3	33:z:576:ARG:HD2	1.79	0.48
2:I:139:MET:SD	2:I:155:GLN:HG2	2.53	0.48
15:C:550:LEU:HD11	15:C:552:PHE:HE1	1.78	0.48
15:C:637:THR:HG21	15:C:687:LEU:HA	1.96	0.48
17:F:56:LEU:HD22	17:F:108:ALA:HB2	1.95	0.48
19:O:58:SER:HB3	19:O:130:PRO:HB3	1.94	0.48
21:R:30:ARG:HG3	21:R:77:ILE:HD11	1.94	0.48
21:R:64:ARG:HA	21:R:67:VAL:HG12	1.96	0.48
24:D:112:ALA:HB1	24:D:204:GLY:HA3	1.94	0.48
11:S:50:PRO:HB2	24:D:105:PRO:CD	2.42	0.48
15:C:344:LEU:HD22	15:C:617:ILE:HG21	1.96	0.48
15:C:582:TYR:HD1	15:C:601:VAL:HG13	1.77	0.48
16:T:182:GLN:HG2	16:T:207:VAL:HG11	1.94	0.48
18:B:100:ILE:HG23	18:B:102:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:125:ALA:HB2	24:D:152:THR:HG22	1.94	0.48
27:Q:4:ARG:HH21	27:Q:83:LEU:HG	1.79	0.48
32:q:141:ASP:OD1	32:q:142:GLU:N	2.46	0.48
32:p:106:VAL:HG12	32:p:120:THR:HG21	1.95	0.48
1:A:428:LYS:NZ	8:Z:12:MET:SD	2.85	0.48
2:I:367:ARG:HG2	2:I:461:MET:HE1	1.96	0.48
2:I:460:PRO:HB3	12:i:24:ARG:HA	1.96	0.48
8:Z:38:ARG:NH2	11:S:127:GLY:HA3	2.29	0.48
14:G:58:LYS:HB3	14:G:62:GLN:HB2	1.96	0.48
14:G:238:PRO:HD3	21:R:134:ARG:HB2	1.95	0.48
15:C:105:PHE:CZ	15:C:181:LEU:HA	2.47	0.48
15:C:729:THR:HG23	15:C:735:MET:HG3	1.96	0.48
19:O:100:ASN:OD1	19:O:101:VAL:N	2.46	0.48
30:n:84:TYR:N	30:n:84:TYR:CD1	2.82	0.48
31:o:49:LYS:HB2	32:q:46:MET:HE3	1.96	0.48
33:z:194:ARG:HA	33:z:219:GLN:HA	1.93	0.48
33:z:244:SER:HB3	33:z:283:THR:HB	1.95	0.48
33:z:387:ILE:HD12	33:z:387:ILE:HA	1.67	0.48
1:A:99:ILE:HG23	1:A:278:LEU:HD11	1.95	0.48
15:C:222:THR:O	15:C:222:THR:HG22	2.14	0.48
15:C:411:GLU:OE1	15:C:588:ASP:N	2.44	0.48
15:C:445:THR:OG1	15:C:517:GLY:N	2.38	0.48
16:T:84:LEU:HD23	16:T:144:LEU:HD11	1.95	0.48
16:T:360:PHE:CE2	16:T:367:PRO:HB3	2.48	0.48
23:E:86:PRO:HD3	23:E:113:ILE:HG23	1.96	0.48
26:c:52:GLY:HA3	26:c:57:ILE:O	2.12	0.48
32:q:21:ALA:HA	32:p:16:ARG:HD2	1.95	0.48
32:p:216:ALA:N	32:p:217:GLU:OE1	2.46	0.48
2:I:46:ASP:CG	2:I:46:ASP:O	2.56	0.48
5:H:74:PHE:CE2	5:H:219:GLU:HB3	2.49	0.48
18:B:149:ASP:OD1	18:B:150:HIS:N	2.45	0.48
18:B:248:GLN:OE1	18:B:248:GLN:N	2.44	0.48
31:o:223:LEU:HD21	32:p:86:ARG:NH1	2.29	0.48
33:z:533:PHE:HD1	33:z:537:ARG:HB2	1.77	0.48
16:T:135:MET:HE1	16:T:170:VAL:HG23	1.95	0.48
16:T:181:ILE:HG12	16:T:215:THR:HB	1.96	0.48
22:U:116:TYR:HE1	24:D:117:PRO:HA	1.78	0.48
25:X:33:ALA:HA	25:X:86:LEU:HD21	1.95	0.48
32:p:61:VAL:HG22	32:p:79:ILE:HD13	1.96	0.48
33:z:124:ARG:HH12	33:z:156:LEU:HD11	1.79	0.48
33:z:554:TRP:HA	33:z:554:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:10:ASN:OD1	7:Y:10:ASN:N	2.45	0.48
7:Y:32:GLU:N	7:Y:32:GLU:OE2	2.47	0.48
8:Z:40:SER:OG	11:S:30:CYS:O	2.26	0.48
11:S:106:VAL:O	11:S:107:SER:OG	2.25	0.48
12:i:41:LEU:C	12:i:41:LEU:HD23	2.38	0.48
14:G:47:LEU:HD21	14:G:390:GLY:N	2.29	0.48
15:C:212:LYS:HE3	15:C:274:THR:HG23	1.95	0.48
15:C:251:TYR:HB3	18:B:108:TYR:CD2	2.48	0.48
16:T:86:GLN:HG3	17:F:160:PRO:HD3	1.95	0.48
17:F:18:TRP:HZ3	17:F:44:PHE:HB2	1.79	0.48
17:F:161:GLU:O	17:F:164:VAL:HB	2.14	0.48
21:R:114:ASP:OD1	21:R:115:TYR:N	2.38	0.48
23:E:163:GLY:H	24:D:161:LYS:HA	1.79	0.48
28:k:51:LEU:O	28:k:55:LYS:HG2	2.14	0.48
28:k:90:GLU:HB3	28:k:97:ILE:HD12	1.95	0.48
32:q:18:THR:CG2	32:q:22:LEU:HD11	2.43	0.48
32:q:137:CYS:SG	32:q:151:LEU:HB3	2.54	0.48
33:z:533:PHE:CD1	33:z:533:PHE:C	2.92	0.48
14:G:71:ASP:HB3	14:G:78:GLN:NE2	2.29	0.47
14:G:225:ARG:O	14:G:252:GLY:N	2.33	0.47
15:C:169:ASP:O	15:C:173:CYS:N	2.47	0.47
18:B:68:TYR:CZ	19:O:147:LYS:HG2	2.48	0.47
23:E:173:ARG:N	23:E:173:ARG:CD	2.77	0.47
33:z:380:PRO:HA	33:z:388:GLN:HB2	1.96	0.47
1:A:339:ALA:HB2	1:A:465:PHE:CZ	2.49	0.47
2:I:344:SER:HB3	2:I:412:TYR:HD1	1.78	0.47
3:J:86:ASN:OD1	3:J:86:ASN:N	2.47	0.47
8:Z:2:THR:C	8:Z:4:ALA:H	2.22	0.47
14:G:69:ARG:NH2	23:E:188:CYS:SG	2.81	0.47
15:C:228:ALA:HA	15:C:232:ALA:HB3	1.95	0.47
15:C:429:THR:HG23	15:C:548:ASN:O	2.14	0.47
16:T:216:ILE:HB	16:T:279:THR:HG22	1.96	0.47
22:U:100:ILE:HG22	24:D:103:LEU:HB2	1.96	0.47
25:X:22:ALA:O	25:X:26:VAL:HG23	2.14	0.47
27:Q:11:MET:HE1	27:Q:14:LEU:HB2	1.95	0.47
1:A:71:LEU:HD11	18:B:237:ASN:HD21	1.78	0.47
1:A:337:LEU:HD11	1:A:340:ILE:HD11	1.96	0.47
2:I:157:LEU:HA	2:I:160:TYR:CD2	2.49	0.47
3:J:71:PHE:O	3:J:75:VAL:HG23	2.14	0.47
4:N:173:ARG:HD2	4:N:178:LYS:HG2	1.97	0.47
5:H:150:SER:O	5:H:154:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:287:PHE:HB3	14:G:198:ILE:HD12	1.96	0.47
11:S:121:LEU:HD23	11:S:121:LEU:H	1.78	0.47
37:i:201:CDL:H1	37:i:201:CDL:OB5	2.14	0.47
14:G:96:LEU:HB3	14:G:283:PRO:HG2	1.97	0.47
16:T:58:LYS:HE3	16:T:66:VAL:HG21	1.95	0.47
16:T:99:PHE:CD1	16:T:106:PRO:HG3	2.49	0.47
17:F:26:GLU:CD	17:F:27:HIS:H	2.22	0.47
31:o:112:ASN:ND2	31:o:220:ILE:HG21	2.29	0.47
2:I:216:TYR:O	2:I:221:ALA:HB3	2.14	0.47
6:K:28:ILE:O	6:K:31:MET:HB2	2.15	0.47
10:W:25:GLY:O	10:W:29:PHE:N	2.48	0.47
14:G:247:PHE:CG	14:G:274:ILE:HD11	2.49	0.47
15:C:159:MET:O	15:C:159:MET:HG3	2.14	0.47
15:C:440:PHE:CD2	15:C:469:VAL:HG12	2.49	0.47
15:C:658:ARG:HD3	15:C:668:LEU:HD23	1.96	0.47
16:T:282:LEU:HD22	16:T:360:PHE:HE1	1.78	0.47
18:B:125:TYR:CE1	18:B:213:LEU:HD22	2.49	0.47
1:A:139:ASN:ND2	35:A:502:FMN:H1'1	2.28	0.47
2:I:125:PHE:HE1	2:I:162:ILE:HB	1.79	0.47
3:J:70:ILE:O	3:J:74:GLU:HG3	2.15	0.47
10:W:30:LEU:O	10:W:34:VAL:HB	2.15	0.47
12:i:39:MET:O	12:i:39:MET:SD	2.72	0.47
14:G:116:LEU:HD12	14:G:138:ARG:NH2	2.29	0.47
14:G:152:ARG:NH1	23:E:192:ALA:CB	2.70	0.47
15:C:113:ILE:HD11	19:O:138:LYS:HG3	1.96	0.47
32:q:184:ASN:HB3	32:q:185:PRO:HD3	1.96	0.47
32:p:6:ARG:HD2	32:p:6:ARG:HA	1.69	0.47
2:I:125:PHE:CD1	2:I:162:ILE:HG22	2.49	0.47
4:N:133:SER:OG	9:V:44:GLU:OE1	2.23	0.47
14:G:175:ILE:HG22	14:G:279:LEU:HD11	1.96	0.47
14:G:197:ARG:O	14:G:201:GLN:HB2	2.15	0.47
14:G:372:HIS:HB3	29:r:2:ALA:HB1	1.96	0.47
15:C:287:LEU:HB3	15:C:306:ASP:HB3	1.96	0.47
15:C:423:TYR:HA	15:C:428:ASN:HD21	1.79	0.47
24:D:111:HIS:HE1	34:D:301:SF4:S4	2.38	0.47
24:D:133:CYS:HA	34:D:301:SF4:S2	2.55	0.47
26:c:16:VAL:HG23	26:c:91:ASN:HD21	1.80	0.47
28:k:95:LEU:HD13	28:k:118:HIS:CG	2.50	0.47
28:k:114:TYR:O	28:k:118:HIS:ND1	2.46	0.47
32:q:62:ALA:O	32:q:65:ALA:N	2.37	0.47
1:A:273:VAL:O	1:A:277:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TYR:HB2	1:A:416:TRP:CD1	2.50	0.47
2:I:143:TYR:HE2	2:I:207:ASP:HB2	1.79	0.47
2:I:146:ILE:HD12	4:N:151:TRP:CZ3	2.50	0.47
4:N:67:PHE:HE1	5:H:122:ILE:HD13	1.79	0.47
14:G:321:SER:O	14:G:321:SER:OG	2.28	0.47
38:G:601:PEV:O1P	38:G:601:PEV:H52	2.14	0.47
15:C:125:GLU:HG3	15:C:126:LYS:HG3	1.95	0.47
15:C:431:ILE:HG13	15:C:634:GLU:HB3	1.96	0.47
15:C:582:TYR:CD1	15:C:601:VAL:HG13	2.49	0.47
15:C:639:GLN:OE1	15:C:690:THR:HG21	2.15	0.47
17:F:53:VAL:HG23	17:F:54:GLN:N	2.30	0.47
17:F:155:VAL:HG23	17:F:168:PRO:HG2	1.96	0.47
27:Q:64:TYR:HE2	27:Q:70:ARG:HG2	1.79	0.47
28:k:47:VAL:HG22	28:k:112:ILE:HG23	1.95	0.47
32:p:128:ILE:HG12	32:p:145:ILE:HD13	1.96	0.47
1:A:96:THR:OG1	1:A:171:GLY:O	2.33	0.47
1:A:267:ASN:OD1	1:A:268:VAL:N	2.48	0.47
6:K:79:ILE:HA	6:K:82:ILE:CG2	2.44	0.47
8:Z:12:MET:O	8:Z:14:SER:N	2.48	0.47
37:i:201:CDL:H512	37:i:201:CDL:CB3	2.34	0.47
14:G:356:ARG:HB2	17:F:58:ASP:OD2	2.15	0.47
15:C:292:THR:C	15:C:303:ILE:HG22	2.38	0.47
15:C:444:GLY:N	15:C:472:VAL:O	2.43	0.47
33:z:491:ALA:HB1	33:z:494:LYS:HE2	1.96	0.47
2:I:185:PHE:HZ	6:K:18:ILE:HG13	1.80	0.47
2:I:411:PHE:CD1	2:I:411:PHE:C	2.93	0.47
3:J:5:PHE:CD1	3:J:8:ILE:HD11	2.50	0.47
3:J:71:PHE:CE1	3:J:103:LEU:HD21	2.50	0.47
4:N:68:VAL:HG21	6:K:77:LEU:HD13	1.96	0.47
8:Z:134:ALA:HB2	13:j:50:GLU:HG2	1.97	0.47
14:G:152:ARG:HH12	23:E:192:ALA:HB2	1.77	0.47
14:G:312:HIS:HE1	24:D:171:ALA:O	1.98	0.47
15:C:178:GLU:CD	15:C:314:ARG:HH22	2.23	0.47
15:C:310:PRO:HA	15:C:645:PRO:HD2	1.97	0.47
16:T:251:THR:HG21	16:T:347:LEU:HD12	1.95	0.47
21:R:99:LEU:O	21:R:103:MET:HG2	2.15	0.47
22:U:51:LEU:HD11	22:U:60:LYS:HG2	1.96	0.47
32:q:9:TYR:C	32:q:11:VAL:H	2.22	0.47
32:p:86:ARG:HH22	32:p:88:ASP:H	1.61	0.47
33:z:245:MET:HE1	33:z:247:LEU:HB3	1.97	0.47
1:A:340:ILE:HG12	1:A:379:VAL:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:27:GLU:CD	5:H:200:ARG:HE	2.23	0.47
13:j:29:ARG:CA	33:z:121:VAL:CG2	2.65	0.47
14:G:62:GLN:O	14:G:65:PRO:HD2	2.15	0.47
14:G:254:ARG:HD3	29:r:9:ALA:HB1	1.97	0.47
15:C:328:ILE:CD1	15:C:333:ARG:HG2	2.45	0.47
22:U:49:ALA:HB2	22:U:64:LYS:HB2	1.96	0.47
32:q:164:ALA:HB3	32:q:167:ALA:HB2	1.97	0.47
32:p:84:VAL:HG12	32:p:86:ARG:HB2	1.97	0.47
14:G:239:TYR:HB3	21:R:131:PRO:CA	2.45	0.46
18:B:42:LYS:HG2	18:B:45:LEU:HG	1.97	0.46
21:R:126:ILE:O	21:R:126:ILE:HG13	2.15	0.46
1:A:234:ALA:HB2	1:A:246:PRO:HG3	1.98	0.46
1:A:480:GLU:OE1	8:Z:11:GLY:N	2.47	0.46
6:K:85:ARG:O	6:K:86:VAL:C	2.57	0.46
12:i:18:MET:O	12:i:20:SER:N	2.48	0.46
15:C:262:GLY:O	15:C:265:ILE:HD12	2.15	0.46
16:T:184:SER:O	16:T:219:PRO:HD2	2.15	0.46
24:D:92:VAL:HG23	24:D:92:VAL:O	2.16	0.46
33:z:136:GLU:CG	33:z:253:GLY:H	2.27	0.46
2:I:459:GLU:HG3	2:I:460:PRO:HD2	1.96	0.46
36:I:501:T7X:O13	36:I:501:T7X:O6	2.33	0.46
5:H:200:ARG:HD3	5:H:236:MET:SD	2.55	0.46
7:Y:12:ILE:O	7:Y:14:THR:N	2.47	0.46
7:Y:44:PRO:HD2	8:Z:129:ARG:CZ	2.45	0.46
13:j:5:TRP:CD1	13:j:5:TRP:H	2.33	0.46
15:C:343:ARG:HB3	15:C:647:VAL:HG21	1.97	0.46
15:C:455:ASN:ND2	15:C:479:ASN:OD1	2.44	0.46
16:T:119:VAL:HG11	22:U:140:LEU:HG	1.97	0.46
24:D:180:GLY:C	24:D:182:ASN:H	2.23	0.46
31:o:94:ASN:O	31:o:116:ARG:N	2.47	0.46
33:z:142:SER:O	33:z:146:LYS:N	2.45	0.46
4:N:173:ARG:HA	4:N:177:VAL:HG13	1.98	0.46
5:H:169:GLU:OE2	8:Z:71:ARG:NE	2.33	0.46
5:H:291:ARG:CG	5:H:291:ARG:O	2.62	0.46
6:K:21:ILE:HA	6:K:31:MET:SD	2.56	0.46
6:K:79:ILE:CA	6:K:82:ILE:HG22	2.44	0.46
14:G:155:ALA:O	14:G:157:PHE:N	2.49	0.46
14:G:367:ASP:O	14:G:371:LYS:HG3	2.15	0.46
16:T:253:PHE:CE2	16:T:255:PRO:HG3	2.51	0.46
23:E:188:CYS:SG	23:E:189:PRO:HD3	2.55	0.46
26:c:20:PRO:HD3	26:c:86:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:129:PRO:CD	33:z:170:ASN:HB3	2.45	0.46
37:i:201:CDL:H241	37:i:201:CDL:C76	2.46	0.46
14:G:121:HIS:HE1	14:G:203:LEU:HD21	1.81	0.46
15:C:108:HIS:HB3	15:C:111:LEU:HB2	1.97	0.46
16:T:253:PHE:HA	16:T:352:LEU:O	2.16	0.46
24:D:113:LEU:HD13	24:D:198:GLU:HG3	1.98	0.46
28:k:70:HIS:CD2	28:k:107:SER:HB2	2.51	0.46
1:A:192:LEU:HG	1:A:220:ILE:HD11	1.98	0.46
1:A:343:GLY:HA3	1:A:373:GLY:H	1.80	0.46
2:I:17:LEU:HD23	2:I:20:PHE:CE1	2.51	0.46
3:J:62:TYR:O	3:J:66:ILE:HG12	2.16	0.46
4:N:59:GLY:HA3	5:H:115:SER:HB3	1.97	0.46
13:j:59:LYS:O	13:j:63:ARG:N	2.43	0.46
14:G:74:SER:HB2	14:G:334:PRO:HG2	1.97	0.46
14:G:266:GLU:OE1	14:G:270:GLN:NE2	2.49	0.46
15:C:337:ASP:HB2	15:C:734:ILE:HD12	1.97	0.46
17:F:14:LEU:HD23	17:F:15:PRO:HD2	1.98	0.46
17:F:71:PHE:HE2	17:F:94:GLU:HA	1.80	0.46
24:D:134:PRO:HG2	24:D:163:ILE:HD11	1.98	0.46
27:Q:6:SER:HA	27:Q:9:LYS:HE2	1.98	0.46
33:z:136:GLU:HG2	33:z:253:GLY:H	1.81	0.46
1:A:228:ILE:HG21	1:A:401:SER:HA	1.98	0.46
1:A:401:SER:O	1:A:403:GLY:N	2.48	0.46
1:A:406:THR:H	15:C:117:CYS:HA	1.80	0.46
1:A:418:ILE:HG21	1:A:435:LEU:HD13	1.97	0.46
2:I:314:LYS:HD3	2:I:314:LYS:HA	1.77	0.46
2:I:345:LEU:CD2	2:I:349:ILE:HD11	2.45	0.46
5:H:16:LEU:HD23	5:H:86:LEU:HG	1.97	0.46
5:H:74:PHE:HB3	5:H:127:SER:HB3	1.97	0.46
6:K:41:ALA:O	6:K:45:ASN:HB2	2.15	0.46
7:Y:78:TYR:O	7:Y:82:MET:HG2	2.15	0.46
37:i:201:CDL:C51	37:i:201:CDL:CB3	2.90	0.46
15:C:381:VAL:HG11	15:C:575:LEU:H	1.81	0.46
22:U:68:THR:OG1	22:U:69:GLN:N	2.48	0.46
23:E:108:LEU:HA	23:E:108:LEU:HD23	1.71	0.46
23:E:155:MET:HG2	23:E:190:PRO:HG2	1.97	0.46
23:E:175:CYS:C	23:E:177:ARG:N	2.74	0.46
27:Q:4:ARG:CZ	27:Q:87:GLU:HB2	2.46	0.46
27:Q:91:LYS:HD2	27:Q:91:LYS:HA	1.70	0.46
1:A:392:ARG:NH1	18:B:168:GLU:OE2	2.48	0.46
15:C:331:LYS:O	15:C:335:CYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:386:GLN:NE2	15:C:588:ASP:OD1	2.49	0.46
18:B:51:GLU:C	18:B:53:ASN:H	2.23	0.46
32:p:47:ASN:HB3	32:p:68:ILE:HG23	1.97	0.46
32:p:104:SER:OG	32:p:105:LEU:N	2.49	0.46
1:A:354:ILE:HD12	1:A:368:VAL:HG22	1.97	0.46
2:I:114:PHE:CG	2:I:260:PRO:HG3	2.51	0.46
5:H:78:PRO:HB2	5:H:227:LEU:HD23	1.97	0.46
5:H:87:VAL:HG22	5:H:109:TYR:OH	2.16	0.46
5:H:162:VAL:HG12	5:H:163:GLY:N	2.31	0.46
10:W:30:LEU:HD23	10:W:34:VAL:HG21	1.98	0.46
12:i:19:TYR:O	12:i:19:TYR:CG	2.69	0.46
14:G:112:LEU:HD21	14:G:141:LEU:HB2	1.98	0.46
14:G:161:GLY:HA3	14:G:295:CYS:SG	2.56	0.46
15:C:514:ILE:HG22	15:C:542:VAL:HG11	1.98	0.46
16:T:254:GLN:HG2	16:T:287:VAL:HA	1.98	0.46
17:F:10:SER:OG	17:F:45:LEU:HD21	2.16	0.46
17:F:158:ASP:OD2	23:E:140:ARG:NE	2.48	0.46
32:q:92:VAL:HG22	32:q:108:VAL:CG2	2.46	0.46
33:z:322:TYR:CD1	33:z:322:TYR:C	2.94	0.46
33:z:489:TRP:HE3	33:z:508:ILE:CG2	2.28	0.46
1:A:396:PHE:CD1	18:B:170:GLU:HB3	2.51	0.46
1:A:421:ARG:NH1	1:A:431:GLU:OE1	2.49	0.46
2:I:70:ALA:HA	2:I:94:TYR:HE1	1.81	0.46
4:N:11:LEU:HD23	4:N:11:LEU:HA	1.76	0.46
5:H:186:VAL:HA	5:H:189:MET:HE3	1.98	0.46
11:S:78:ARG:HH22	15:C:186:MET:HE3	1.80	0.46
14:G:87:GLU:O	21:R:127:PRO:HG3	2.16	0.46
14:G:354:LYS:HD2	14:G:355:ILE:H	1.81	0.46
17:F:180:PHE:CZ	24:D:131:ALA:HB1	2.50	0.46
32:q:79:ILE:HG22	32:q:83:CYS:SG	2.55	0.46
32:p:90:ASN:ND2	32:p:117:VAL:O	2.49	0.46
2:I:39:PHE:CZ	26:c:60:PRO:HB2	2.50	0.45
2:I:136:MET:O	2:I:140:ILE:HG12	2.17	0.45
10:W:17:VAL:O	10:W:17:VAL:HG22	2.16	0.45
14:G:153:MET:HG2	23:E:97:GLU:OE2	2.15	0.45
14:G:341:PHE:CE2	14:G:343:VAL:HG23	2.51	0.45
15:C:192:ARG:CZ	15:C:192:ARG:HB2	2.46	0.45
15:C:242:ARG:NH2	18:B:115:SER:HB3	2.30	0.45
16:T:63:ARG:NH2	23:E:177:ARG:HD3	2.32	0.45
16:T:316:LYS:NZ	16:T:345:ASN:OD1	2.33	0.45
16:T:344:ILE:O	16:T:348:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:60:ILE:HG21	18:B:75:PRO:HB2	1.97	0.45
23:E:160:ASN:HB2	23:E:184:TYR:HD2	1.80	0.45
24:D:159:MET:O	24:D:162:CYS:HB3	2.16	0.45
31:o:212:GLU:HA	31:o:215:LYS:HD3	1.96	0.45
32:q:83:CYS:HB3	32:q:104:SER:H	1.81	0.45
1:A:235:LEU:HA	1:A:235:LEU:HD12	1.69	0.45
2:I:86:LEU:HD13	4:N:150:VAL:HG21	1.97	0.45
2:I:367:ARG:CG	2:I:461:MET:HE1	2.46	0.45
2:I:484:SER:N	2:I:485:PRO:HD2	2.32	0.45
6:K:10:SER:OG	6:K:41:ALA:O	2.34	0.45
8:Z:5:MET:HG3	15:C:196:THR:OG1	2.15	0.45
37:i:201:CDL:H761	37:i:201:CDL:H241	1.96	0.45
21:R:88:GLU:O	21:R:92:GLU:HG3	2.16	0.45
22:U:118:LEU:HB3	24:D:206:ARG:HG2	1.96	0.45
32:q:68:ILE:HG13	32:q:86:ARG:HG2	1.98	0.45
1:A:432:ILE:HD11	1:A:473:ILE:HD12	1.97	0.45
2:I:39:PHE:CG	26:c:57:ILE:HD13	2.51	0.45
5:H:71:PHE:HB2	5:H:75:ARG:CZ	2.46	0.45
7:Y:18:LEU:HD23	7:Y:18:LEU:HA	1.72	0.45
7:Y:103:CYS:HB2	7:Y:104:PRO:HD3	1.97	0.45
8:Z:127:SER:OG	8:Z:128:GLY:N	2.50	0.45
15:C:572:ALA:C	15:C:574:ALA:H	2.22	0.45
16:T:84:LEU:HD21	16:T:142:ILE:HD13	1.98	0.45
23:E:93:CYS:O	23:E:96:VAL:N	2.49	0.45
32:q:77:SER:OG	32:q:98:THR:O	2.26	0.45
14:G:44:ILE:HG22	14:G:45:GLY:N	2.31	0.45
15:C:171:PRO:HB3	24:D:173:PRO:HG3	1.97	0.45
19:O:82:LEU:HD13	25:X:132:TYR:CE1	2.51	0.45
33:z:236:PRO:HB3	33:z:497:ILE:HG13	1.99	0.45
33:z:490:THR:HG22	33:z:511:TRP:HE1	1.81	0.45
12:i:9:GLY:HA3	12:i:43:ALA:HB2	1.97	0.45
15:C:361:TRP:CZ2	15:C:619:PRO:HD2	2.51	0.45
15:C:556:TYR:HB2	15:C:559:GLN:HB2	1.98	0.45
16:T:253:PHE:O	16:T:255:PRO:HD3	2.16	0.45
23:E:155:MET:HA	23:E:185:VAL:HB	1.99	0.45
23:E:155:MET:HE3	23:E:195:LEU:HB2	1.98	0.45
23:E:175:CYS:C	23:E:177:ARG:H	2.23	0.45
32:q:107:HIS:CE1	42:q:802:BCT:O2	2.44	0.45
2:I:332:ILE:HG22	2:I:425:LEU:CD2	2.36	0.45
3:J:66:ILE:HG21	4:N:166:ALA:HB2	1.97	0.45
5:H:101:SER:O	5:H:101:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:141:LEU:HD21	14:G:178:PHE:CE2	2.52	0.45
15:C:329:SER:HB3	15:C:452:ALA:HB3	1.98	0.45
15:C:413:THR:HB	15:C:417:VAL:HG21	1.98	0.45
15:C:632:ASN:HD21	15:C:634:GLU:HG2	1.82	0.45
18:B:130:CYS:SG	18:B:131:GLY:N	2.89	0.45
24:D:123:CYS:SG	24:D:152:THR:HG21	2.57	0.45
25:X:33:ALA:O	25:X:37:ILE:HG13	2.17	0.45
27:Q:62:ALA:HB2	27:Q:89:LEU:HD13	1.98	0.45
28:k:107:SER:HB3	28:k:110:LEU:HD12	1.98	0.45
32:q:105:LEU:C	32:q:107:HIS:N	2.75	0.45
33:z:122:GLN:OE1	33:z:172:ALA:CA	2.63	0.45
3:J:18:VAL:HG11	5:H:13:ILE:HG21	1.98	0.45
7:Y:37:LEU:HD23	7:Y:37:LEU:HA	1.81	0.45
7:Y:82:MET:HE3	7:Y:87:ASN:HA	1.98	0.45
21:R:28:ASN:O	21:R:28:ASN:ND2	2.50	0.45
21:R:127:PRO:HB2	21:R:129:HIS:CE1	2.52	0.45
31:o:55:GLN:H	32:p:40:SER:HB2	1.82	0.45
31:o:120:HIS:CG	31:o:121:ALA:N	2.84	0.45
32:q:16:ARG:HD3	32:q:16:ARG:HA	1.53	0.45
32:p:48:VAL:HG12	32:p:49:PHE:N	2.32	0.45
2:I:195:SER:HA	6:K:46:PHE:CZ	2.52	0.45
3:J:81:TRP:CZ3	5:H:160:ILE:HD11	2.52	0.45
4:N:37:THR:HG21	6:K:40:LEU:HD11	1.98	0.45
5:H:151:ILE:O	5:H:155:LEU:HG	2.17	0.45
5:H:182:PRO:HB2	8:Z:61:MET:HE2	1.98	0.45
14:G:38:GLU:O	14:G:371:LYS:NZ	2.42	0.45
14:G:113:ASN:HD21	14:G:335:LYS:CE	2.29	0.45
16:T:220:ALA:O	16:T:221:THR:C	2.59	0.45
16:T:379:ILE:HG23	16:T:382:ARG:HD2	1.97	0.45
22:U:138:HIS:C	22:U:140:LEU:H	2.25	0.45
31:o:120:HIS:CD2	31:o:121:ALA:H	2.34	0.45
32:p:80:TRP:HZ3	32:p:214:HIS:CE1	2.35	0.45
32:p:111:SER:OG	32:p:112:ASN:N	2.50	0.45
33:z:346:ASP:HB2	33:z:352:THR:HG21	1.97	0.45
33:z:392:PHE:O	33:z:392:PHE:CD1	2.70	0.45
5:H:98:MET:HG2	9:V:27:TYR:HB2	1.99	0.45
7:Y:51:ASP:OD1	7:Y:51:ASP:N	2.49	0.45
16:T:69:ILE:HD12	16:T:91:MET:HE1	1.99	0.45
22:U:72:ARG:HD2	24:D:93:THR:O	2.17	0.45
25:X:78:LEU:HD23	25:X:78:LEU:HA	1.85	0.45
32:q:116:LYS:HB2	32:q:118:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:p:193:THR:OG1	32:p:196:GLU:HG3	2.16	0.45
32:p:216:ALA:O	32:p:218:ASN:N	2.50	0.45
1:A:91:LEU:HD11	1:A:279:ARG:HG2	1.99	0.45
1:A:307:LYS:HB2	1:A:327:CYS:O	2.17	0.45
2:I:345:LEU:CD2	2:I:349:ILE:CD1	2.94	0.45
4:N:34:PHE:CD2	4:N:57:TYR:HB3	2.51	0.45
5:H:291:ARG:C	5:H:293:ASP:H	2.25	0.45
7:Y:68:HIS:HA	7:Y:75:MET:HE2	1.99	0.45
14:G:146:GLU:OE1	24:D:104:SER:N	2.50	0.45
31:o:112:ASN:HD22	31:o:114:GLN:HG2	1.81	0.45
31:o:158:ILE:HG22	31:o:162:SER:OG	2.17	0.45
32:q:120:THR:HG23	32:q:137:CYS:O	2.17	0.45
33:z:390:LEU:HD23	33:z:390:LEU:O	2.17	0.45
35:A:502:FMN:C9	35:A:502:FMN:O2'	2.66	0.44
2:I:80:HIS:HD2	2:I:84:ASN:HB2	1.82	0.44
2:I:241:ILE:HA	2:I:270:LYS:HD2	1.99	0.44
2:I:354:LEU:HD23	2:I:475:PHE:HE2	1.81	0.44
5:H:202:PRO:O	5:H:289:ARG:HA	2.16	0.44
38:G:601:PEV:O3	38:G:601:PEV:C31	2.65	0.44
15:C:431:ILE:HG22	15:C:457:ARG:HG3	1.98	0.44
19:O:52:ARG:HD3	19:O:78:PHE:HB3	1.98	0.44
23:E:91:LEU:O	23:E:129:GLY:HA3	2.17	0.44
24:D:163:ILE:HG12	34:D:301:SF4:S3	2.56	0.44
32:q:45:LEU:HD13	32:q:63:PRO:HA	1.98	0.44
32:p:100:ILE:HG22	32:p:104:SER:HB3	1.99	0.44
2:I:369:THR:HB	2:I:372:LYS:HD2	1.99	0.44
14:G:209:VAL:HG12	14:G:368:PHE:HE1	1.82	0.44
15:C:63:ALA:HB1	19:O:135:LEU:HG	2.00	0.44
15:C:95:CYS:SG	15:C:102:ILE:HD11	2.58	0.44
15:C:311:GLU:OE1	22:U:149:ARG:NH2	2.41	0.44
17:F:153:VAL:O	17:F:153:VAL:HG23	2.16	0.44
17:F:177:TYR:CG	19:O:104:SER:HB2	2.52	0.44
26:c:43:ILE:HG13	30:n:92:ALA:HB1	1.99	0.44
31:o:79:VAL:HB	31:o:97:VAL:HG13	1.98	0.44
1:A:143:SER:HB3	1:A:227:TYR:HA	1.99	0.44
1:A:407:PRO:HA	15:C:161:PHE:CD2	2.52	0.44
4:N:47:ASP:N	4:N:47:ASP:OD1	2.50	0.44
7:Y:43:ASP:HB2	8:Z:129:ARG:NH2	2.29	0.44
14:G:64:LEU:HD22	14:G:159:ARG:HD3	1.99	0.44
14:G:182:PHE:CE2	14:G:186:ILE:HD11	2.51	0.44
15:C:721:ASN:O	15:C:722:PHE:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:288:PHE:CE2	16:T:370:LEU:HD12	2.53	0.44
17:F:114:GLU:HG3	17:F:133:LEU:HD12	1.98	0.44
18:B:135:CYS:HB3	18:B:140:SER:CB	2.47	0.44
22:U:101:THR:OG1	22:U:102:ASP:N	2.51	0.44
32:p:99:ASN:HB2	32:p:127:THR:HA	1.99	0.44
33:z:508:ILE:HG22	33:z:509:PHE:N	2.32	0.44
2:I:59:LEU:O	2:I:63:LEU:HG	2.17	0.44
2:I:73:ALA:HB3	2:I:74:PRO:HD3	2.00	0.44
2:I:249:TRP:HZ2	6:K:25:ARG:HD3	1.81	0.44
4:N:124:TYR:HB2	8:Z:97:PHE:CD1	2.52	0.44
4:N:180:GLN:HG3	4:N:181:ASP:H	1.81	0.44
5:H:8:GLU:HB3	9:V:29:ILE:HG21	2.00	0.44
5:H:34:VAL:CG1	24:D:83:THR:HG23	2.48	0.44
14:G:202:ARG:O	14:G:203:LEU:HD12	2.17	0.44
14:G:237:ALA:CB	21:R:133:HIS:HA	2.48	0.44
16:T:90:LYS:HE2	16:T:90:LYS:HB3	1.90	0.44
17:F:41:LEU:HD12	17:F:41:LEU:C	2.41	0.44
23:E:86:PRO:CD	23:E:113:ILE:HG23	2.48	0.44
24:D:197:LYS:H	24:D:197:LYS:HG3	1.60	0.44
26:c:20:PRO:HB2	26:c:25:VAL:HB	2.00	0.44
32:q:137:CYS:HB2	32:q:155:VAL:O	2.16	0.44
32:q:220:LYS:O	32:q:224:VAL:HG23	2.18	0.44
33:z:122:GLN:CG	33:z:172:ALA:HB3	2.31	0.44
33:z:526:ARG:NH2	33:z:526:ARG:HG2	2.33	0.44
2:I:110:MET:HE3	2:I:110:MET:HB2	1.82	0.44
2:I:117:GLN:NE2	2:I:117:GLN:HA	2.33	0.44
2:I:186:SER:HB3	2:I:239:PHE:CB	2.48	0.44
4:N:190:PHE:HB2	4:N:194:ILE:H	1.82	0.44
14:G:71:ASP:HB3	14:G:78:GLN:CD	2.43	0.44
15:C:361:TRP:CZ3	15:C:618:LEU:HD22	2.52	0.44
18:B:181:ILE:HG23	18:B:198:PHE:HB2	1.99	0.44
30:n:84:TYR:HD1	30:n:84:TYR:N	2.16	0.44
31:o:112:ASN:HD22	31:o:114:GLN:HE21	1.66	0.44
33:z:505:GLU:CD	33:z:505:GLU:N	2.76	0.44
33:z:526:ARG:HG2	33:z:526:ARG:HH21	1.82	0.44
1:A:142:GLU:OE1	1:A:147:THR:HG22	2.17	0.44
1:A:345:SER:OG	1:A:393:LEU:HD22	2.18	0.44
2:I:333:GLY:HA3	2:I:345:LEU:HB2	2.00	0.44
3:J:88:ILE:HB	3:J:92:GLY:HA3	1.99	0.44
4:N:127:TYR:HE1	9:V:48:ALA:HB1	1.82	0.44
6:K:56:MET:SD	6:K:59:GLN:HB2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:23:ASP:O	14:G:97:ARG:NH1	2.48	0.44
11:S:91:LYS:O	11:S:95:VAL:HG22	2.17	0.44
14:G:119:THR:HA	14:G:122:ALA:HB3	1.98	0.44
15:C:208:GLY:HA2	15:C:255:LEU:HG	1.98	0.44
15:C:328:ILE:HB	15:C:332:THR:OG1	2.17	0.44
15:C:520:LEU:HD22	15:C:715:PHE:HE1	1.82	0.44
16:T:243:LEU:HB2	16:T:298:TYR:OH	2.17	0.44
32:p:82:GLY:HA3	32:p:103:ASN:OD1	2.18	0.44
1:A:68:LEU:HD11	1:A:298:LEU:HD11	1.99	0.44
1:A:307:LYS:HB3	18:B:233:PRO:O	2.17	0.44
3:J:70:ILE:HG21	4:N:163:MET:HG3	1.98	0.44
4:N:29:PHE:HA	4:N:32:LEU:HB2	2.00	0.44
5:H:28:ARG:NE	23:E:114:ILE:HD11	2.33	0.44
5:H:287:PHE:CZ	24:D:76:MET:HB3	2.52	0.44
5:H:300:TRP:O	5:H:305:PRO:HD3	2.18	0.44
23:E:184:TYR:CD1	23:E:184:TYR:N	2.86	0.44
28:k:66:THR:O	28:k:69:VAL:HG12	2.18	0.44
31:o:127:THR:OG1	31:o:128:GLY:N	2.51	0.44
31:o:244:PHE:O	31:o:247:SER:OG	2.25	0.44
32:q:78:SER:HB2	32:q:211:ALA:CB	2.48	0.44
32:p:78:SER:O	32:p:100:ILE:HG12	2.17	0.44
33:z:325:TYR:CG	33:z:325:TYR:O	2.70	0.44
33:z:542:LYS:HE3	33:z:568:ALA:HB1	1.98	0.44
33:z:574:ARG:HA	33:z:579:VAL:HG22	2.00	0.44
2:I:380:LEU:HG	2:I:458:TYR:CE1	2.53	0.44
7:Y:15:SER:OG	9:V:53:ASP:OD2	2.28	0.44
7:Y:17:VAL:HG23	7:Y:79:VAL:HG11	1.98	0.44
14:G:32:MET:HE2	14:G:32:MET:HB3	1.86	0.44
14:G:45:GLY:HA2	14:G:48:HIS:HB2	2.00	0.44
14:G:121:HIS:CD2	14:G:383:GLY:HA3	2.53	0.44
14:G:200:LYS:O	14:G:204:VAL:HG23	2.17	0.44
15:C:394:MET:SD	15:C:683:VAL:HG11	2.57	0.44
15:C:443:ILE:O	15:C:445:THR:OG1	2.34	0.44
17:F:118:MET:SD	17:F:143:LEU:HD13	2.57	0.44
20:P:41:THR:HG21	20:P:52:SER:HB2	1.99	0.44
20:P:70:VAL:O	20:P:86:PHE:HA	2.18	0.44
32:q:46:MET:HG3	32:p:220:LYS:HZ3	1.82	0.44
33:z:473:LEU:HD12	33:z:473:LEU:HA	1.72	0.44
1:A:145:PRO:HB3	18:B:132:THR:HG21	1.99	0.44
1:A:156:HIS:O	1:A:157:ASP:HB3	2.18	0.44
1:A:232:GLU:HG3	1:A:265:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HD2	1:A:354:ILE:HG12	2.00	0.44
11:S:121:LEU:HG	11:S:122:ASP:H	1.83	0.44
15:C:345:SER:HB2	15:C:648:GLY:HA3	2.00	0.44
15:C:573:LYS:HE2	15:C:573:LYS:HB2	1.78	0.44
17:F:46:LYS:C	17:F:47:LEU:HG	2.43	0.44
18:B:164:PHE:HE2	18:B:214:ARG:HB3	1.83	0.44
23:E:186:PRO:HG3	24:D:185:PHE:C	2.42	0.44
24:D:75:GLU:HA	24:D:75:GLU:OE1	2.17	0.44
28:k:78:ASP:O	28:k:82:THR:HG23	2.18	0.44
33:z:319:LYS:CD	33:z:488:ARG:HD3	2.47	0.44
1:A:146:GLY:C	1:A:376:ALA:HB1	2.42	0.43
4:N:64:LEU:O	4:N:68:VAL:HG23	2.17	0.43
5:H:33:PHE:CD1	9:V:8:ALA:HB2	2.53	0.43
6:K:59:GLN:NE2	13:j:7:ILE:HG23	2.24	0.43
8:Z:125:TYR:HB3	8:Z:127:SER:O	2.18	0.43
11:S:112:VAL:HG22	17:F:82:TYR:CE1	2.53	0.43
12:i:10:ALA:O	12:i:36:VAL:HB	2.18	0.43
13:j:30:GLU:HG3	13:j:33:ASP:H	1.82	0.43
15:C:438:ASP:N	15:C:511:ASN:O	2.31	0.43
15:C:572:ALA:O	15:C:573:LYS:HB2	2.18	0.43
15:C:584:MET:HG3	15:C:603:GLN:OE1	2.18	0.43
15:C:649:ASP:OD1	15:C:651:ARG:NH1	2.31	0.43
17:F:177:TYR:CD1	19:O:104:SER:HB2	2.53	0.43
18:B:32:LEU:HD22	20:P:90:ASP:HB3	2.00	0.43
21:R:86:VAL:HA	21:R:89:LEU:HB2	2.01	0.43
26:c:57:ILE:HG22	26:c:61:SER:H	1.81	0.43
28:k:69:VAL:HG23	28:k:74:ASP:OD2	2.18	0.43
33:z:140:LYS:O	33:z:140:LYS:HD2	2.18	0.43
2:I:72:GLY:O	2:I:76:LEU:N	2.51	0.43
2:I:255:GLU:HA	2:I:316:LYS:HD2	2.00	0.43
3:J:113:ARG:CD	4:N:176:LYS:HE3	2.48	0.43
5:H:161:CYS:SG	5:H:314:VAL:HG11	2.58	0.43
7:Y:72:GLN:O	7:Y:76:ASP:N	2.45	0.43
8:Z:47:MET:O	8:Z:48:ALA:HB3	2.18	0.43
14:G:54:LEU:HD11	23:E:168:SER:HB2	1.99	0.43
15:C:74:ILE:HD12	15:C:87:LYS:HA	2.00	0.43
15:C:413:THR:HG21	15:C:563:LEU:HD21	2.00	0.43
15:C:698:PHE:HE2	27:Q:18:LEU:HD21	1.82	0.43
16:T:212:PRO:C	16:T:213:GLU:HG3	2.43	0.43
16:T:251:THR:O	16:T:289:THR:OG1	2.36	0.43
17:F:171:MET:HG2	19:O:95:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:65:LEU:HD23	22:U:65:LEU:H	1.84	0.43
23:E:186:PRO:HB2	24:D:185:PHE:CE2	2.53	0.43
23:E:209:ARG:NH1	23:E:211:ASP:OD2	2.43	0.43
31:o:51:ASP:HB3	32:p:227:PHE:CE2	2.54	0.43
32:q:83:CYS:HB2	32:q:104:SER:HB2	2.00	0.43
2:I:26:ILE:HD13	4:N:157:LEU:HD11	2.00	0.43
4:N:190:PHE:O	4:N:191:ARG:HG2	2.19	0.43
5:H:23:LEU:HD12	5:H:277:LEU:HD13	2.01	0.43
5:H:175:LYS:HD2	5:H:252:LEU:HD22	2.01	0.43
14:G:324:ALA:HA	14:G:344:SER:O	2.18	0.43
15:C:209:PRO:HD3	15:C:255:LEU:HD23	2.00	0.43
15:C:212:LYS:HZ2	15:C:274:THR:HG22	1.83	0.43
16:T:252:LYS:H	16:T:350:ASP:CB	2.31	0.43
17:F:66:SER:HB3	19:O:108:PHE:HA	2.00	0.43
19:O:74:TRP:CH2	19:O:130:PRO:HD3	2.53	0.43
21:R:57:VAL:HA	21:R:60:PHE:CE2	2.54	0.43
23:E:108:LEU:HD13	23:E:113:ILE:HG21	2.00	0.43
31:o:68:VAL:HA	31:o:86:VAL:HG22	2.00	0.43
31:o:194:TRP:CZ2	31:o:201:PHE:HB2	2.53	0.43
32:q:43:ARG:NH2	32:p:214:HIS:O	2.51	0.43
1:A:212:SER:OG	1:A:213:GLY:N	2.51	0.43
36:I:501:T7X:O16	36:I:501:T7X:P1	2.76	0.43
3:J:113:ARG:HG2	4:N:167:ILE:CG2	2.48	0.43
5:H:95:ASP:HB3	5:H:98:MET:SD	2.59	0.43
6:K:34:SER:O	6:K:38:MET:HG2	2.19	0.43
11:S:43:THR:HG22	22:U:69:GLN:N	2.33	0.43
14:G:321:SER:HA	14:G:348:ASN:HA	1.99	0.43
15:C:278:PHE:CZ	15:C:282:ALA:HB3	2.53	0.43
15:C:281:LYS:O	15:C:308:ARG:NH1	2.50	0.43
15:C:396:LEU:O	15:C:400:VAL:HG22	2.18	0.43
16:T:335:SER:O	16:T:335:SER:OG	2.31	0.43
23:E:135:MET:HG3	23:E:135:MET:O	2.18	0.43
31:o:230:GLU:HB3	32:q:36:ARG:NH1	2.33	0.43
32:q:104:SER:C	32:q:105:LEU:HD22	2.44	0.43
33:z:109:LEU:HD23	33:z:109:LEU:H	1.83	0.43
33:z:127:ASN:O	33:z:128:GLN:HB3	2.17	0.43
33:z:240:GLU:HA	33:z:240:GLU:OE2	2.18	0.43
1:A:204:LEU:O	1:A:210:CYS:N	2.47	0.43
1:A:348:PRO:HB3	1:A:460:GLY:HA3	2.00	0.43
1:A:406:THR:HG21	15:C:162:LEU:HG	2.00	0.43
12:i:31:HIS:NE2	37:i:201:CDL:H611	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:91:VAL:HG23	15:C:136:MET:O	2.19	0.43
15:C:111:LEU:HD12	15:C:223:ARG:HG2	2.00	0.43
15:C:170:CYS:HB2	15:C:171:PRO:HD3	2.00	0.43
16:T:60:THR:HG23	16:T:61:GLY:N	2.33	0.43
16:T:218:ARG:HB2	16:T:281:GLU:HA	2.01	0.43
20:P:96:ILE:HG22	20:P:103:ARG:HG2	1.99	0.43
23:E:155:MET:SD	23:E:195:LEU:HD22	2.59	0.43
24:D:73:LEU:H	24:D:73:LEU:CD1	2.30	0.43
28:k:99:ASP:N	28:k:99:ASP:OD1	2.49	0.43
31:o:139:VAL:HG13	31:o:156:CYS:HB2	2.01	0.43
32:q:51:LYS:HD2	32:q:70:ASP:HB2	2.00	0.43
33:z:141:GLU:O	33:z:145:LYS:N	2.51	0.43
33:z:304:ILE:HD12	33:z:304:ILE:HA	1.76	0.43
33:z:456:LEU:O	33:z:459:PRO:HD2	2.18	0.43
1:A:231:GLU:OE2	1:A:231:GLU:CA	2.67	0.43
2:I:348:GLY:HA2	2:I:409:SER:OG	2.18	0.43
5:H:175:LYS:HE2	5:H:175:LYS:HB3	1.76	0.43
5:H:287:PHE:CE2	38:G:601:PEV:H372	2.53	0.43
15:C:582:TYR:HA	15:C:601:VAL:HG13	1.99	0.43
15:C:721:ASN:C	15:C:723:TYR:H	2.27	0.43
15:C:723:TYR:O	15:C:735:MET:HB3	2.19	0.43
17:F:14:LEU:HD21	17:F:41:LEU:HD13	2.01	0.43
18:B:160:LYS:HE2	18:B:160:LYS:HB2	1.81	0.43
24:D:114:ARG:HB3	24:D:122:ARG:HD2	2.00	0.43
24:D:146:GLU:H	24:D:146:GLU:CD	2.26	0.43
33:z:316:LYS:HA	33:z:316:LYS:HD3	1.81	0.43
1:A:120:LEU:O	1:A:123:SER:OG	2.35	0.43
5:H:45:SER:O	22:U:40:LEU:HD23	2.18	0.43
37:i:201:CDL:H372	37:i:201:CDL:C15	2.48	0.43
14:G:84:LEU:HD22	21:R:129:HIS:O	2.18	0.43
14:G:132:LEU:HD23	14:G:132:LEU:HA	1.80	0.43
14:G:169:LEU:HD23	14:G:169:LEU:HA	1.76	0.43
14:G:364:GLN:CD	17:F:110:TRP:HB2	2.43	0.43
15:C:176:GLY:O	15:C:182:GLN:NE2	2.51	0.43
15:C:252:VAL:HG11	18:B:90:VAL:HG11	2.00	0.43
15:C:448:ARG:HE	15:C:479:ASN:HD21	1.67	0.43
17:F:56:LEU:HD21	17:F:59:ILE:HG13	1.99	0.43
18:B:180:MET:HA	18:B:199:GLU:HA	2.00	0.43
19:O:146:TRP:CZ2	19:O:148:GLY:HA2	2.54	0.43
24:D:47:GLU:HG2	24:D:48:GLU:N	2.33	0.43
28:k:54:VAL:O	28:k:60:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:42:HIS:CG	32:q:42:HIS:O	2.72	0.43
32:p:87:GLY:HA3	32:p:92:VAL:CG2	2.49	0.43
32:p:203:SER:HB2	32:p:207:TYR:CZ	2.54	0.43
1:A:305:VAL:HG11	1:A:327:CYS:SG	2.58	0.43
2:I:380:LEU:CD2	2:I:380:LEU:O	2.66	0.43
7:Y:49:CYS:HB2	7:Y:52:LYS:HB2	1.99	0.43
12:i:53:ASP:O	12:i:57:LYS:N	2.45	0.43
14:G:89:LEU:HD22	14:G:325:SER:HB2	2.01	0.43
15:C:251:TYR:HE2	18:B:90:VAL:HG22	1.83	0.43
16:T:194:SER:HB3	16:T:342:ASP:O	2.19	0.43
16:T:275:SER:OG	16:T:280:TYR:OH	2.22	0.43
24:D:50:GLU:O	24:D:54:LYS:HG2	2.18	0.43
25:X:98:HIS:O	25:X:102:GLN:N	2.41	0.43
32:p:102:ASP:HB3	32:p:103:ASN:H	1.65	0.43
1:A:246:PRO:HD2	34:A:501:SF4:S2	2.58	0.43
5:H:29:LYS:HD2	9:V:11:PRO:HG2	1.99	0.43
5:H:241:GLY:HA2	5:H:244:THR:HG22	2.01	0.43
8:Z:85:ILE:HD11	9:V:45:TRP:HZ2	1.84	0.43
14:G:30:LEU:HD11	14:G:378:VAL:HG11	2.01	0.43
15:C:222:THR:HG22	15:C:226:ARG:HG3	2.01	0.43
15:C:400:VAL:O	15:C:405:SER:OG	2.27	0.43
24:D:77:VAL:O	24:D:77:VAL:CG1	2.66	0.43
25:X:77:LEU:HD12	25:X:77:LEU:HA	1.91	0.43
26:c:89:PHE:HB3	26:c:90:PRO:HD2	2.00	0.43
27:Q:46:LEU:HD23	27:Q:48:ILE:HG12	2.00	0.43
28:k:110:LEU:HA	28:k:113:GLU:CG	2.48	0.43
31:o:194:TRP:NE1	31:o:201:PHE:HD1	2.16	0.43
1:A:258:LEU:H	1:A:263:THR:HG21	1.84	0.43
2:I:451:THR:N	2:I:452:PRO:HD3	2.34	0.43
4:N:51:MET:HE3	5:H:109:TYR:HB2	2.01	0.43
6:K:79:ILE:C	6:K:82:ILE:HG22	2.44	0.43
14:G:118:LEU:HD23	14:G:118:LEU:HA	1.82	0.43
15:C:196:THR:O	15:C:196:THR:HG23	2.19	0.43
15:C:213:THR:HB	15:C:215:MET:SD	2.59	0.43
18:B:170:GLU:O	18:B:171:CYS:C	2.62	0.43
22:U:126:GLY:H	22:U:132:ILE:HD12	1.83	0.43
31:o:132:ALA:O	31:o:134:ILE:HG12	2.18	0.43
32:q:42:HIS:HB2	32:p:63:PRO:HB2	2.01	0.43
32:p:32:LYS:HD2	32:p:34:TYR:CE2	2.54	0.43
1:A:241:GLY:HA3	18:B:70:GLN:HG2	2.01	0.42
1:A:410:GLU:HB2	15:C:161:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:LEU:HA	2:I:123:PHE:HE1	1.83	0.42
2:I:125:PHE:CE1	2:I:162:ILE:CB	3.02	0.42
2:I:346:LEU:HD13	2:I:493:MET:HB2	2.01	0.42
7:Y:20:ALA:HB2	7:Y:82:MET:HG3	2.01	0.42
14:G:65:PRO:HB2	23:E:164:TYR:CE2	2.54	0.42
14:G:96:LEU:HD23	14:G:96:LEU:HA	1.90	0.42
16:T:111:LEU:HD11	17:F:158:ASP:HB3	2.01	0.42
21:R:37:TYR:HB2	21:R:65:LEU:HD13	2.01	0.42
23:E:83:SER:O	23:E:83:SER:OG	2.35	0.42
24:D:110:GLU:HB3	24:D:182:ASN:HB3	2.01	0.42
25:X:25:ARG:HD2	25:X:76:ASP:OD1	2.18	0.42
31:o:175:ILE:O	31:o:193:LEU:HA	2.19	0.42
32:q:184:ASN:HD22	32:p:184:ASN:H	1.66	0.42
2:I:48:PRO:HB2	26:c:55:PRO:HB2	2.01	0.42
2:I:422:ALA:HB1	2:I:425:LEU:HB3	2.01	0.42
5:H:22:PHE:HD1	5:H:51:PRO:HG2	1.83	0.42
7:Y:75:MET:O	7:Y:79:VAL:HG22	2.20	0.42
8:Z:72:ARG:O	8:Z:76:GLU:HG2	2.20	0.42
11:S:104:PHE:O	21:R:59:SER:OG	2.32	0.42
37:i:201:CDL:H132	37:i:201:CDL:OA7	2.18	0.42
15:C:220:GLN:HG2	15:C:246:GLU:HB3	2.01	0.42
17:F:19:VAL:O	17:F:19:VAL:HG22	2.19	0.42
17:F:138:PHE:HE2	17:F:142:PRO:HD3	1.84	0.42
22:U:98:HIS:NE2	24:D:100:LYS:HD2	2.35	0.42
24:D:141:GLU:HB2	24:D:154:ARG:HB2	2.01	0.42
1:A:103:MET:HE2	1:A:122:TRP:CH2	2.55	0.42
1:A:145:PRO:HB2	1:A:345:SER:HB2	2.00	0.42
1:A:407:PRO:HG3	15:C:158:VAL:HG22	2.01	0.42
2:I:259:THR:N	2:I:260:PRO:HD2	2.34	0.42
2:I:459:GLU:HG3	2:I:460:PRO:CD	2.49	0.42
3:J:96:MET:SD	4:N:152:PHE:HZ	2.42	0.42
5:H:321:PHE:O	5:H:323:TRP:N	2.53	0.42
11:S:72:TYR:OH	14:G:291:ASP:OD1	2.27	0.42
16:T:84:LEU:HD21	16:T:142:ILE:HG21	2.01	0.42
16:T:305:PRO:HB3	16:T:307:TYR:CE2	2.54	0.42
17:F:18:TRP:CD1	17:F:37:TYR:HB3	2.54	0.42
21:R:90:ILE:HG22	21:R:94:ARG:HH22	1.84	0.42
24:D:55:GLU:O	24:D:58:LYS:HG2	2.19	0.42
26:c:57:ILE:O	26:c:61:SER:HB3	2.19	0.42
27:Q:89:LEU:HD23	27:Q:89:LEU:HA	1.87	0.42
31:o:234:TYR:CD1	32:p:24:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:q:86:ARG:NH2	32:p:101:GLN:O	2.53	0.42
1:A:245:LYS:HD3	1:A:404:GLN:HB2	2.00	0.42
2:I:354:LEU:HD11	2:I:472:THR:HG23	1.97	0.42
2:I:361:ALA:CB	2:I:468:LEU:HD23	2.46	0.42
5:H:89:TRP:CZ2	5:H:237:ILE:HG22	2.55	0.42
5:H:178:TRP:O	5:H:182:PRO:HD2	2.18	0.42
13:j:41:TYR:CZ	13:j:45:LEU:HD11	2.54	0.42
14:G:306:MET:O	14:G:306:MET:SD	2.77	0.42
15:C:603:GLN:NE2	15:C:653:ASP:HA	2.34	0.42
15:C:658:ARG:O	15:C:661:SER:OG	2.23	0.42
17:F:59:ILE:HB	17:F:111:TRP:HB3	2.01	0.42
18:B:134:PRO:HB2	39:B:301:FES:S2	2.59	0.42
23:E:193:GLU:HG2	23:E:193:GLU:H	1.47	0.42
31:o:197:ASN:HB2	31:o:198:PRO:HD3	2.01	0.42
33:z:273:LEU:HD21	33:z:554:TRP:HB3	2.00	0.42
33:z:293:VAL:HG21	33:z:427:TYR:HB2	2.02	0.42
33:z:470:LEU:O	33:z:474:ILE:HG13	2.19	0.42
1:A:102:GLU:OE1	1:A:282:PRO:HG2	2.20	0.42
1:A:145:PRO:HD2	1:A:345:SER:CB	2.49	0.42
1:A:209:ALA:N	1:A:214:TYR:O	2.52	0.42
1:A:228:ILE:CG2	1:A:400:GLU:O	2.67	0.42
2:I:153:GLU:HA	2:I:153:GLU:OE2	2.19	0.42
5:H:304:LEU:HB3	5:H:305:PRO:HD3	2.01	0.42
11:S:32:HIS:CD2	11:S:36:LEU:HD22	2.53	0.42
14:G:147:ARG:HG2	14:G:168:PRO:HG3	2.01	0.42
14:G:210:THR:HG1	21:R:22:GLY:HA3	1.85	0.42
14:G:223:MET:SD	14:G:385:GLN:HA	2.60	0.42
14:G:231:TRP:CZ2	17:F:78:LEU:HD11	2.55	0.42
16:T:70:VAL:HA	16:T:94:GLN:HB3	2.02	0.42
25:X:19:LEU:HD22	25:X:72:PRO:HG3	2.01	0.42
31:o:77:ASN:HB2	31:o:95:GLY:H	1.84	0.42
33:z:264:GLU:O	33:z:268:LEU:HD13	2.20	0.42
33:z:319:LYS:HG3	33:z:488:ARG:CG	2.49	0.42
2:I:110:MET:SD	2:I:361:ALA:HB2	2.60	0.42
2:I:309:ALA:HA	2:I:318:LEU:HD12	2.02	0.42
5:H:169:GLU:O	5:H:173:ALA:N	2.53	0.42
6:K:13:ILE:HG22	6:K:41:ALA:HB2	2.02	0.42
11:S:54:ASP:OD1	11:S:54:ASP:N	2.53	0.42
11:S:56:GLU:HA	24:D:220:LEU:HD13	2.01	0.42
37:i:201:CDL:C62	37:i:201:CDL:H802	2.49	0.42
13:j:70:ARG:O	13:j:71:LYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:231:TRP:CZ2	17:F:78:LEU:HD21	2.54	0.42
15:C:544:ARG:HG2	15:C:547:TRP:HB3	2.02	0.42
15:C:707:LYS:HG2	15:C:708:GLU:H	1.84	0.42
16:T:208:LEU:HD23	16:T:208:LEU:HA	1.88	0.42
18:B:97:ALA:HA	18:B:100:ILE:HG22	2.02	0.42
21:R:131:PRO:O	21:R:132:GLN:C	2.62	0.42
23:E:169:TYR:CD1	23:E:169:TYR:N	2.83	0.42
32:q:46:MET:HG3	32:p:220:LYS:NZ	2.34	0.42
33:z:114:ASN:O	33:z:115:TRP:HB2	2.19	0.42
33:z:302:GLN:CD	33:z:302:GLN:N	2.74	0.42
33:z:557:ILE:CG2	33:z:560:PRO:HB3	2.50	0.42
1:A:414:TRP:CE3	15:C:164:MET:HE2	2.55	0.42
2:I:197:ILE:HD12	2:I:233:ILE:HD12	2.01	0.42
2:I:298:SER:OG	2:I:331:CYS:HB3	2.20	0.42
4:N:66:LEU:HD12	4:N:66:LEU:HA	1.86	0.42
5:H:89:TRP:HZ2	5:H:237:ILE:HG22	1.84	0.42
6:K:60:VAL:O	6:K:64:LEU:HG	2.20	0.42
14:G:114:HIS:O	14:G:118:LEU:HB2	2.19	0.42
14:G:306:MET:HE2	15:C:166:HIS:CD2	2.54	0.42
16:T:282:LEU:HD22	16:T:360:PHE:CE1	2.54	0.42
17:F:146:ASP:HB3	19:O:117:PHE:CZ	2.54	0.42
19:O:76:ILE:HG13	19:O:108:PHE:CE2	2.53	0.42
21:R:28:ASN:O	21:R:32:VAL:HG12	2.20	0.42
22:U:56:LYS:HG3	22:U:57:PHE:CD1	2.54	0.42
24:D:182:ASN:C	24:D:184:GLU:H	2.27	0.42
24:D:193:LEU:HD12	24:D:193:LEU:HA	1.78	0.42
31:o:57:GLN:HG3	31:o:58:ILE:HG13	2.02	0.42
33:z:135:LEU:CD2	33:z:169:VAL:HG13	2.50	0.42
33:z:300:ASN:HB2	33:z:303:GLU:HB3	2.01	0.42
1:A:224:ALA:HB3	18:B:114:TYR:HB3	2.01	0.42
3:J:57:PHE:CE2	6:K:86:VAL:HA	2.55	0.42
7:Y:21:SER:O	7:Y:25:ILE:HG12	2.20	0.42
7:Y:43:ASP:OD1	7:Y:43:ASP:N	2.53	0.42
7:Y:74:GLU:HB3	7:Y:99:PHE:HA	2.01	0.42
37:i:201:CDL:H112	37:i:201:CDL:CA6	2.46	0.42
15:C:329:SER:N	15:C:453:MET:HE3	2.35	0.42
16:T:167:LEU:HB2	16:T:180:TYR:OH	2.19	0.42
17:F:155:VAL:O	17:F:168:PRO:HD2	2.19	0.42
32:q:114:SER:O	32:q:114:SER:OG	2.36	0.42
32:p:133:VAL:HB	32:p:150:THR:HG23	2.00	0.42
33:z:125:ASN:ND2	33:z:171:LEU:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:247:LEU:HD23	33:z:247:LEU:N	2.31	0.42
1:A:142:GLU:CD	1:A:150:ASP:HB2	2.45	0.42
1:A:396:PHE:HD1	18:B:170:GLU:HB3	1.83	0.42
2:I:123:PHE:CD1	2:I:123:PHE:C	2.97	0.42
2:I:247:HIS:HD2	2:I:251:PRO:HG2	1.84	0.42
2:I:330:ILE:N	2:I:330:ILE:HD13	2.34	0.42
4:N:121:SER:OG	4:N:122:LEU:N	2.52	0.42
5:H:152:GLY:O	5:H:156:ILE:HG12	2.20	0.42
8:Z:38:ARG:HD3	8:Z:38:ARG:HA	1.72	0.42
11:S:59:VAL:HG13	11:S:59:VAL:O	2.20	0.42
15:C:203:VAL:HG11	20:P:91:LEU:HG	2.02	0.42
15:C:225:VAL:HG23	15:C:248:ILE:CG2	2.49	0.42
15:C:421:LEU:HD11	15:C:702:LEU:HB2	2.01	0.42
17:F:100:SER:HB3	17:F:124:ILE:O	2.20	0.42
17:F:109:GLY:HA2	17:F:126:HIS:CE1	2.55	0.42
17:F:158:ASP:OD1	17:F:159:ASP:N	2.53	0.42
31:o:55:GLN:OE1	32:q:64:SER:HB3	2.20	0.42
33:z:448:GLU:HA	33:z:541:GLN:HE22	1.85	0.42
5:H:277:LEU:HD23	5:H:277:LEU:HA	1.86	0.42
7:Y:45:ASN:HA	8:Z:130:TRP:CD1	2.55	0.42
8:Z:112:MET:HB3	8:Z:117:GLY:HA3	2.02	0.42
9:V:49:MET:HA	9:V:52:ARG:HG2	2.01	0.42
14:G:210:THR:HA	21:R:21:VAL:HG12	2.01	0.42
15:C:722:PHE:O	15:C:722:PHE:CG	2.73	0.42
16:T:348:THR:OG1	16:T:349:THR:N	2.52	0.42
26:c:61:SER:HA	26:c:64:THR:HG22	2.01	0.42
31:o:122:ALA:N	31:o:149:SER:OG	2.39	0.42
31:o:223:LEU:HD21	32:p:86:ARG:HH11	1.84	0.42
32:q:20:GLN:C	32:q:22:LEU:N	2.76	0.42
32:q:162:MET:O	32:q:180:VAL:HA	2.20	0.42
33:z:263:PRO:HB3	33:z:500:ALA:HB1	2.02	0.42
33:z:399:LEU:HD13	33:z:410:VAL:HG23	2.02	0.42
33:z:569:LEU:HD23	33:z:569:LEU:H	1.83	0.42
1:A:406:THR:OG1	1:A:409:ARG:NH2	2.53	0.41
1:A:474:ARG:O	1:A:478:GLU:HG2	2.20	0.41
3:J:63:LEU:HA	3:J:63:LEU:HD23	1.77	0.41
14:G:45:GLY:HA2	14:G:48:HIS:CB	2.50	0.41
16:T:67:SER:HB2	16:T:93:SER:HB3	2.02	0.41
23:E:69:ILE:HA	23:E:72:VAL:HG12	2.01	0.41
25:X:44:TYR:OH	25:X:94:LYS:O	2.31	0.41
31:o:120:HIS:O	31:o:148:ARG:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:z:309:LYS:HD2	33:z:309:LYS:HA	1.87	0.41
33:z:435:ILE:HD13	33:z:435:ILE:HA	1.88	0.41
33:z:559:ILE:O	33:z:559:ILE:CG2	2.67	0.41
1:A:404:GLN:O	15:C:116:ASN:HA	2.20	0.41
2:I:274:PHE:HZ	2:I:327:VAL:HG13	1.84	0.41
4:N:47:ASP:HB2	5:H:105:ILE:HD13	2.02	0.41
5:H:289:ARG:HG3	14:G:126:GLY:HA3	2.02	0.41
6:K:14:PHE:CE1	6:K:38:MET:HE3	2.55	0.41
37:i:201:CDL:H402	37:i:201:CDL:C44	2.50	0.41
15:C:590:ASN:HB3	15:C:593:LYS:HG3	2.02	0.41
16:T:128:GLU:O	16:T:129:ASP:HB3	2.20	0.41
17:F:176:ARG:NH2	24:D:138:ILE:O	2.53	0.41
18:B:189:GLY:C	18:B:191:GLU:H	2.28	0.41
24:D:111:HIS:CD2	24:D:111:HIS:N	2.87	0.41
28:k:70:HIS:HA	28:k:107:SER:HA	2.02	0.41
28:k:90:GLU:HB2	28:k:95:LEU:O	2.20	0.41
31:o:76:PRO:HB2	32:p:42:HIS:N	2.35	0.41
33:z:180:VAL:HA	33:z:187:VAL:HA	2.03	0.41
2:I:332:ILE:CG2	2:I:425:LEU:HD11	2.50	0.41
5:H:187:LEU:HD11	5:H:276:PHE:CZ	2.55	0.41
5:H:208:ALA:O	5:H:209:GLU:C	2.63	0.41
11:S:32:HIS:HD2	11:S:36:LEU:HD22	1.85	0.41
37:i:201:CDL:H411	37:i:201:CDL:C21	2.51	0.41
14:G:149:SER:OG	14:G:150:GLY:N	2.54	0.41
15:C:111:LEU:HD11	15:C:267:ILE:HD12	1.88	0.41
16:T:55:LEU:HB3	16:T:56:ALA:H	1.55	0.41
16:T:126:ARG:NH1	16:T:153:ASN:O	2.53	0.41
16:T:318:MET:HE3	16:T:318:MET:HB2	1.85	0.41
17:F:64:TYR:HB2	17:F:67:ARG:HD2	2.03	0.41
24:D:114:ARG:N	24:D:176:ALA:O	2.39	0.41
27:Q:77:LEU:HB3	27:Q:81:GLN:HB2	2.02	0.41
28:k:46:VAL:O	28:k:50:VAL:HG13	2.20	0.41
32:q:145:ILE:HD12	32:q:151:LEU:HD21	2.02	0.41
32:q:205:THR:O	32:q:209:ASN:ND2	2.53	0.41
32:p:87:GLY:HA3	32:p:92:VAL:HG23	2.01	0.41
33:z:492:ARG:HD3	33:z:507:ASP:HB2	2.03	0.41
2:I:374:ILE:HG22	2:I:446:ARG:HD3	2.03	0.41
3:J:68:PHE:CD1	5:H:145:VAL:HG22	2.56	0.41
14:G:88:LYS:N	21:R:130:VAL:HG11	2.36	0.41
14:G:210:THR:OG1	21:R:22:GLY:HA3	2.21	0.41
38:G:601:PEV:O31	38:G:601:PEV:C3	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:350:ARG:HG3	15:C:615:ASN:HA	2.03	0.41
15:C:384:ALA:HA	15:C:584:MET:HB3	2.03	0.41
15:C:427:MET:HB3	15:C:634:GLU:HA	2.03	0.41
15:C:516:VAL:HB	15:C:552:PHE:CD1	2.54	0.41
16:T:83:TYR:CD2	17:F:160:PRO:HB3	2.54	0.41
16:T:156:PHE:CE1	16:T:196:MET:HB3	2.55	0.41
16:T:215:THR:OG1	16:T:275:SER:O	2.26	0.41
33:z:395:LEU:O	33:z:399:LEU:HG	2.20	0.41
33:z:541:GLN:O	33:z:576:ARG:NH1	2.54	0.41
1:A:397:TYR:O	1:A:401:SER:HB3	2.20	0.41
2:I:125:PHE:CE1	2:I:162:ILE:CG2	3.04	0.41
2:I:354:LEU:HD11	2:I:472:THR:CG2	2.50	0.41
5:H:94:PHE:CZ	9:V:22:MET:HE2	2.56	0.41
8:Z:112:MET:HE3	13:j:57:ILE:HD13	2.01	0.41
15:C:444:GLY:O	15:C:471:TYR:HE1	2.04	0.41
16:T:82:ARG:HG2	16:T:108:HIS:NE2	2.35	0.41
16:T:233:TRP:HB3	16:T:297:MET:HE1	2.02	0.41
18:B:127:LEU:HD22	18:B:183:VAL:HG12	2.02	0.41
21:R:44:ILE:O	21:R:47:VAL:HG22	2.20	0.41
32:q:88:ASP:OD1	32:q:89:VAL:N	2.53	0.41
32:q:117:VAL:O	32:q:118:HIS:ND1	2.52	0.41
33:z:130:GLU:H	33:z:135:LEU:HD21	1.85	0.41
33:z:545:TRP:HA	33:z:548:PHE:HD2	1.85	0.41
33:z:559:ILE:HD12	33:z:559:ILE:N	2.35	0.41
1:A:127:LYS:HD3	1:A:127:LYS:HA	1.84	0.41
1:A:169:GLY:HA3	1:A:216:PHE:CE1	2.55	0.41
14:G:271:SER:O	14:G:275:ILE:HG12	2.21	0.41
15:C:372:ILE:HD11	15:C:664:SER:HB2	2.03	0.41
15:C:445:THR:O	15:C:446:GLN:C	2.64	0.41
15:C:517:GLY:O	15:C:520:LEU:HG	2.21	0.41
15:C:682:SER:O	27:Q:17:LEU:HD11	2.21	0.41
16:T:80:LEU:HG	16:T:144:LEU:HD13	2.02	0.41
18:B:74:ILE:HB	18:B:75:PRO:HD3	2.02	0.41
32:q:67:VAL:HG23	32:q:67:VAL:O	2.20	0.41
32:q:81:TYR:OH	32:q:214:HIS:ND1	2.36	0.41
32:q:118:HIS:ND1	32:q:118:HIS:O	2.50	0.41
1:A:272:ALA:O	1:A:275:PRO:HD2	2.20	0.41
3:J:61:PHE:CZ	5:H:139:ARG:HG2	2.55	0.41
5:H:23:LEU:HB2	9:V:15:ILE:HD12	2.02	0.41
8:Z:115:VAL:HG12	8:Z:116:PRO:HD3	2.03	0.41
11:S:78:ARG:HD3	14:G:294:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:74:ILE:N	15:C:85:VAL:O	2.50	0.41
15:C:164:MET:HG3	15:C:195:PHE:CD1	2.55	0.41
15:C:438:ASP:O	15:C:439:LEU:HD23	2.20	0.41
15:C:735:MET:O	15:C:738:CYS:HB2	2.20	0.41
15:C:741:VAL:O	15:C:741:VAL:CG1	2.67	0.41
16:T:221:THR:HB	16:T:229:ILE:HG13	2.03	0.41
22:U:55:ASP:OD2	22:U:59:ASN:HB2	2.20	0.41
25:X:16:SER:OG	25:X:76:ASP:OD2	2.23	0.41
26:c:48:GLY:O	26:c:61:SER:OG	2.34	0.41
32:q:206:ASN:HA	32:q:209:ASN:HD21	1.86	0.41
33:z:345:LYS:HE2	33:z:345:LYS:HB2	1.91	0.41
33:z:540:THR:HG21	33:z:543:GLN:HB2	2.01	0.41
1:A:437:GLU:OE2	15:C:153:LYS:NZ	2.54	0.41
1:A:446:THR:HG21	1:A:451:GLY:HA3	2.02	0.41
3:J:113:ARG:HD3	4:N:176:LYS:HE3	2.02	0.41
5:H:269:PHE:HE2	9:V:19:LEU:HD23	1.86	0.41
14:G:61:LEU:HD21	14:G:316:TYR:HE1	1.84	0.41
14:G:240:ASP:C	14:G:242:TYR:N	2.79	0.41
15:C:161:PHE:O	15:C:164:MET:HB3	2.21	0.41
15:C:162:LEU:O	15:C:166:HIS:HB2	2.20	0.41
15:C:331:LYS:HD2	15:C:725:THR:HG22	2.03	0.41
18:B:203:PRO:O	18:B:207:VAL:HG22	2.21	0.41
23:E:96:VAL:HA	23:E:99:MET:HE3	2.02	0.41
32:q:73:ILE:HG21	32:q:79:ILE:HD11	2.02	0.41
32:q:167:ALA:CB	32:q:182:GLY:HA2	2.50	0.41
1:A:224:ALA:O	18:B:114:TYR:HB3	2.20	0.41
2:I:36:GLY:HA3	2:I:123:PHE:CD1	2.55	0.41
2:I:53:ASN:HD21	26:c:52:GLY:CA	2.29	0.41
4:N:58:ILE:HG13	5:H:116:LEU:HD21	2.03	0.41
4:N:173:ARG:HD2	4:N:178:LYS:CG	2.51	0.41
5:H:139:ARG:HB3	5:H:292:TYR:CZ	2.56	0.41
5:H:227:LEU:HD12	5:H:227:LEU:HA	1.81	0.41
5:H:261:LYS:HG3	5:H:263:ILE:H	1.86	0.41
5:H:287:PHE:HA	5:H:288:PRO:HD3	1.84	0.41
7:Y:88:GLU:OE1	9:V:39:HIS:HE1	2.04	0.41
11:S:32:HIS:NE2	24:D:85:LYS:HE2	2.36	0.41
11:S:51:ALA:HB2	24:D:105:PRO:HB3	2.02	0.41
11:S:124:ARG:HD2	11:S:124:ARG:HA	1.74	0.41
37:i:201:CDL:C51	37:i:201:CDL:CB6	2.99	0.41
14:G:89:LEU:HD21	14:G:327:THR:HG22	2.03	0.41
14:G:123:MET:HE2	14:G:123:MET:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:159:ARG:HH22	24:D:170:GLU:CD	2.29	0.41
14:G:199:TRP:O	14:G:200:LYS:C	2.62	0.41
14:G:248:ASP:HB3	29:r:16:ALA:HB1	2.02	0.41
14:G:293:LYS:O	14:G:294:LEU:HD23	2.20	0.41
14:G:387:ILE:HD13	14:G:387:ILE:HA	1.91	0.41
15:C:85:VAL:HB	15:C:89:PHE:CD2	2.55	0.41
15:C:212:LYS:CE	15:C:274:THR:CG2	2.98	0.41
15:C:260:LEU:HD12	15:C:263:ASN:ND2	2.36	0.41
15:C:489:PRO:HD3	15:C:714:PRO:HA	2.03	0.41
16:T:90:LYS:O	16:T:90:LYS:HG2	2.21	0.41
16:T:115:LEU:O	19:O:88:LEU:HD22	2.21	0.41
16:T:147:ARG:HA	16:T:147:ARG:HD3	1.77	0.41
16:T:222:MET:HE3	16:T:222:MET:HB2	1.93	0.41
16:T:358:LEU:HD12	16:T:358:LEU:H	1.85	0.41
17:F:109:GLY:HA2	17:F:126:HIS:HE1	1.84	0.41
18:B:147:LEU:HB2	18:B:206:VAL:HG11	2.03	0.41
22:U:80:SER:O	22:U:84:TYR:HB3	2.20	0.41
22:U:90:PRO:HA	22:U:120:HIS:CD2	2.55	0.41
22:U:100:ILE:CG2	24:D:103:LEU:HB2	2.49	0.41
22:U:133:TYR:CD2	24:D:200:LEU:HD22	2.56	0.41
23:E:88:THR:HB	23:E:98:MET:SD	2.61	0.41
23:E:185:VAL:HG11	23:E:195:LEU:HA	2.02	0.41
24:D:47:GLU:HG2	24:D:48:GLU:H	1.86	0.41
24:D:145:ARG:HG2	24:D:149:SER:O	2.20	0.41
24:D:145:ARG:NH2	24:D:151:ARG:HG3	2.36	0.41
24:D:159:MET:HB3	24:D:164:TYR:OH	2.21	0.41
27:Q:13:GLU:HG2	27:Q:63:ARG:HB2	2.03	0.41
28:k:77:LEU:HD13	28:k:81:ASP:HB3	2.02	0.41
31:o:84:VAL:HG22	31:o:105:ILE:HB	2.02	0.41
31:o:175:ILE:HB	31:o:205:LEU:HD11	2.02	0.41
31:o:214:PRO:O	31:o:218:VAL:HG22	2.21	0.41
32:q:17:GLU:HG2	32:p:19:GLY:C	2.46	0.41
32:q:140:GLU:HB3	32:q:159:LYS:HG2	2.02	0.41
33:z:140:LYS:HD2	33:z:140:LYS:C	2.46	0.41
33:z:198:LEU:O	33:z:202:ILE:HG13	2.21	0.41
33:z:232:GLY:HA2	33:z:317:HIS:HA	2.02	0.41
33:z:322:TYR:HB3	33:z:485:ILE:HB	2.03	0.41
33:z:557:ILE:HD12	33:z:557:ILE:HA	1.92	0.41
1:A:53:THR:OG1	1:A:54:HIS:N	2.53	0.41
3:J:71:PHE:HE1	3:J:103:LEU:HD21	1.86	0.41
14:G:37:VAL:HG21	14:G:378:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:44:ILE:CG2	14:G:392:VAL:HG12	2.51	0.41
14:G:84:LEU:HD22	21:R:130:VAL:HA	2.02	0.41
15:C:427:MET:HE3	15:C:553:LEU:HB3	2.03	0.41
15:C:740:ALA:C	15:C:742:LEU:N	2.78	0.41
16:T:125:PRO:HG3	40:T:501:NDP:H2A	2.02	0.41
17:F:87:ARG:HH12	17:F:89:GLN:HE21	1.69	0.41
23:E:90:GLY:C	23:E:95:ALA:HB2	2.46	0.41
24:D:164:TYR:CD1	24:D:164:TYR:N	2.89	0.41
25:X:25:ARG:HA	25:X:28:ASP:HB2	2.03	0.41
31:o:54:GLY:HA2	32:q:42:HIS:NE2	2.36	0.41
31:o:153:GLU:HB3	31:o:172:THR:HG22	2.03	0.41
32:q:179:GLU:HB2	32:q:191:LYS:HE2	2.02	0.41
32:p:29:LEU:O	32:p:31:GLY:N	2.49	0.41
33:z:257:LEU:HD23	33:z:257:LEU:HA	1.85	0.41
33:z:589:LEU:HD23	33:z:589:LEU:HA	1.79	0.41
2:I:77:THR:O	2:I:77:THR:OG1	2.31	0.40
3:J:100:LEU:HD12	3:J:100:LEU:HA	1.69	0.40
5:H:183:LEU:HD21	5:H:314:VAL:HG21	2.02	0.40
5:H:201:ALA:C	5:H:203:PHE:N	2.72	0.40
6:K:15:ILE:HA	6:K:18:ILE:HG22	2.02	0.40
6:K:31:MET:O	6:K:35:ILE:HG12	2.22	0.40
14:G:133:TRP:CH2	14:G:192:MET:HE3	2.56	0.40
15:C:111:LEU:HD11	15:C:227:PHE:HB2	2.02	0.40
15:C:324:ASN:HB2	15:C:327:TRP:O	2.20	0.40
16:T:289:THR:HG23	16:T:292:GLU:H	1.86	0.40
18:B:136:MET:HE2	18:B:136:MET:HB3	1.94	0.40
21:R:47:VAL:CG2	21:R:54:ARG:HB2	2.51	0.40
21:R:60:PHE:O	21:R:64:ARG:HG3	2.21	0.40
31:o:141:VAL:HA	31:o:158:ILE:HB	2.02	0.40
32:p:130:HIS:O	32:p:148:GLY:N	2.54	0.40
32:p:162:MET:HE2	32:p:200:ILE:HG21	2.03	0.40
33:z:228:ALA:HB1	33:z:238:ILE:HB	2.02	0.40
33:z:377:LYS:O	33:z:378:LYS:HG2	2.21	0.40
1:A:401:SER:C	1:A:403:GLY:N	2.79	0.40
2:I:364:LEU:HB3	2:I:465:LYS:HD3	2.03	0.40
5:H:24:VAL:HG12	5:H:233:TYR:HD2	1.83	0.40
5:H:200:ARG:HD2	5:H:233:TYR:HE1	1.87	0.40
5:H:310:TRP:O	5:H:314:VAL:HG23	2.21	0.40
14:G:46:LEU:HD23	23:E:135:MET:SD	2.61	0.40
14:G:73:VAL:HG12	23:E:96:VAL:HG21	2.03	0.40
14:G:209:VAL:HG12	14:G:368:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:246:ASP:H	14:G:277:GLN:NE2	2.19	0.40
15:C:227:PHE:HB2	15:C:267:ILE:HD11	1.94	0.40
15:C:419:ALA:HB3	15:C:568:ILE:HD11	2.02	0.40
16:T:128:GLU:C	16:T:130:SER:N	2.80	0.40
16:T:158:ASP:HA	16:T:162:HIS:HB2	2.03	0.40
33:z:300:ASN:HA	33:z:328:THR:HA	2.02	0.40
1:A:105:LYS:HB3	1:A:105:LYS:HE2	1.92	0.40
1:A:304:HIS:HB2	1:A:379:VAL:O	2.21	0.40
4:N:61:ILE:O	4:N:64:LEU:HB2	2.20	0.40
4:N:164:ILE:O	4:N:168:VAL:HG12	2.20	0.40
5:H:158:VAL:HG21	5:H:246:PHE:HB3	2.02	0.40
8:Z:51:LEU:HD23	8:Z:51:LEU:HA	1.83	0.40
37:i:201:CDL:H212	37:i:201:CDL:C41	2.50	0.40
14:G:119:THR:HG21	14:G:134:ALA:HB2	2.02	0.40
15:C:202:VAL:CG1	15:C:215:MET:HB2	2.52	0.40
15:C:450:GLU:OE2	15:C:555:GLN:HB3	2.21	0.40
17:F:18:TRP:CZ2	17:F:40:GLN:HB3	2.57	0.40
17:F:47:LEU:CA	21:R:95:ASP:HB3	2.47	0.40
17:F:69:ARG:NH1	17:F:91:SER:O	2.55	0.40
21:R:18:THR:OG1	21:R:23:LEU:O	2.33	0.40
22:U:74:ARG:HB2	22:U:99:PHE:CE1	2.56	0.40
25:X:59:ILE:O	25:X:63:ILE:HG13	2.22	0.40
32:q:45:LEU:HD12	32:q:45:LEU:HA	1.88	0.40
33:z:130:GLU:CD	33:z:130:GLU:N	2.79	0.40
33:z:554:TRP:HA	33:z:554:TRP:HE3	1.87	0.40
33:z:566:LEU:HD23	33:z:566:LEU:HA	1.90	0.40
1:A:82:ARG:HG2	18:B:244:PRO:HB2	2.04	0.40
1:A:268:VAL:HA	1:A:271:VAL:HG12	2.03	0.40
1:A:433:ASP:OD1	1:A:466:ARG:NH2	2.42	0.40
2:I:186:SER:HB3	2:I:239:PHE:HB2	2.03	0.40
2:I:265:LEU:HA	2:I:269:PRO:HG2	2.04	0.40
2:I:292:GLN:HE21	2:I:292:GLN:HA	1.86	0.40
2:I:330:ILE:HG23	2:I:345:LEU:HG	2.03	0.40
3:J:107:PHE:HE2	5:H:305:PRO:HG3	1.86	0.40
4:N:143:LEU:HD23	4:N:148:TYR:HE2	1.86	0.40
5:H:258:PRO:HD2	5:H:263:ILE:HD11	2.02	0.40
6:K:61:PHE:O	6:K:65:VAL:HG23	2.22	0.40
8:Z:115:VAL:HG13	8:Z:116:PRO:HD3	2.04	0.40
12:i:29:MET:SD	12:i:34:GLU:OE2	2.80	0.40
12:i:56:LEU:HD12	12:i:56:LEU:HA	1.80	0.40
13:j:37:LEU:HD22	13:j:37:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:248:ASP:O	14:G:270:GLN:HG3	2.20	0.40
15:C:371:ILE:HG21	15:C:599:PHE:CG	2.57	0.40
15:C:447:PRO:HD2	15:C:478:PHE:CZ	2.55	0.40
15:C:516:VAL:HG21	15:C:533:VAL:HG11	2.03	0.40
17:F:116:TRP:HZ3	17:F:131:ARG:HG3	1.87	0.40
23:E:141:LYS:HE2	23:E:141:LYS:HB3	1.75	0.40
1:A:393:LEU:HD23	1:A:393:LEU:HA	1.80	0.40
4:N:52:ILE:HD13	4:N:52:ILE:HA	1.88	0.40
9:V:49:MET:O	9:V:53:ASP:HB2	2.20	0.40
14:G:54:LEU:HB3	14:G:66:TYR:OH	2.22	0.40
14:G:90:LEU:HA	14:G:90:LEU:HD23	1.84	0.40
14:G:117:ALA:HB1	14:G:386:ASP:OD1	2.22	0.40
15:C:693:ARG:CZ	15:C:695:PRO:HG3	2.51	0.40
16:T:218:ARG:HB2	16:T:280:TYR:O	2.22	0.40
17:F:97:ARG:NH2	25:X:76:ASP:HB3	2.28	0.40
17:F:129:LEU:HD23	25:X:80:PHE:CZ	2.57	0.40
19:O:40:GLY:O	19:O:43:SER:OG	2.40	0.40
22:U:56:LYS:NZ	22:U:92:GLU:OE1	2.44	0.40
23:E:191:THR:HG21	23:E:193:GLU:HG3	2.02	0.40
31:o:165:MET:HE3	31:o:166:GLU:HG3	2.04	0.40
31:o:211:LEU:O	31:o:214:PRO:HD2	2.21	0.40
31:o:236:THR:HG22	32:q:38:GLN:NE2	2.36	0.40
32:p:98:THR:HG21	32:p:122:ILE:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/486 (88%)	381 (89%)	46 (11%)	0	100	100
2	I	479/499 (96%)	465 (97%)	13 (3%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100	100
4	N	145/205 (71%)	125 (86%)	19 (13%)	1 (1%)	18	51
5	H	316/325 (97%)	284 (90%)	32 (10%)	0	100	100
6	K	83/100 (83%)	81 (98%)	2 (2%)	0	100	100
7	Y	96/106 (91%)	88 (92%)	7 (7%)	1 (1%)	12	43
8	Z	138/143 (96%)	110 (80%)	28 (20%)	0	100	100
9	V	55/65 (85%)	52 (94%)	3 (6%)	0	100	100
10	W	35/65 (54%)	31 (89%)	4 (11%)	0	100	100
11	S	99/131 (76%)	86 (87%)	13 (13%)	0	100	100
12	i	61/81 (75%)	57 (93%)	3 (5%)	1 (2%)	7	35
13	j	66/83 (80%)	63 (96%)	2 (3%)	1 (2%)	8	36
14	G	380/394 (96%)	348 (92%)	32 (8%)	0	100	100
15	C	691/748 (92%)	617 (89%)	73 (11%)	1 (0%)	48	79
16	T	326/402 (81%)	280 (86%)	46 (14%)	0	100	100
17	F	176/190 (93%)	151 (86%)	25 (14%)	0	100	100
18	B	217/255 (85%)	184 (85%)	33 (15%)	0	100	100
19	O	109/154 (71%)	102 (94%)	7 (6%)	0	100	100
20	P	69/110 (63%)	64 (93%)	5 (7%)	0	100	100
21	R	119/169 (70%)	104 (87%)	14 (12%)	1 (1%)	16	48
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	18	51
24	D	175/222 (79%)	159 (91%)	14 (8%)	2 (1%)	11	41
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100
26	c	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
27	Q	90/97 (93%)	81 (90%)	9 (10%)	0	100	100
28	k	76/122 (62%)	74 (97%)	2 (3%)	0	100	100
29	r	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
30	n	25/113 (22%)	24 (96%)	0	1 (4%)	2	20
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	191 (86%)	28 (13%)	3 (1%)	9	37
32	q	226/275 (82%)	196 (87%)	27 (12%)	3 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	z	495/610 (81%)	476 (96%)	15 (3%)	4 (1%)	16	48
All	All	6177/7436 (83%)	5565 (90%)	591 (10%)	21 (0%)	37	67

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	q	108	VAL
2	I	59	LEU
13	j	26	SER
15	C	272	ALA
24	D	120	GLU
30	n	81	ASN
32	q	23	ASP
32	q	106	VAL
32	p	30	GLN
32	p	102	ASP
32	p	217	GLU
7	Y	103	CYS
33	z	128	GLN
12	i	19	TYR
23	E	189	PRO
24	D	73	LEU
4	N	183	PHE
33	z	385	PRO
33	z	250	PRO
33	z	129	PRO
21	R	120	ILE

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	349/396 (88%)	348 (100%)	1 (0%)	86	84
2	I	399/416 (96%)	365 (92%)	34 (8%)	10	33
3	J	87/106 (82%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	133/186 (72%)	132 (99%)	1 (1%)	73	76
5	H	266/272 (98%)	264 (99%)	2 (1%)	73	76
6	K	74/86 (86%)	74 (100%)	0	100	100
7	Y	88/94 (94%)	88 (100%)	0	100	100
8	Z	112/115 (97%)	112 (100%)	0	100	100
9	V	48/53 (91%)	48 (100%)	0	100	100
10	W	30/53 (57%)	29 (97%)	1 (3%)	33	56
11	S	92/118 (78%)	92 (100%)	0	100	100
12	i	50/66 (76%)	37 (74%)	13 (26%)	0	3
13	j	62/73 (85%)	57 (92%)	5 (8%)	11	35
14	G	328/340 (96%)	325 (99%)	3 (1%)	70	74
15	C	576/625 (92%)	570 (99%)	6 (1%)	68	74
16	T	271/334 (81%)	269 (99%)	2 (1%)	76	77
17	F	168/179 (94%)	163 (97%)	5 (3%)	36	57
18	B	188/220 (86%)	186 (99%)	2 (1%)	65	73
19	O	93/128 (73%)	93 (100%)	0	100	100
20	P	62/97 (64%)	62 (100%)	0	100	100
21	R	108/148 (73%)	106 (98%)	2 (2%)	50	66
22	U	104/133 (78%)	104 (100%)	0	100	100
23	E	129/184 (70%)	121 (94%)	8 (6%)	16	42
24	D	157/191 (82%)	152 (97%)	5 (3%)	34	56
25	X	92/114 (81%)	92 (100%)	0	100	100
26	c	79/84 (94%)	78 (99%)	1 (1%)	61	71
27	Q	82/85 (96%)	81 (99%)	1 (1%)	63	72
28	k	73/112 (65%)	73 (100%)	0	100	100
30	n	21/84 (25%)	19 (90%)	2 (10%)	8	30
31	o	171/211 (81%)	171 (100%)	0	100	100
32	p	181/228 (79%)	177 (98%)	4 (2%)	45	63
32	q	184/228 (81%)	179 (97%)	5 (3%)	39	59
33	z	440/534 (82%)	404 (92%)	36 (8%)	10	35
All	All	5297/6293 (84%)	5158 (97%)	139 (3%)	41	60

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
2	I	35	HIS
2	I	83	TRP
2	I	86	LEU
2	I	120	PHE
2	I	127	VAL
2	I	131	LEU
2	I	155	GLN
2	I	157	LEU
2	I	182	LEU
2	I	197	ILE
2	I	209	LEU
2	I	214	THR
2	I	230	ILE
2	I	241	ILE
2	I	248	MET
2	I	252	ASP
2	I	261	VAL
2	I	264	PHE
2	I	267	ILE
2	I	290	LEU
2	I	315	VAL
2	I	322	SER
2	I	331	CYS
2	I	336	CYS
2	I	345	LEU
2	I	356	THR
2	I	395	MET
2	I	411	PHE
2	I	415	PHE
2	I	427	LEU
2	I	428	VAL
2	I	438	PHE
2	I	443	LEU
2	I	464	ASN
4	N	190	PHE
5	H	290	TYR
5	H	298	LEU
10	W	26	VAL
12	i	8	VAL
12	i	17	GLN
12	i	19	TYR

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Mol	Chain	Res	Type
12	i	21	ASN
12	i	26	LEU
12	i	28	TYR
12	i	36	VAL
12	i	39	MET
12	i	50	VAL
12	i	53	ASP
12	i	60	LEU
12	i	62	VAL
12	i	64	LEU
13	j	7	ILE
13	j	39	GLU
13	j	42	LEU
13	j	46	HIS
13	j	57	ILE
14	G	68	ASP
14	G	73	VAL
14	G	310	ILE
15	C	104	ARG
15	C	218	CYS
15	C	266	ASP
15	C	270	VAL
15	C	275	SER
15	C	601	VAL
16	T	147	ARG
16	T	153	ASN
17	F	19	VAL
17	F	39	PHE
17	F	42	LEU
17	F	47	LEU
17	F	49	THR
18	B	110	VAL
18	B	181	ILE
21	R	122	ASN
21	R	132	GLN
23	E	89	PHE
23	E	93	CYS
23	E	130	THR
23	E	153	ILE
23	E	172	VAL
23	E	183	ILE
23	E	188	CYS

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Mol	Chain	Res	Type
23	E	193	GLU
24	D	73	LEU
24	D	152	THR
24	D	156	ASP
24	D	174	VAL
24	D	197	LYS
26	c	46	THR
27	Q	19	CYS
30	n	83	ASN
30	n	84	TYR
32	q	14	TRP
32	q	16	ARG
32	q	102	ASP
32	q	107	HIS
32	q	108	VAL
32	p	17	GLU
32	p	29	LEU
32	p	30	GLN
32	p	207	TYR
33	z	107	GLU
33	z	109	LEU
33	z	111	THR
33	z	112	VAL
33	z	120	GLU
33	z	122	GLN
33	z	127	ASN
33	z	170	ASN
33	z	173	LEU
33	z	182	LYS
33	z	187	VAL
33	z	243	ILE
33	z	249	THR
33	z	293	VAL
33	z	302	GLN
33	z	304	ILE
33	z	317	HIS
33	z	323	ILE
33	z	333	THR
33	z	337	VAL
33	z	387	ILE
33	z	403	ASP
33	z	408	VAL

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Mol	Chain	Res	Type
33	z	413	VAL
33	z	467	ILE
33	z	473	LEU
33	z	490	THR
33	z	510	SER
33	z	515	ILE
33	z	520	THR
33	z	533	PHE
33	z	569	LEU
33	z	577	PHE
33	z	580	ASP
33	z	582	TYR
33	z	597	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	441	GLN
2	I	53	ASN
2	I	80	HIS
2	I	117	GLN
2	I	208	GLN
2	I	247	HIS
2	I	276	ASN
2	I	291	GLN
2	I	292	GLN
2	I	312	GLN
4	N	25	HIS
4	N	73	HIS
4	N	136	ASN
4	N	180	GLN
5	H	143	GLN
5	H	174	GLN
6	K	27	ASN
6	K	43	ASN
6	K	59	GLN
7	Y	45	ASN
7	Y	87	ASN
8	Z	63	GLN
9	V	34	HIS
9	V	39	HIS
9	V	42	HIS

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Mol	Chain	Res	Type
11	S	69	ASN
12	i	21	ASN
13	j	27	HIS
14	G	78	GLN
14	G	113	ASN
14	G	121	HIS
14	G	277	GLN
14	G	385	GLN
15	C	93	GLN
15	C	165	ASN
15	C	182	GLN
15	C	184	GLN
15	C	284	ASN
15	C	508	ASN
15	C	522	ASN
15	C	538	GLN
15	C	569	GLN
15	C	605	HIS
15	C	606	HIS
15	C	716	GLN
16	T	117	GLN
16	T	153	ASN
16	T	182	GLN
16	T	209	ASN
16	T	291	HIS
16	T	340	ASN
17	F	40	GLN
17	F	76	ASN
17	F	125	ASN
18	B	33	ASN
18	B	81	GLN
18	B	84	ASN
18	B	118	ASN
18	B	126	HIS
18	B	196	ASN
18	B	221	HIS
19	O	49	HIS
19	O	77	ASN
20	P	92	ASN
20	P	106	GLN
21	R	66	ASN
21	R	133	HIS

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Mol	Chain	Res	Type
22	U	41	GLN
22	U	46	ASN
22	U	69	GLN
22	U	134	HIS
22	U	138	HIS
23	E	100	HIS
23	E	145	GLN
23	E	166	HIS
23	E	217	ASN
24	D	111	HIS
24	D	190	HIS
25	X	97	HIS
25	X	102	GLN
25	X	131	ASN
26	c	28	ASN
26	c	79	GLN
26	c	91	ASN
27	Q	35	ASN
27	Q	43	ASN
27	Q	88	ASN
30	n	81	ASN
31	o	77	ASN
31	o	94	ASN
31	o	112	ASN
31	o	120	HIS
32	q	33	ASN
32	q	38	GLN
32	q	47	ASN
32	q	72	HIS
32	q	135	HIS
32	q	184	ASN
32	q	206	ASN
32	q	209	ASN
32	q	218	ASN
32	q	223	ASN
32	p	99	ASN
32	p	130	HIS
32	p	160	HIS
32	p	214	HIS
32	p	223	ASN
33	z	127	ASN
33	z	170	ASN

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Mol	Chain	Res	Type
33	z	218	GLN
33	z	241	GLN
33	z	290	HIS
33	z	302	GLN
33	z	541	GLN
33	z	583	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
34	SF4	C	802	15	0,12,12	-	-	-		
36	T7X	c	301	-	37,37,61	0.33	0	47,49,73	0.39	0
38	PEV	G	601	-	27,27,48	0.35	0	30,32,53	0.37	0
34	SF4	A	501	1	0,12,12	-	-	-		
35	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)
37	CDL	i	201	-	89,89,99	0.28	0	95,101,111	0.57	2 (2%)
34	SF4	D	301	24	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	SF4	C	801	15	0,12,12	-	-	-		
40	NDP	T	501	-	49,52,52	0.49	0	66,80,80	0.69	1 (1%)
34	SF4	D	302	24	0,12,12	-	-	-		
36	T7X	I	501	-	42,42,61	0.31	0	52,54,73	0.50	0
39	FES	C	803	15	0,4,4	-	-	-		
39	FES	B	301	-	0,4,4	-	-	-		
34	SF4	E	301	23	0,12,12	-	-	-		
42	BCT	q	802	41	2,3,3	0.60	0	2,3,3	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SF4	C	802	15	-	-	0/6/5/5
36	T7X	c	301	-	-	2/32/56/80	0/1/1/1
38	PEV	G	601	-	-	12/30/30/52	-
34	SF4	A	501	1	-	-	0/6/5/5
37	CDL	i	201	-	-	31/100/100/110	-
35	FMN	A	502	-	-	6/18/18/18	0/3/3/3
34	SF4	D	301	24	-	-	0/6/5/5
34	SF4	C	801	15	-	-	0/6/5/5
40	NDP	T	501	-	-	6/34/77/77	0/5/5/5
36	T7X	I	501	-	-	13/37/61/80	0/1/1/1
34	SF4	D	302	24	-	-	0/6/5/5
39	FES	C	803	15	-	-	0/1/1/1
39	FES	B	301	-	-	-	0/1/1/1
34	SF4	E	301	23	-	-	0/6/5/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	i	201	CDL	OB6-CB5-C51	2.63	117.16	111.50
40	T	501	NDP	O4D-C1D-C2D	-2.40	101.42	106.64
35	A	502	FMN	C4-N3-C2	-2.08	121.79	125.64
37	i	201	CDL	OA6-CA5-C11	2.01	115.82	111.50

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	502	FMN	N10-C1'-C2'-C3'
35	A	502	FMN	O3'-C3'-C4'-C5'
36	I	501	T7X	C6-C1-O1-P1
36	I	501	T7X	C7-O13-P1-O1
36	I	501	T7X	C8-C7-O13-P1
36	I	501	T7X	C12-C10-O16-C8
36	I	501	T7X	O17-C10-O16-C8
37	i	201	CDL	CA3-OA5-PA1-OA4
37	i	201	CDL	OA7-CA5-OA6-CA4
37	i	201	CDL	C11-CA5-OA6-CA4
37	i	201	CDL	CB2-OB2-PB2-OB3
37	i	201	CDL	OB7-CB5-OB6-CB4
37	i	201	CDL	C51-CB5-OB6-CB4
38	G	601	PEV	C2-C1-O3P-P
37	i	201	CDL	O1-C1-CB2-OB2
35	A	502	FMN	C2'-C3'-C4'-C5'
37	i	201	CDL	CA2-C1-CB2-OB2
37	i	201	CDL	O1-C1-CA2-OA2
35	A	502	FMN	O3'-C3'-C4'-O4'
35	A	502	FMN	C2'-C3'-C4'-O4'
37	i	201	CDL	CB2-OB2-PB2-OB5
40	T	501	NDP	C2D-C1D-N1N-C6N
37	i	201	CDL	C1-CB2-OB2-PB2
37	i	201	CDL	OA6-CA4-CA6-OA8
40	T	501	NDP	C2D-C1D-N1N-C2N
37	i	201	CDL	C38-C39-C40-C41
37	i	201	CDL	CA3-CA4-CA6-OA8
36	I	501	T7X	C39-C40-C41-C42
37	i	201	CDL	OB6-CB4-CB6-OB8
37	i	201	CDL	C31-CA7-OA8-CA6
37	i	201	CDL	C1-CA2-OA2-PA1
38	G	601	PEV	O2-C2-C3-O3
37	i	201	CDL	C53-C54-C55-C56
36	I	501	T7X	O16-C8-C9-O18
37	i	201	CDL	C40-C41-C42-C43
36	I	501	T7X	C7-O13-P1-O12
37	i	201	CDL	CB2-OB2-PB2-OB4
37	i	201	CDL	C71-CB7-OB8-CB6
38	G	601	PEV	C5-C4-O4P-P
37	i	201	CDL	CA5-C11-C12-C13
37	i	201	CDL	OA9-CA7-OA8-CA6
40	T	501	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
36	I	501	T7X	C7-C8-C9-O18
38	G	601	PEV	C3-C2-O2-C31
35	A	502	FMN	C5'-O5'-P-O1P
37	i	201	CDL	CB3-OB5-PB2-OB2
38	G	601	PEV	C1-O3P-P-O4P
38	G	601	PEV	C1-C2-C3-O3
38	G	601	PEV	C35-C36-C37-C38
36	I	501	T7X	C38-C39-C40-C41
37	i	201	CDL	CB3-CB4-CB6-OB8
37	i	201	CDL	C41-C42-C43-C44
37	i	201	CDL	CB6-CB4-OB6-CB5
40	T	501	NDP	O4D-C1D-N1N-C2N
37	i	201	CDL	OB9-CB7-OB8-CB6
38	G	601	PEV	C33-C34-C35-C36
37	i	201	CDL	CB2-C1-CA2-OA2
40	T	501	NDP	PN-O3-PA-O1A
37	i	201	CDL	C16-C17-C18-C19
40	T	501	NDP	O4D-C4D-C5D-O5D
36	c	301	T7X	C6-C1-O1-P1
38	G	601	PEV	C32-C33-C34-C35
37	i	201	CDL	CA3-OA5-PA1-OA3
38	G	601	PEV	C1-O3P-P-O1P
36	c	301	T7X	O16-C10-C12-C13
36	I	501	T7X	O18-C11-C31-C32
38	G	601	PEV	O2-C31-C32-C33
36	I	501	T7X	O19-C11-C31-C32
38	G	601	PEV	O31-C31-C32-C33
36	I	501	T7X	C40-C41-C42-C43

There are no ring outliers.

11 monomers are involved in 65 short contacts:

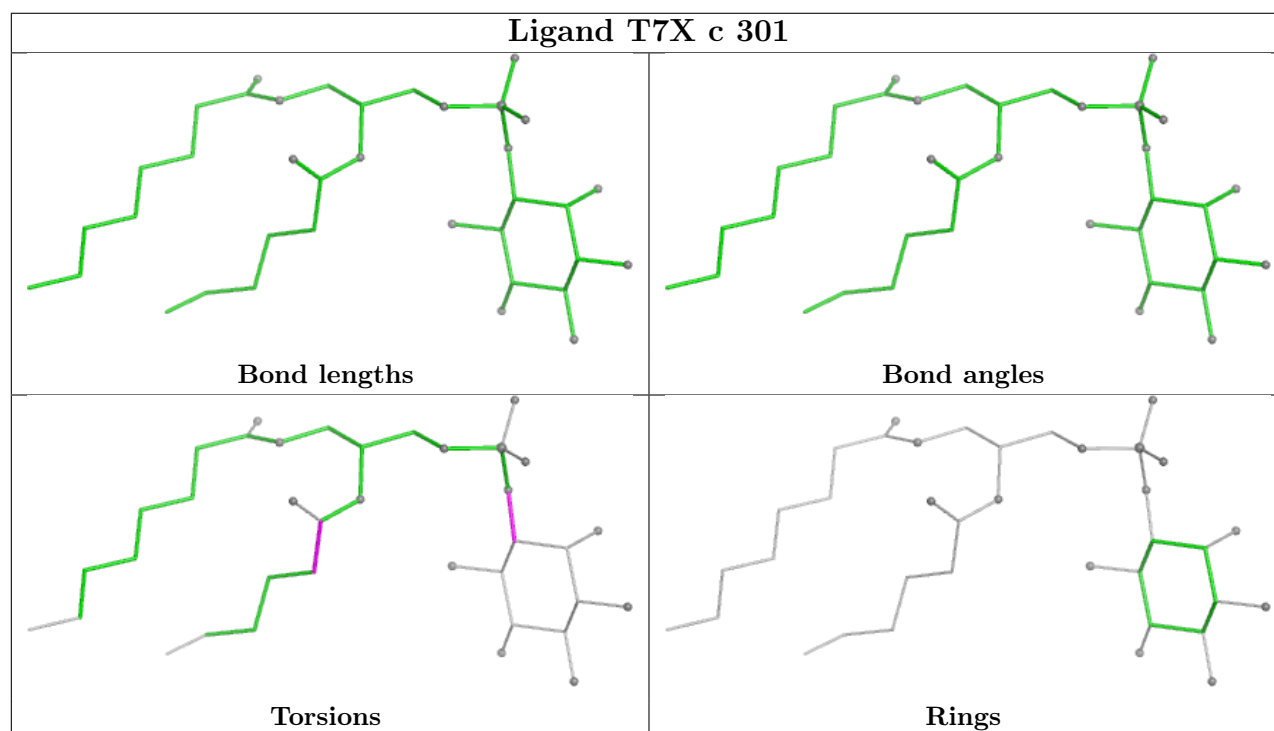
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	G	601	PEV	6	0
34	A	501	SF4	3	0
35	A	502	FMN	3	0
37	i	201	CDL	34	0
34	D	301	SF4	3	0
34	C	801	SF4	1	0
40	T	501	NDP	4	0
36	I	501	T7X	2	0
39	B	301	FES	2	0

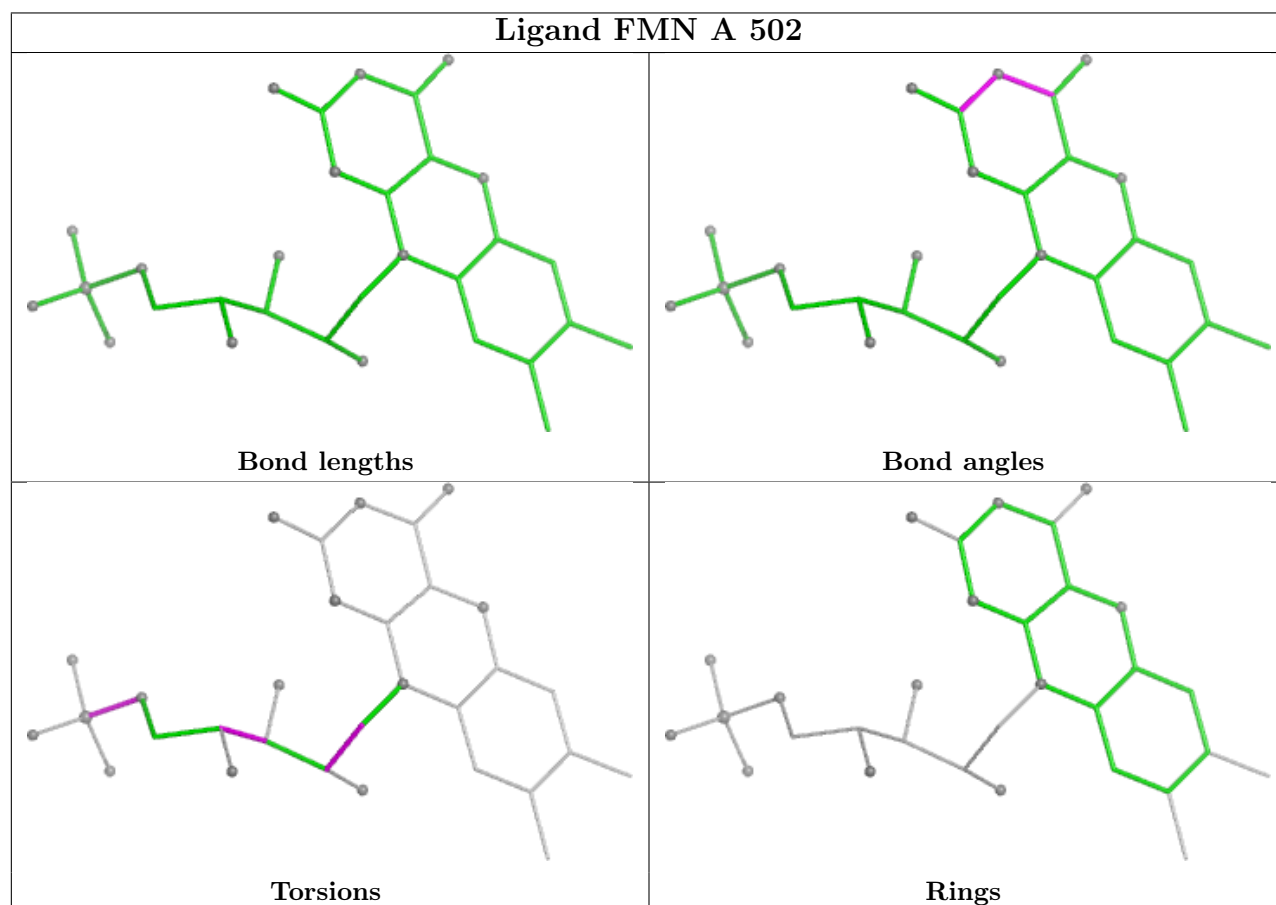
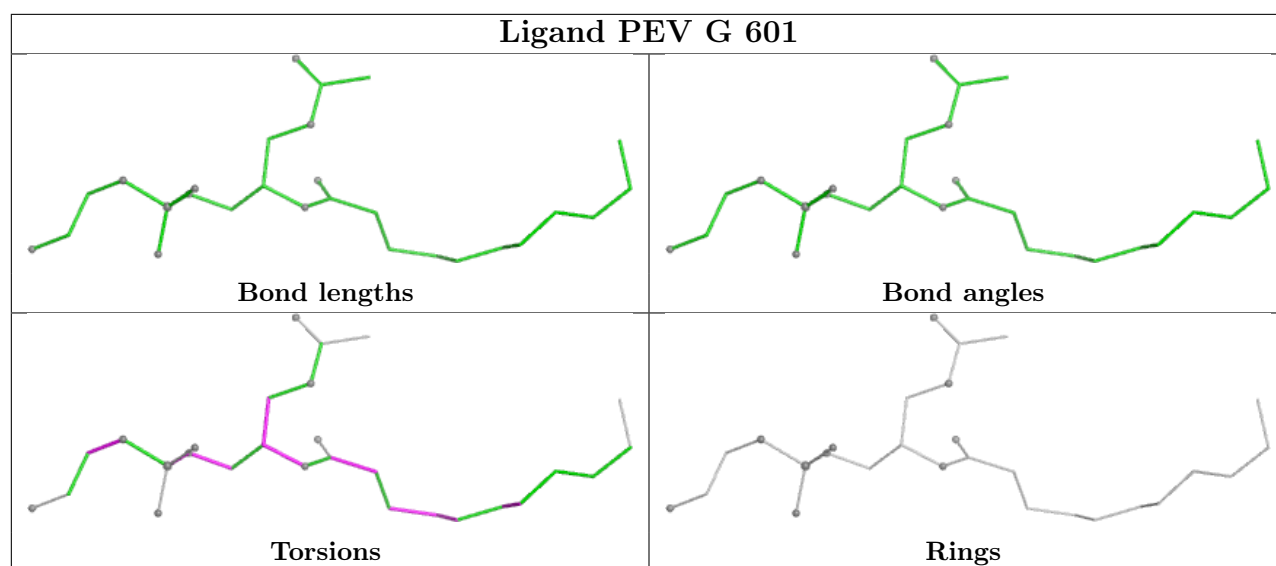
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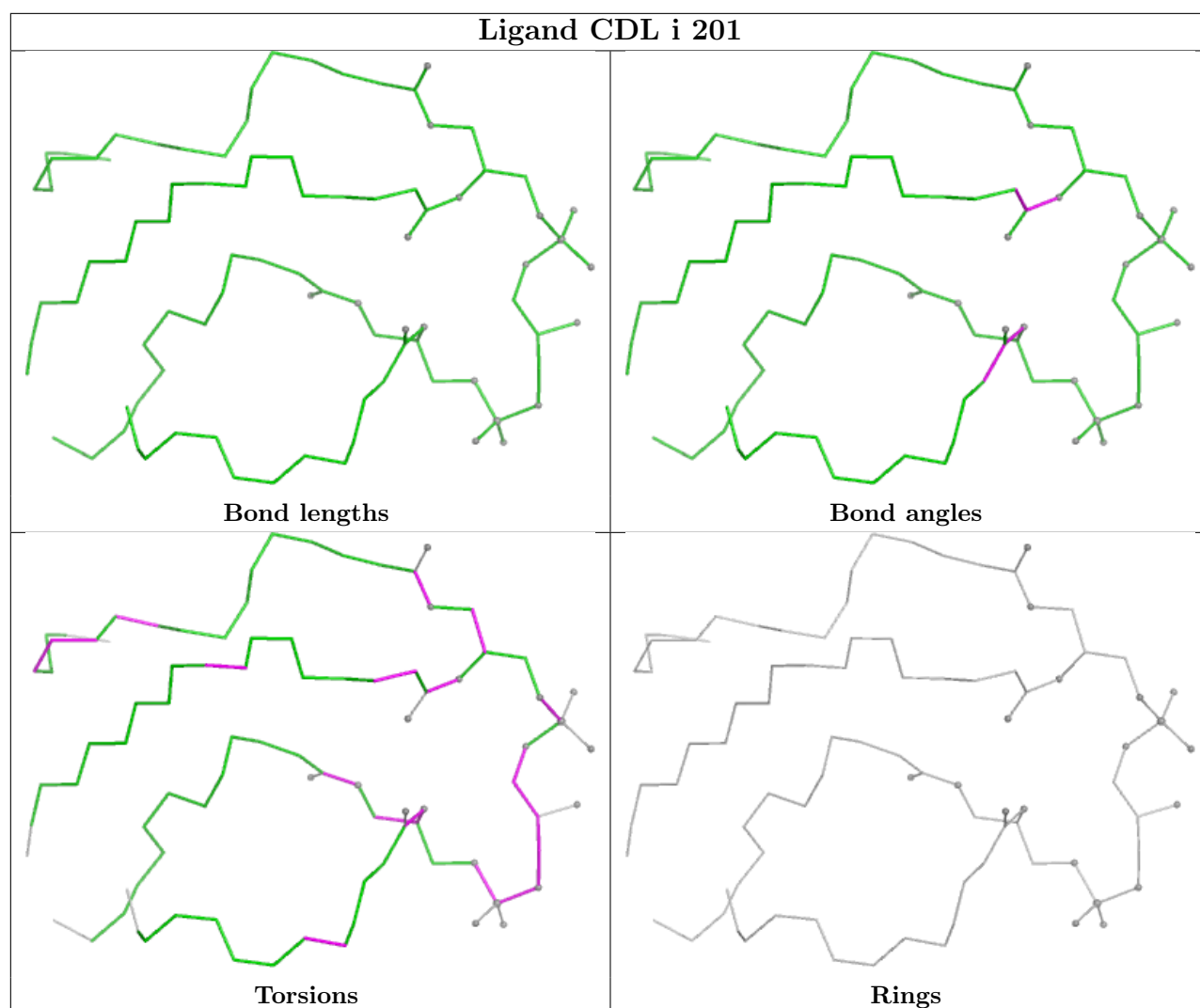
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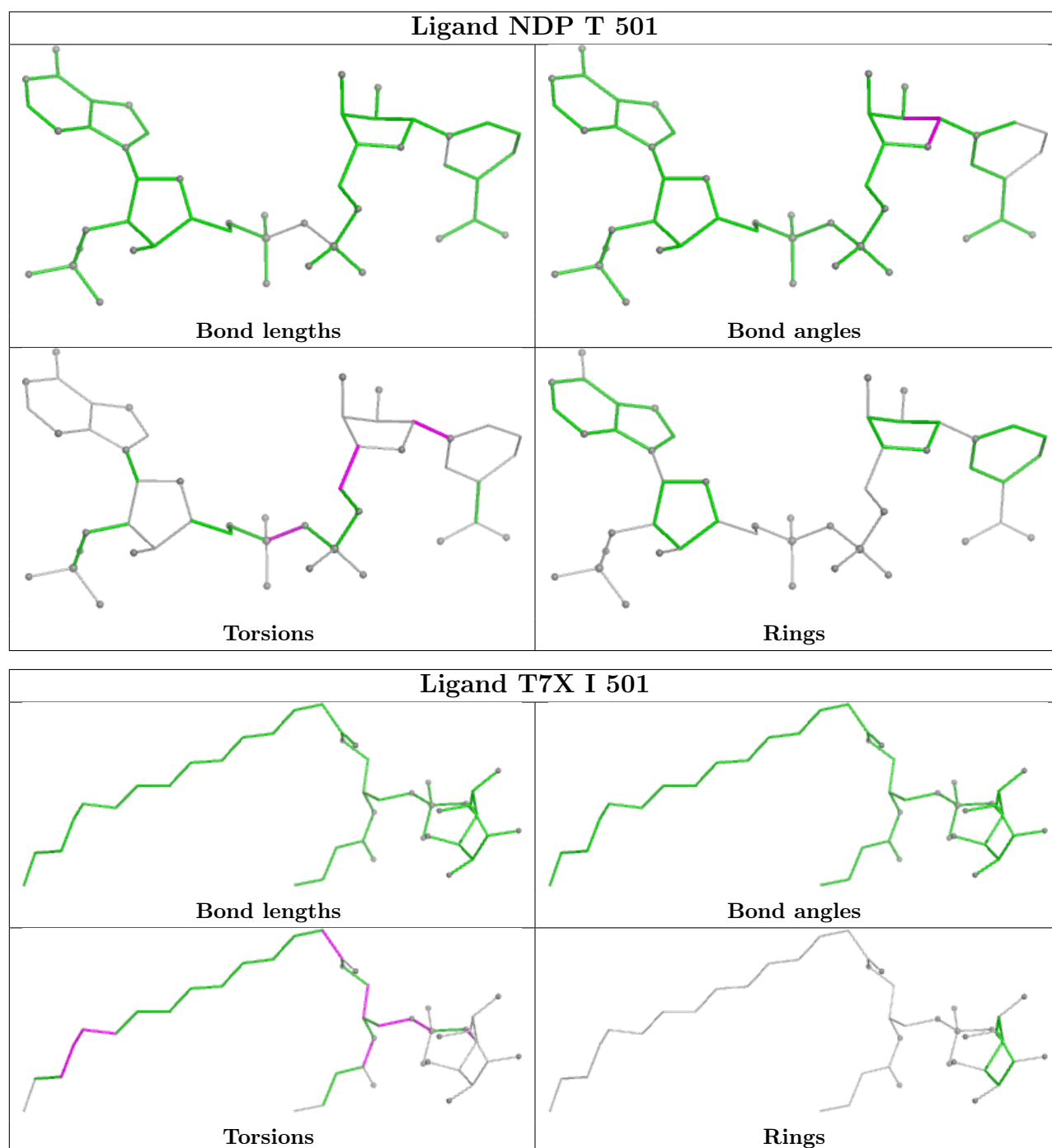
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	301	SF4	6	0
42	q	802	BCT	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	144:GLU	C	145:LYS	N	3.49

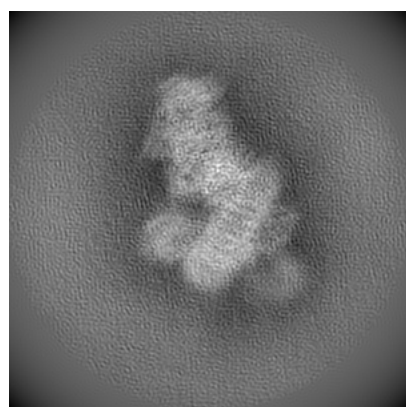
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11615. These allow visual inspection of the internal detail of the map and identification of artifacts.

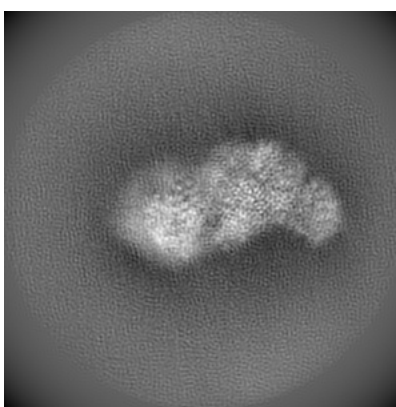
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

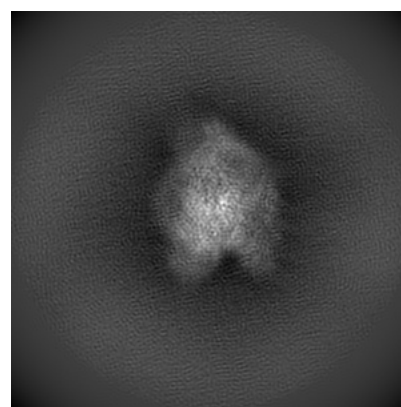
6.1.1 Primary map



X



Y

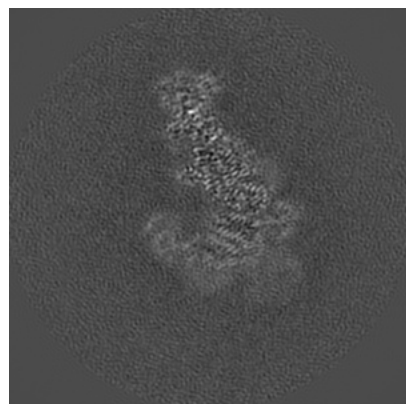


Z

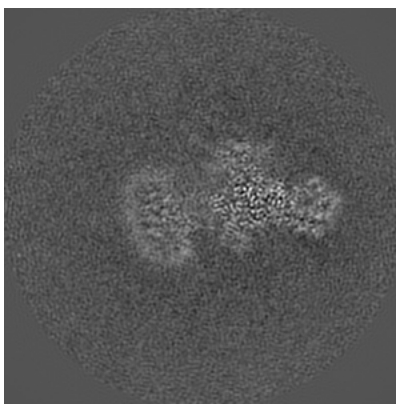
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

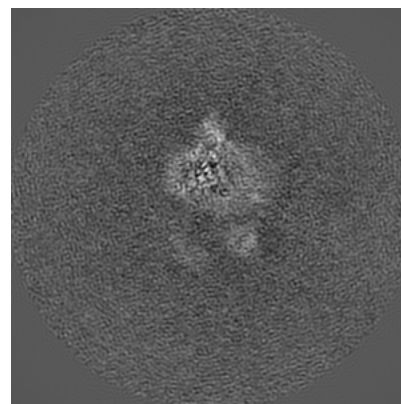
6.2.1 Primary map



X Index: 180



Y Index: 180

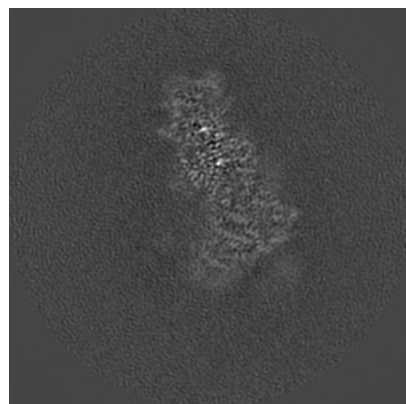


Z Index: 180

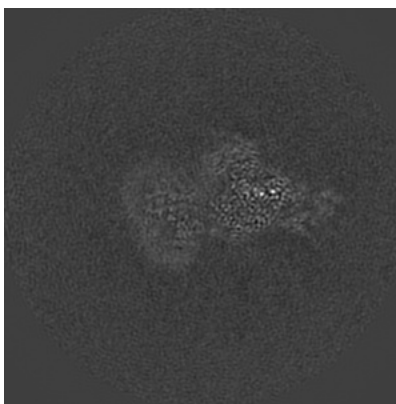
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

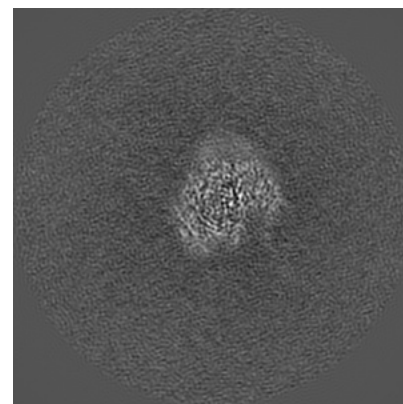
6.3.1 Primary map



X Index: 190



Y Index: 186

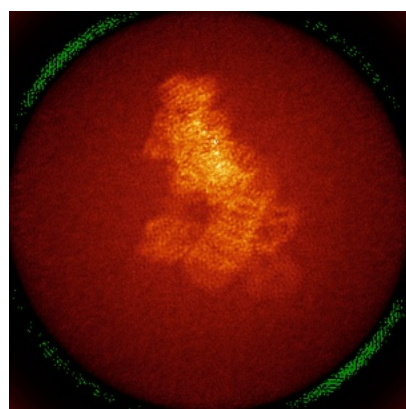


Z Index: 213

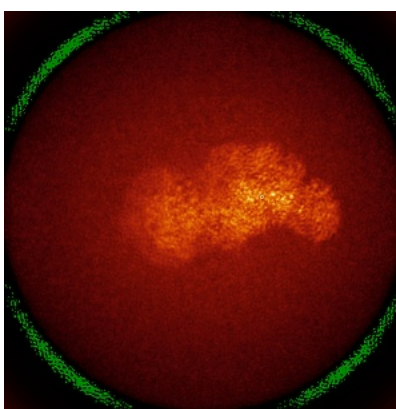
The images above show the largest variance slices of the map in three orthogonal directions.

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

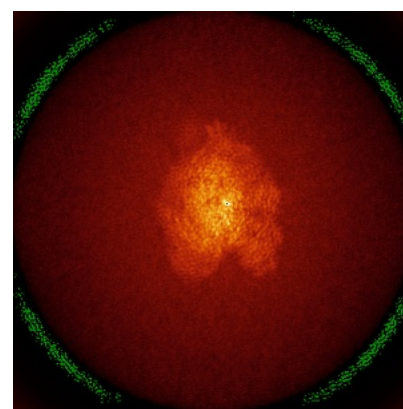
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

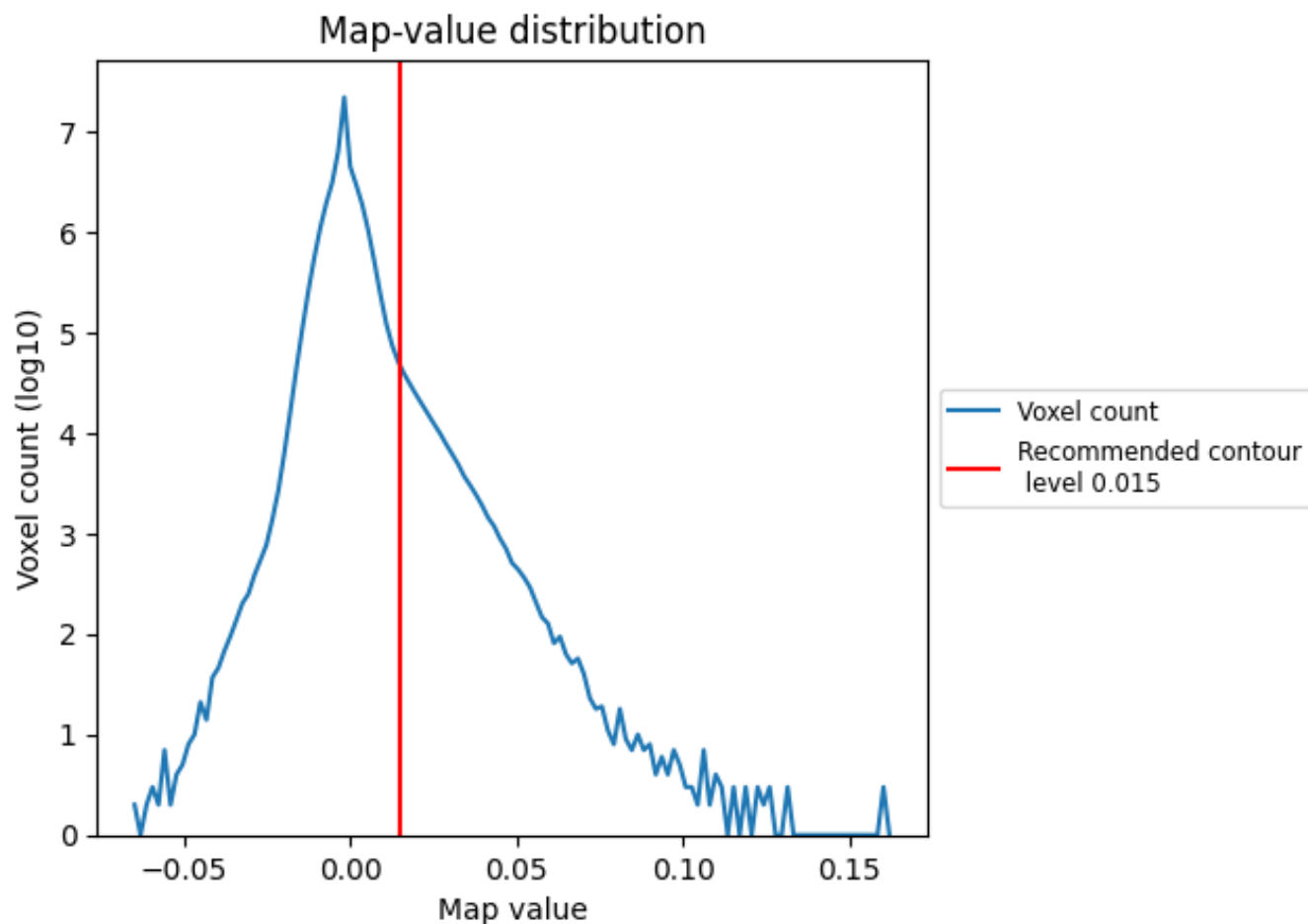
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

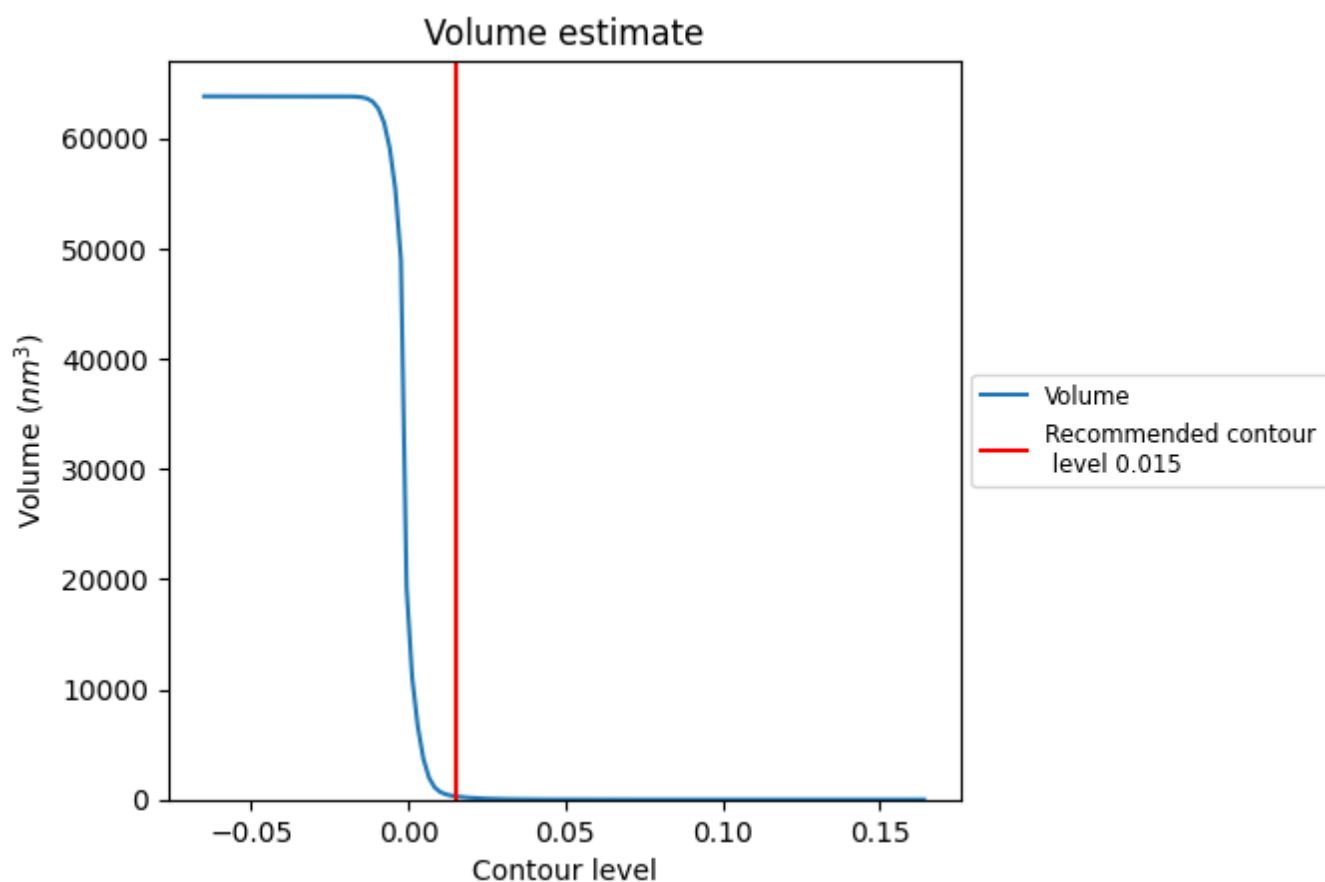
This section contains the results of statistical analysis of the map.

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.

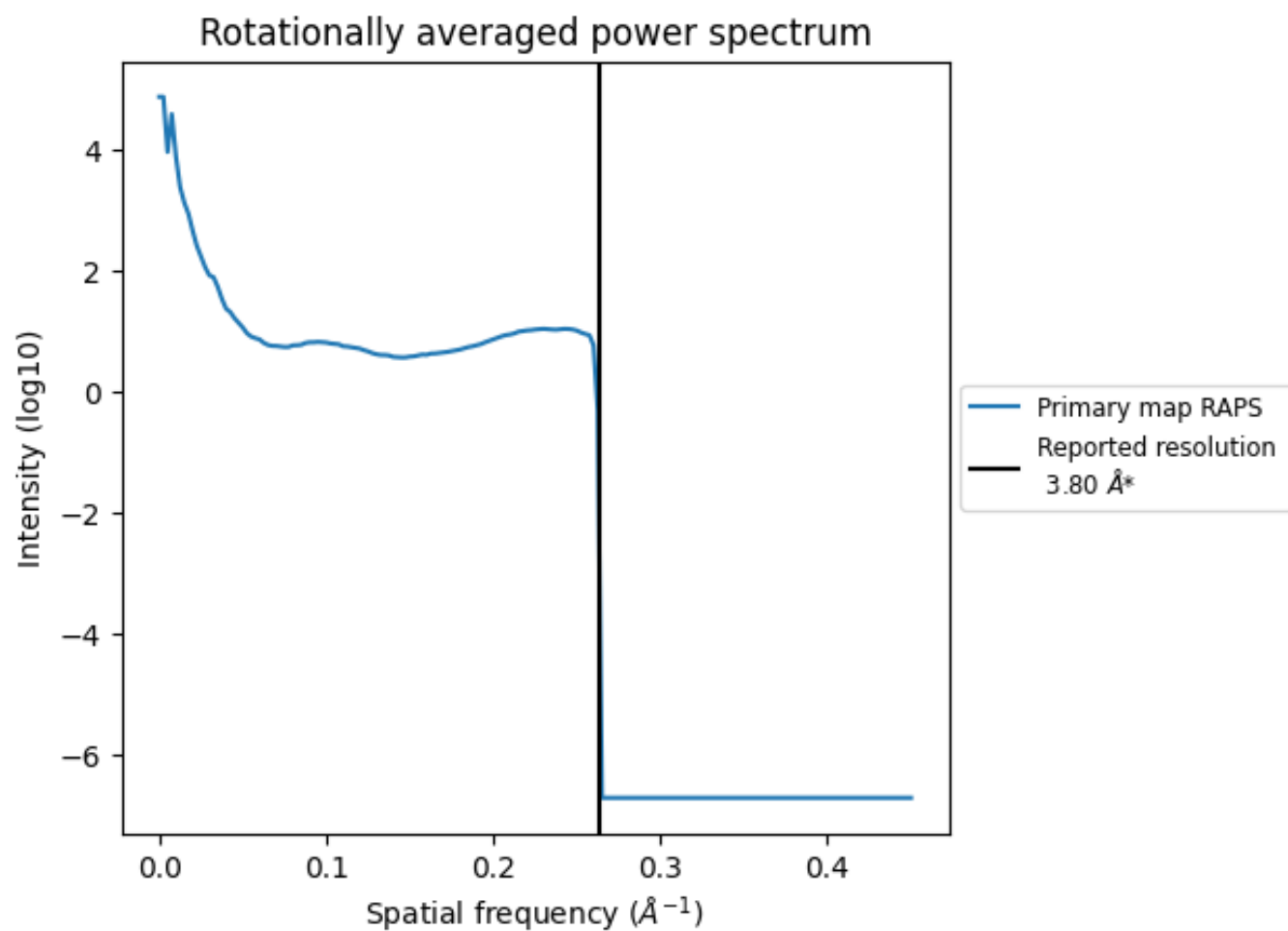
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm^3 ; this corresponds to an approximate mass of 274 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

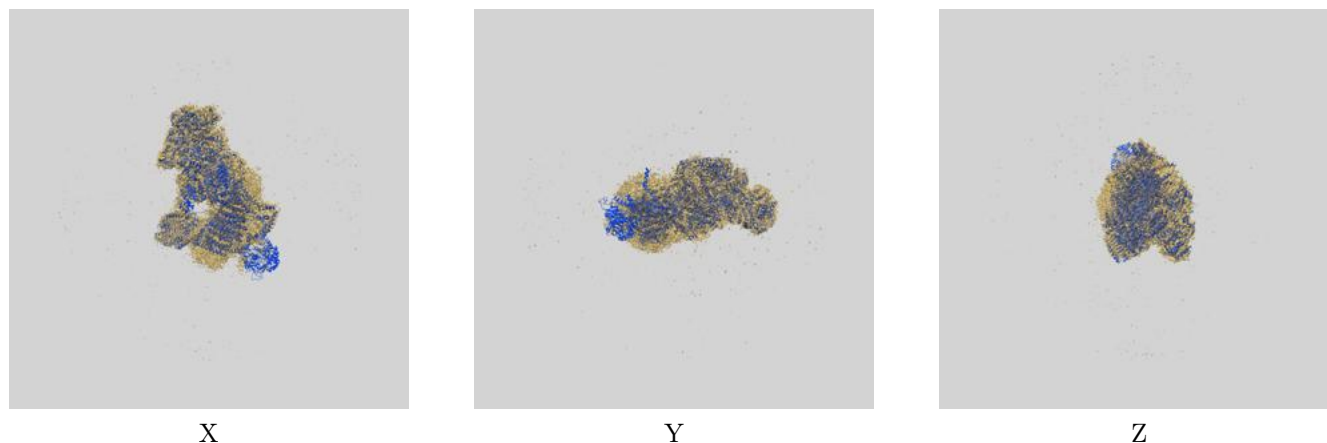
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11615 and PDB model 7A24. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



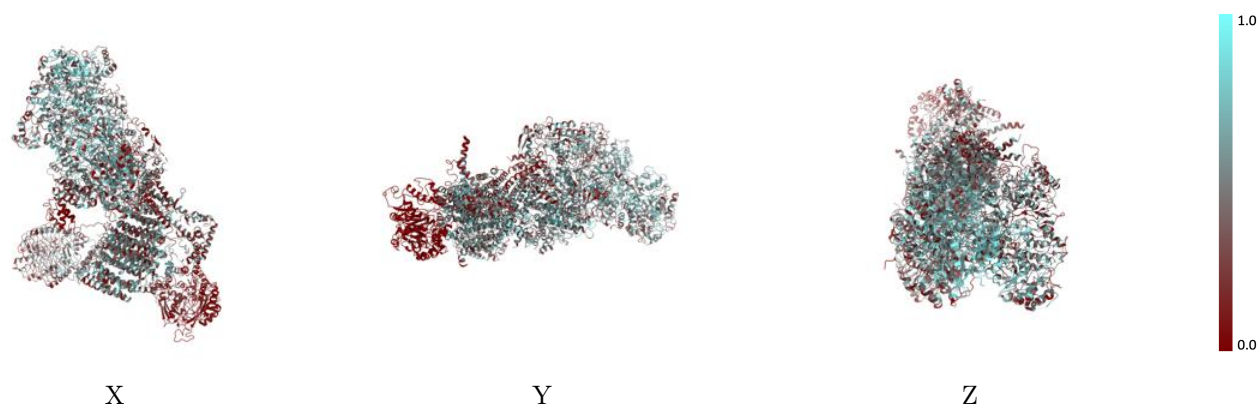
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



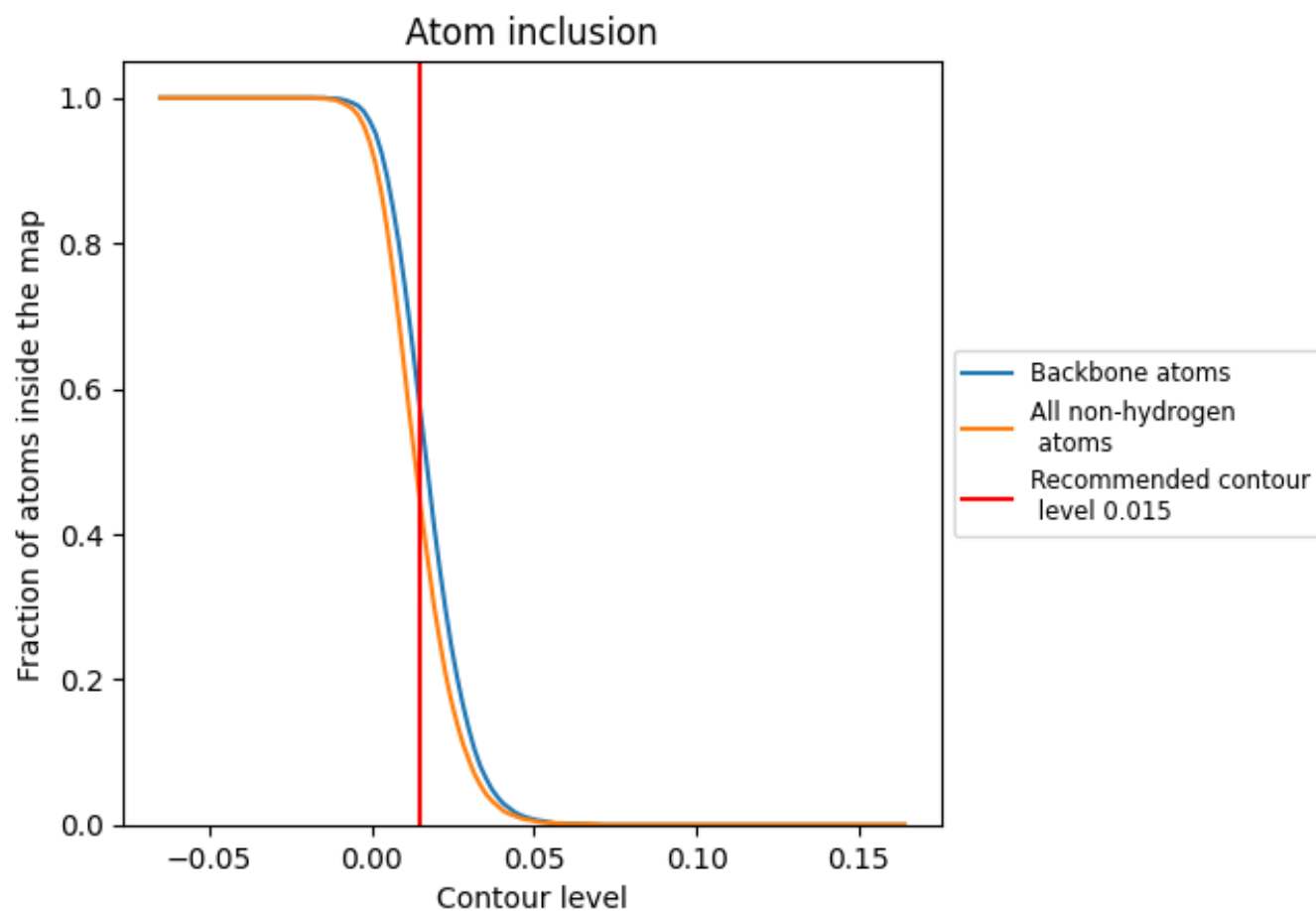
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 44% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4440	 0.2070
A	 0.5070	 0.2170
B	 0.5480	 0.2030
C	 0.5700	 0.2510
D	 0.5610	 0.1890
E	 0.6000	 0.2640
F	 0.5930	 0.2850
G	 0.6280	 0.3100
H	 0.4640	 0.2140
I	 0.5300	 0.3190
J	 0.4150	 0.2400
K	 0.4550	 0.2170
N	 0.3870	 0.2390
O	 0.6150	 0.3120
P	 0.4510	 0.1600
Q	 0.4600	 0.1990
R	 0.4950	 0.2050
S	 0.4550	 0.2110
T	 0.4280	 0.1380
U	 0.2380	 0.0680
V	 0.3470	 0.0900
W	 0.5280	 0.2830
X	 0.3220	 0.1470
Y	 0.3060	 0.0680
Z	 0.3940	 0.1600
c	 0.4890	 0.2340
i	 0.4740	 0.2120
j	 0.4560	 0.2920
k	 0.0980	 0.0790
n	 0.4250	 0.2870
o	 0.3980	 0.1560
p	 0.3520	 0.1240
q	 0.3380	 0.0930
r	 0.4500	 0.1890
z	 0.0330	 0.1250

