Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 04:22 PM EDT

PDB ID	:	9BV3 / pdb_00009bv3
EMDB ID	:	EMD-44930
Title	:	M1B Midnolin-Proteasome
Authors	:	Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on	:	2024-05-19
Resolution	:	2.90 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:

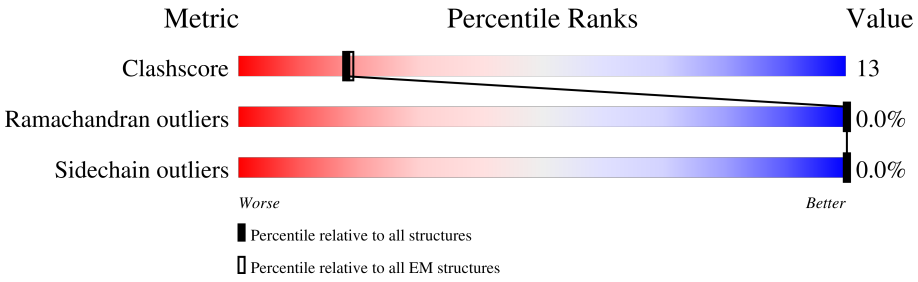
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	y	567	5% 95%
2	U	953	6% 61% 24% 15%
3	V	534	15% 57% 28% 14%
4	W	456	67% 29%
5	X	422	15% 70% 28%
6	Y	389	73% 25%
7	Z	324	6% 67% 22% 11%
8	a	376	20% 66% 33%

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Mol	Chain	Length	Quality of chain
9	b	377	19% 30% 20% 49%
10	c	310	6% 68% 25% 7%
11	d	350	12% 53% 22% 25%
12	e	70	7% 44% 11% 44%
13	A	433	67% 23% 10%
14	B	440	5% 58% 26% 16%
15	C	406	69% 19% 12%
16	D	418	68% 23% 9%
17	E	389	69% 24% 7%
18	F	439	54% 26% 21%
19	G	246	75% 22%
20	H	234	75% 23%
21	I	261	75% 23%
22	J	248	69% 28%
23	L	263	71% 19% 10%
24	M	255	71% 24% 5%
25	N	239	70% 13% 17%
25	n	239	59% 17% 23%
26	O	277	60% 20% 20%
26	o	277	8% 46% 18% 36%
27	P	205	70% 30%
27	p	205	20% 61% 19% 20%
28	Q	201	79% 19%
28	q	201	16% 62% 24% 14%
29	R	263	56% 20% 24%

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Mol	Chain	Length	Quality of chain
29	r	263	
30	S	241	
30	s	241	
31	T	264	
31	t	264	
32	K	241	
33	f	908	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 88575 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 Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	31	Total	C	N	O	S	0	0
			273	164	66	42	1		

There are 101 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-98	MET	-	initiating methionine	UNP Q504T8
y	-97	ASP	-	expression tag	UNP Q504T8
y	-96	TYR	-	expression tag	UNP Q504T8
y	-95	LYS	-	expression tag	UNP Q504T8
y	-94	ASP	-	expression tag	UNP Q504T8
y	-93	ASP	-	expression tag	UNP Q504T8
y	-92	ASP	-	expression tag	UNP Q504T8
y	-91	ASP	-	expression tag	UNP Q504T8
y	-90	LYS	-	expression tag	UNP Q504T8
y	-89	ASP	-	expression tag	UNP Q504T8
y	-88	TYR	-	expression tag	UNP Q504T8
y	-87	LYS	-	expression tag	UNP Q504T8
y	-86	ASP	-	expression tag	UNP Q504T8
y	-85	ASP	-	expression tag	UNP Q504T8
y	-84	ASP	-	expression tag	UNP Q504T8
y	-83	ASP	-	expression tag	UNP Q504T8
y	-82	LYS	-	expression tag	UNP Q504T8
y	-81	GLY	-	expression tag	UNP Q504T8
y	-80	GLY	-	expression tag	UNP Q504T8
y	-79	GLY	-	expression tag	UNP Q504T8
y	-78	GLY	-	expression tag	UNP Q504T8
y	-77	SER	-	expression tag	UNP Q504T8
y	-76	GLY	-	expression tag	UNP Q504T8
y	-75	GLY	-	expression tag	UNP Q504T8
y	-74	GLY	-	expression tag	UNP Q504T8
y	-73	GLY	-	expression tag	UNP Q504T8
y	-72	PHE	-	expression tag	UNP Q504T8
y	-71	GLU	-	expression tag	UNP Q504T8

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Chain	Residue	Modelled	Actual	Comment	Reference
y	-70	THR	-	expression tag	UNP Q504T8
y	-69	SER	-	expression tag	UNP Q504T8
y	-68	LEU	-	expression tag	UNP Q504T8
y	-67	TYR	-	expression tag	UNP Q504T8
y	-66	LYS	-	expression tag	UNP Q504T8
y	-65	LYS	-	expression tag	UNP Q504T8
y	-64	ALA	-	expression tag	UNP Q504T8
y	-63	GLY	-	expression tag	UNP Q504T8
y	-62	LEU	-	expression tag	UNP Q504T8
y	-61	ALA	-	expression tag	UNP Q504T8
y	-60	THR	-	expression tag	UNP Q504T8
y	-59	MET	-	expression tag	UNP Q504T8
y	-58	GLU	-	expression tag	UNP Q504T8
y	-57	LYS	-	expression tag	UNP Q504T8
y	-56	VAL	-	expression tag	UNP Q504T8
y	-55	LEU	-	expression tag	UNP Q504T8
y	-54	VAL	-	expression tag	UNP Q504T8
y	-53	GLU	-	expression tag	UNP Q504T8
y	-52	THR	-	expression tag	UNP Q504T8
y	-51	SER	-	expression tag	UNP Q504T8
y	-50	TYR	-	expression tag	UNP Q504T8
y	-49	PRO	-	expression tag	UNP Q504T8
y	-48	SER	-	expression tag	UNP Q504T8
y	-47	GLN	-	expression tag	UNP Q504T8
y	-46	THR	-	expression tag	UNP Q504T8
y	-45	THR	-	expression tag	UNP Q504T8
y	-44	ARG	-	expression tag	UNP Q504T8
y	-43	LEU	-	expression tag	UNP Q504T8
y	-42	PRO	-	expression tag	UNP Q504T8
y	-41	PRO	-	expression tag	UNP Q504T8
y	-40	ILE	-	expression tag	UNP Q504T8
y	-39	THR	-	expression tag	UNP Q504T8
y	-38	TYR	-	expression tag	UNP Q504T8
y	-37	THR	-	expression tag	UNP Q504T8
y	-36	GLY	-	expression tag	UNP Q504T8
y	-35	ARG	-	expression tag	UNP Q504T8
y	-34	PHE	-	expression tag	UNP Q504T8
y	-33	SER	-	expression tag	UNP Q504T8
y	-32	LEU	-	expression tag	UNP Q504T8
y	-31	GLU	-	expression tag	UNP Q504T8
y	-30	PRO	-	expression tag	UNP Q504T8
y	-29	ALA	-	expression tag	UNP Q504T8

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Chain	Residue	Modelled	Actual	Comment	Reference
y	-28	PRO	-	expression tag	UNP Q504T8
y	-27	ASN	-	expression tag	UNP Q504T8
y	-26	SER	-	expression tag	UNP Q504T8
y	-25	GLY	-	expression tag	UNP Q504T8
y	-24	ASN	-	expression tag	UNP Q504T8
y	-23	THR	-	expression tag	UNP Q504T8
y	-22	LEU	-	expression tag	UNP Q504T8
y	-21	TRP	-	expression tag	UNP Q504T8
y	-20	PRO	-	expression tag	UNP Q504T8
y	-19	GLU	-	expression tag	UNP Q504T8
y	-18	PRO	-	expression tag	UNP Q504T8
y	-17	LEU	-	expression tag	UNP Q504T8
y	-16	PHE	-	expression tag	UNP Q504T8
y	-15	SER	-	expression tag	UNP Q504T8
y	-14	LEU	-	expression tag	UNP Q504T8
y	-13	VAL	-	expression tag	UNP Q504T8
y	-12	SER	-	expression tag	UNP Q504T8
y	-11	GLY	-	expression tag	UNP Q504T8
y	-10	LEU	-	expression tag	UNP Q504T8
y	-9	VAL	-	expression tag	UNP Q504T8
y	-8	SER	-	expression tag	UNP Q504T8
y	-7	MET	-	expression tag	UNP Q504T8
y	-6	THR	-	expression tag	UNP Q504T8
y	-5	ASN	-	expression tag	UNP Q504T8
y	-4	PRO	-	expression tag	UNP Q504T8
y	-3	PRO	-	expression tag	UNP Q504T8
y	-2	ALA	-	expression tag	UNP Q504T8
y	-1	SER	-	expression tag	UNP Q504T8
y	0	SER	-	expression tag	UNP Q504T8
y	1	SER	-	expression tag	UNP Q504T8
y	457	ALA	VAL	conflict	UNP Q504T8

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	812	Total	C	N	O	S	0	0
			6334	4021	1078	1190	45		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	457	Total	C	N	O	S	0	0
			3725	2364	669	679	13		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	438	Total	C	N	O	S	0	0
			3572	2262	610	677	23		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	413	Total	C	N	O	S	0	0
			3259	2073	556	618	12		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	381	Total	C	N	O	S	0	0
			3135	2000	536	582	17		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	261	Total	C	N	O	S	0	0
			2124	1376	348	391	9		

- Molecule 12 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	39	Total	C	N	O	0	0
			345	213	54	78		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	389	Total	C	N	O	S	0	0
			3057	1927	537	575	18		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	371	Total	C	N	O	S	0	0
			2933	1846	499	574	14		

- Molecule 15 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	359	Total	C	N	O	S	0	0
			2834	1790	509	519	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 17 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	362	Total	C	N	O	S	0	0
			2869	1805	508	540	16		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	349	Total	C	N	O	S	0	0
			2724	1721	469	519	15		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	238	Total	C	N	O	S	0	0
			1865	1186	311	355	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	229	Total	C	N	O	S	0	0
			1789	1145	301	337	6		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	254	Total	C	N	O	S	0	0
			2007	1267	345	385	10		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	237	Total	C	N	O	S	0	0
			1868	1168	338	351	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	243	Total	C	N	O	S	0	0
			1909	1208	324	366	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
25	n	183	Total	C	N	O	S	0	0
			1360	849	234	265	12		

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
26	o	176	Total	C	N	O	S	0	0
			1315	823	228	253	11		

- Molecule 27 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
27	p	165	Total	C	N	O	S	0	0
			1271	806	211	237	17		

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
28	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 29 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
29	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 30 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
30	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		
31	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

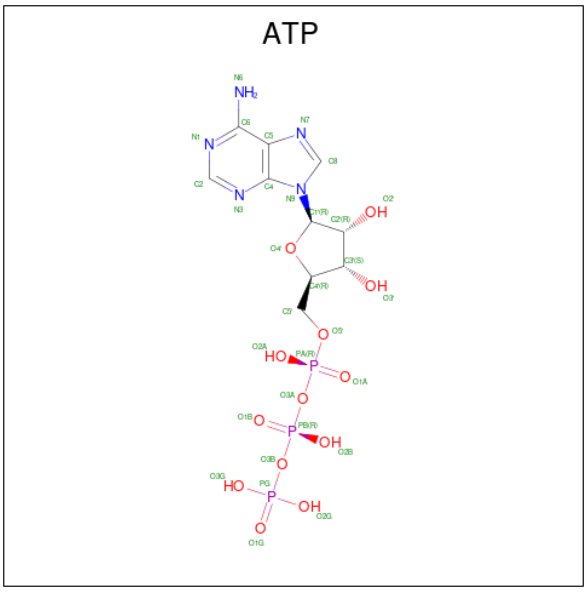
- Molecule 32 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	227	Total	C	N	O	S	0	0
			1736	1093	288	344	11		

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	647	Total	C	N	O	S	0	0
			4942	3141	835	932	34		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

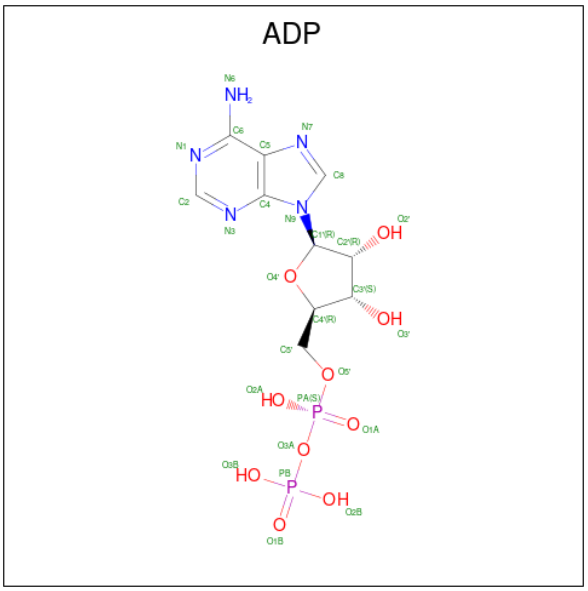


Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



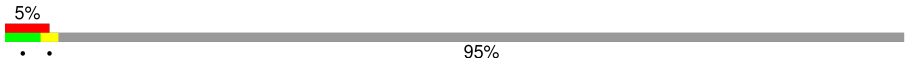
Mol	Chain	Residues	Atoms					AltConf
36	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

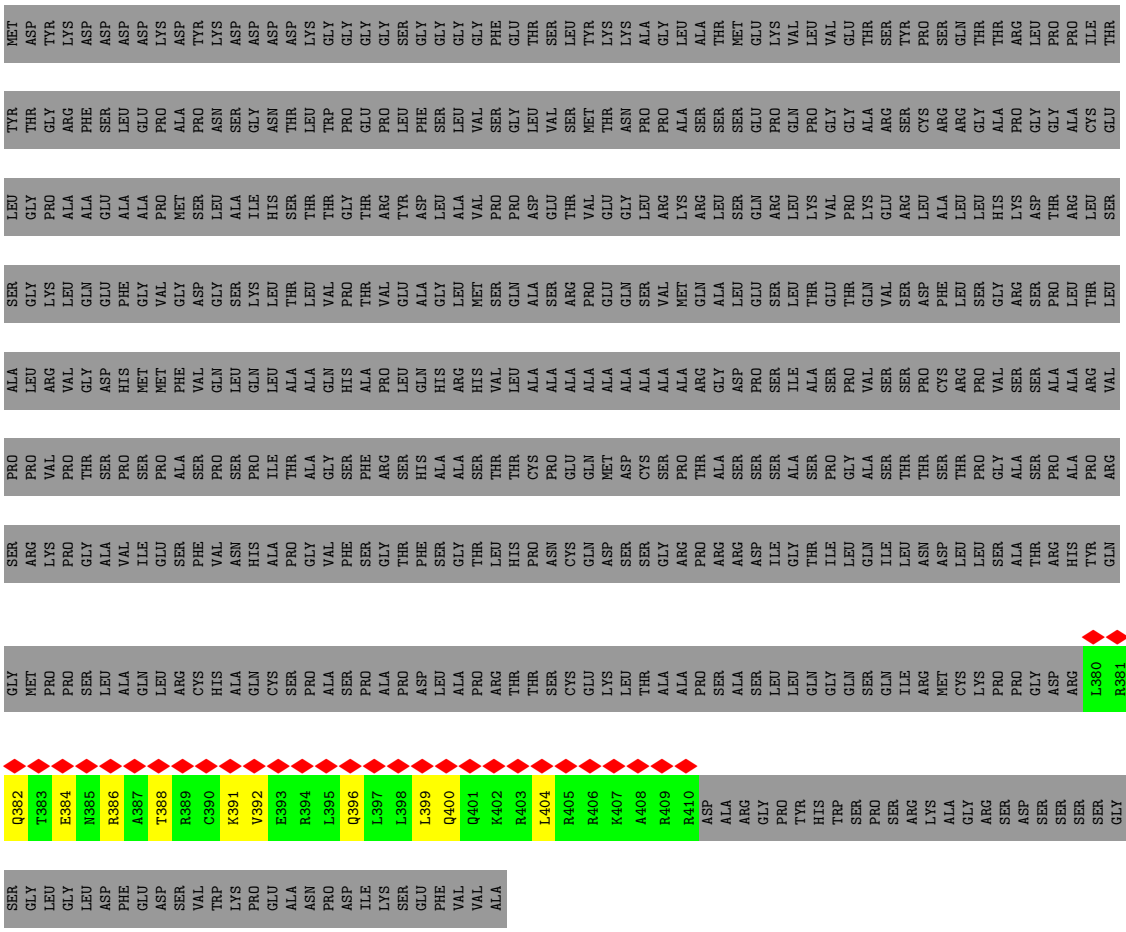
3 Residue-property plots (i)

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

• Molecule 1: Midnolin

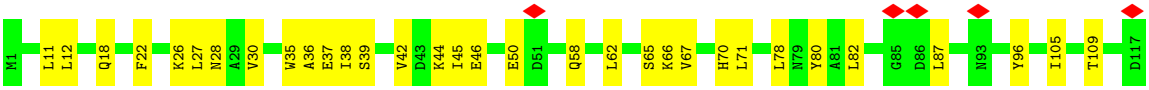
Chain y:

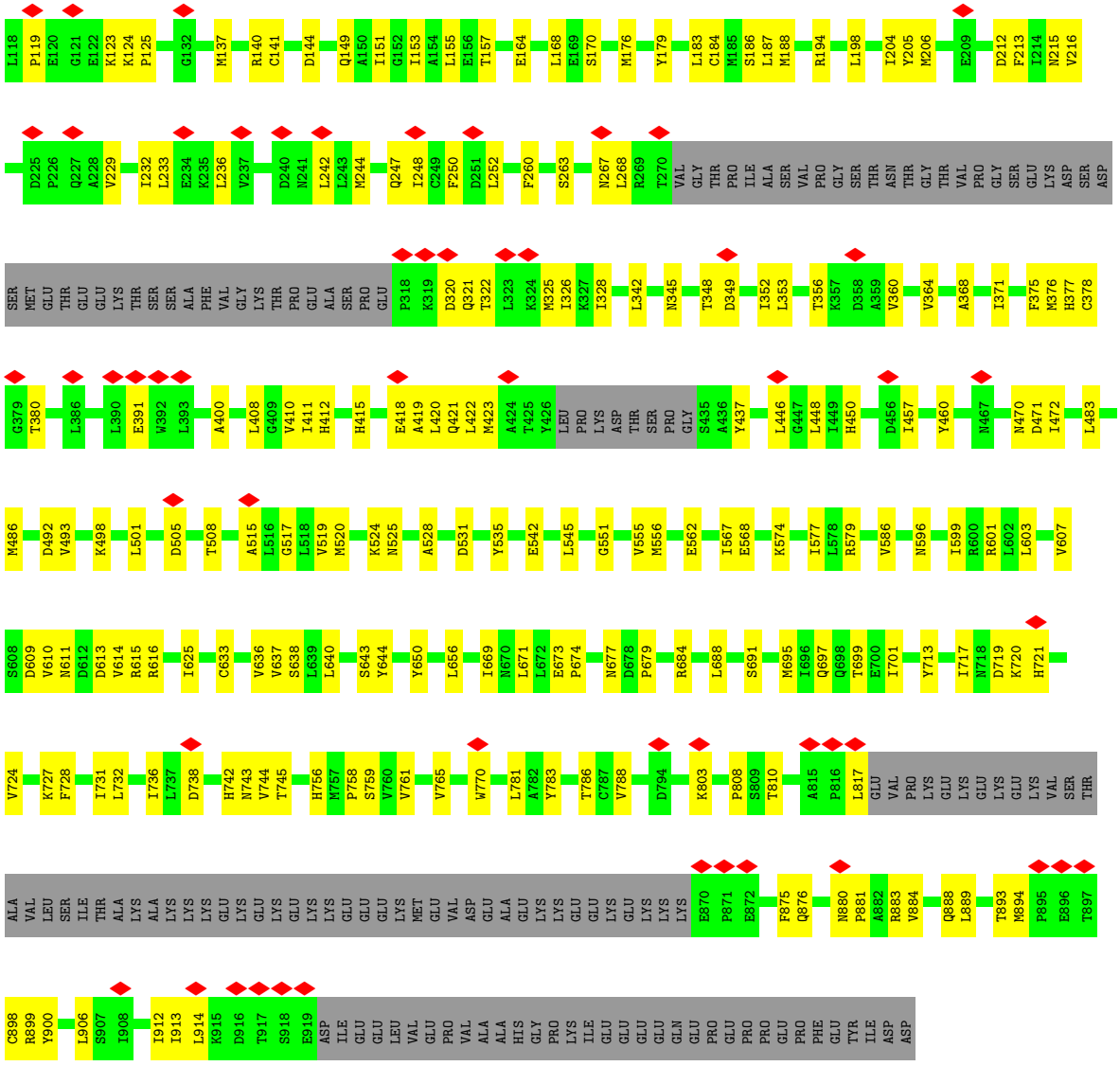




• Molecule 2: 26S proteasome non-ATPase regulatory subunit 1

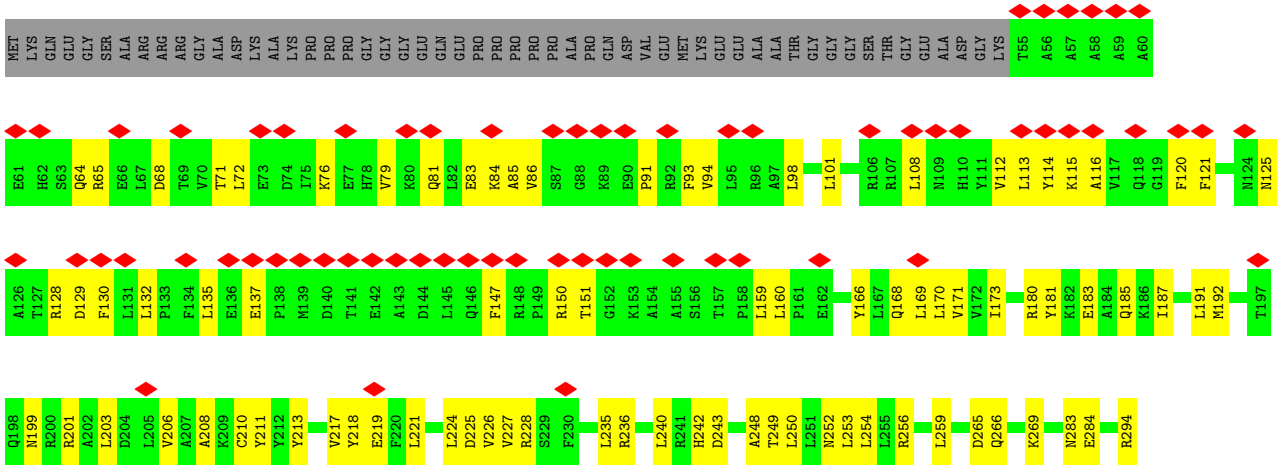
Chain U:

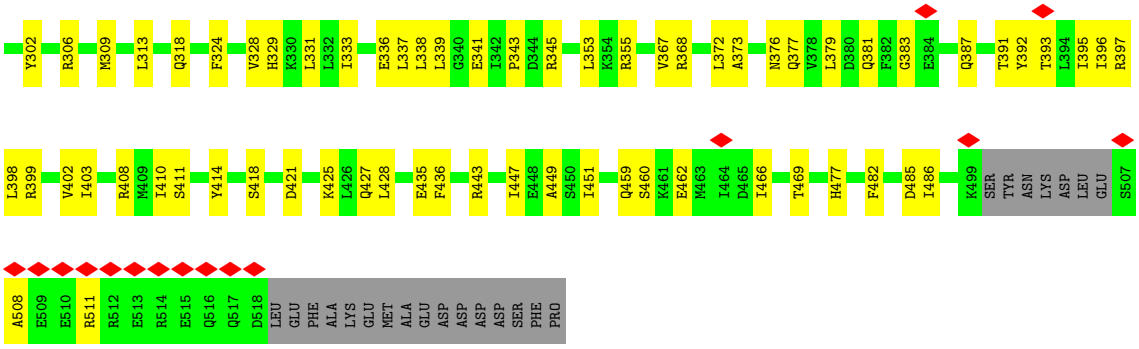




• Molecule 3: 26S proteasome non-ATPase regulatory subunit 3

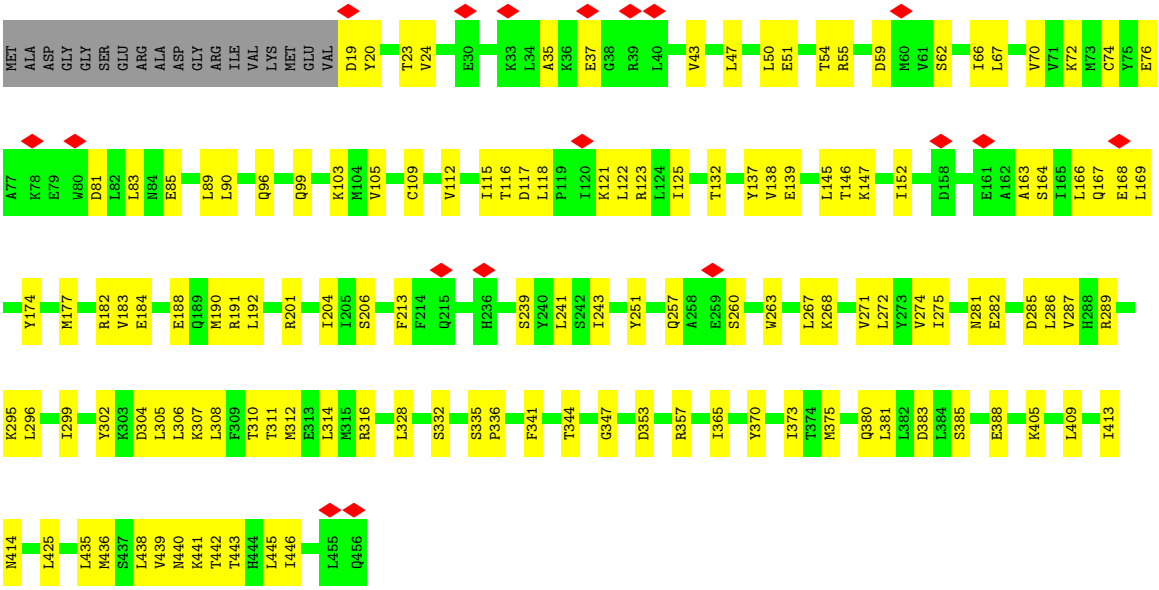
Chain V:





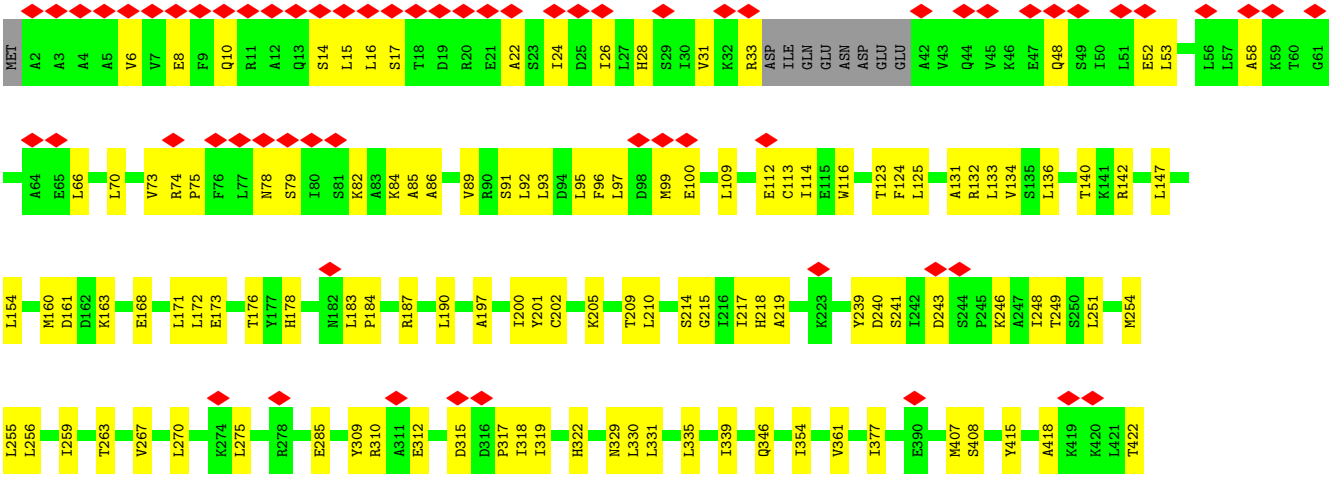
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



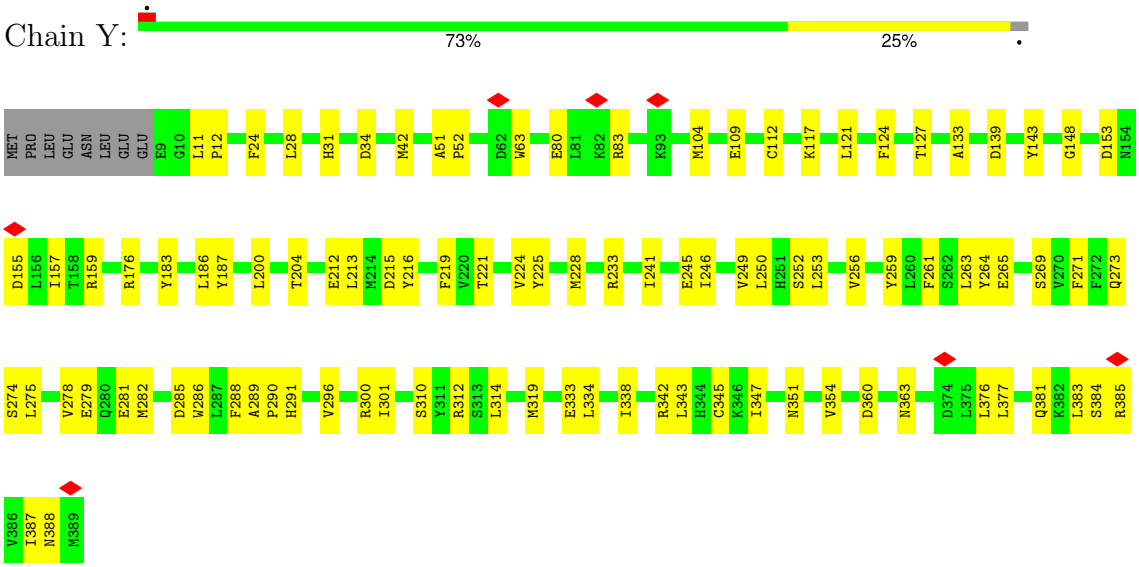
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



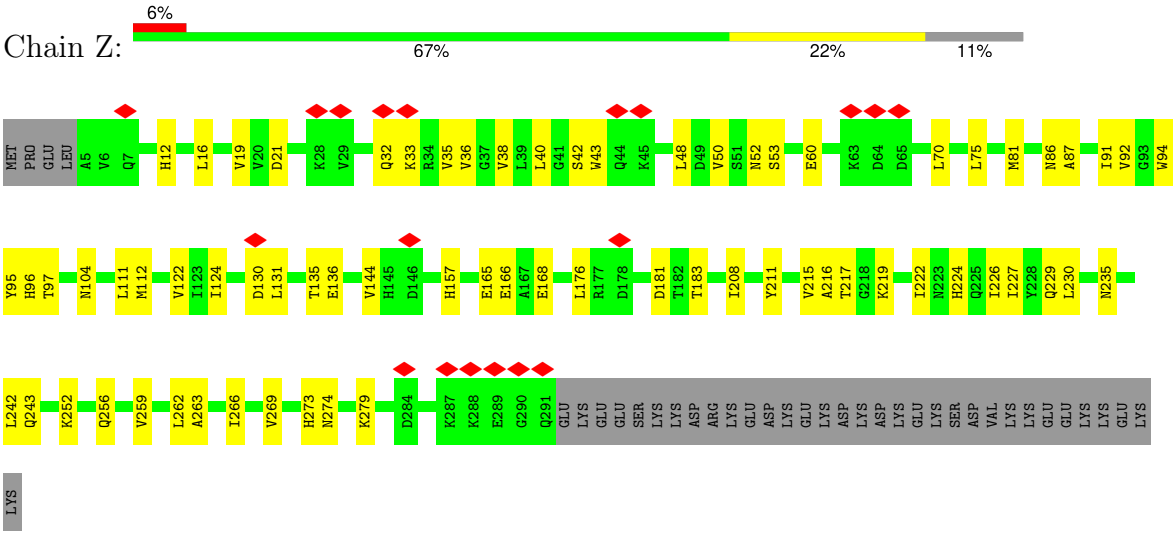
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



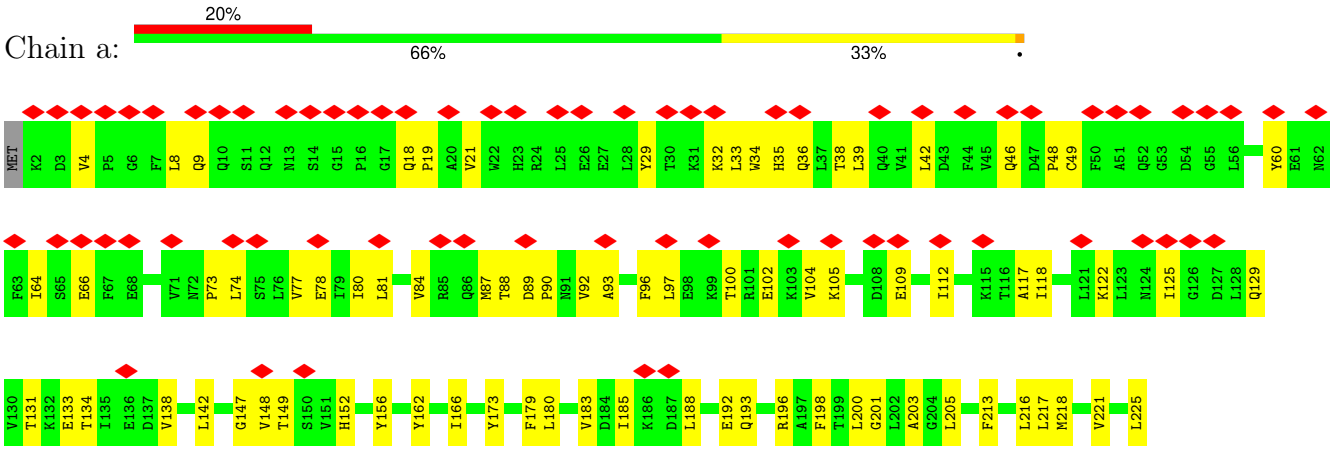
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 7

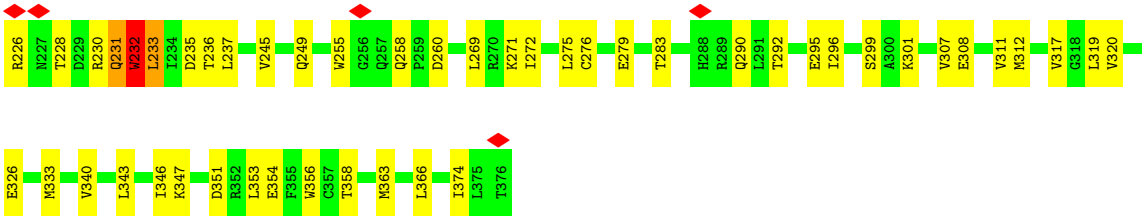
Chain Z:



• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

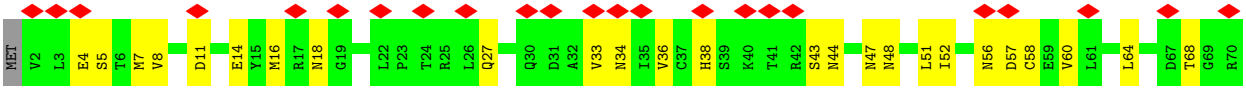
Chain a:

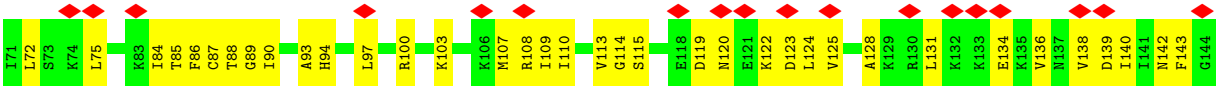


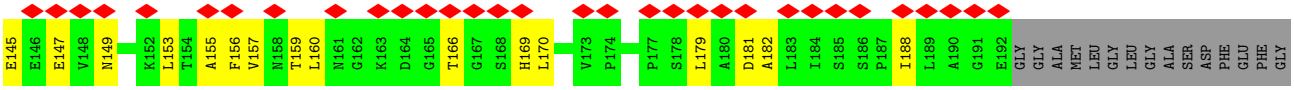


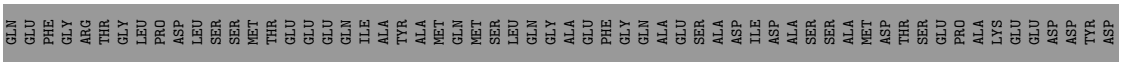
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



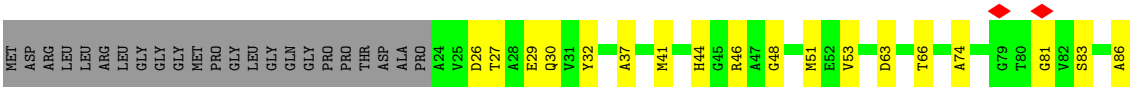


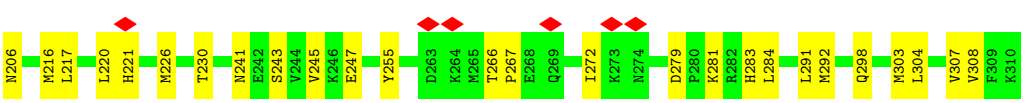




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 14

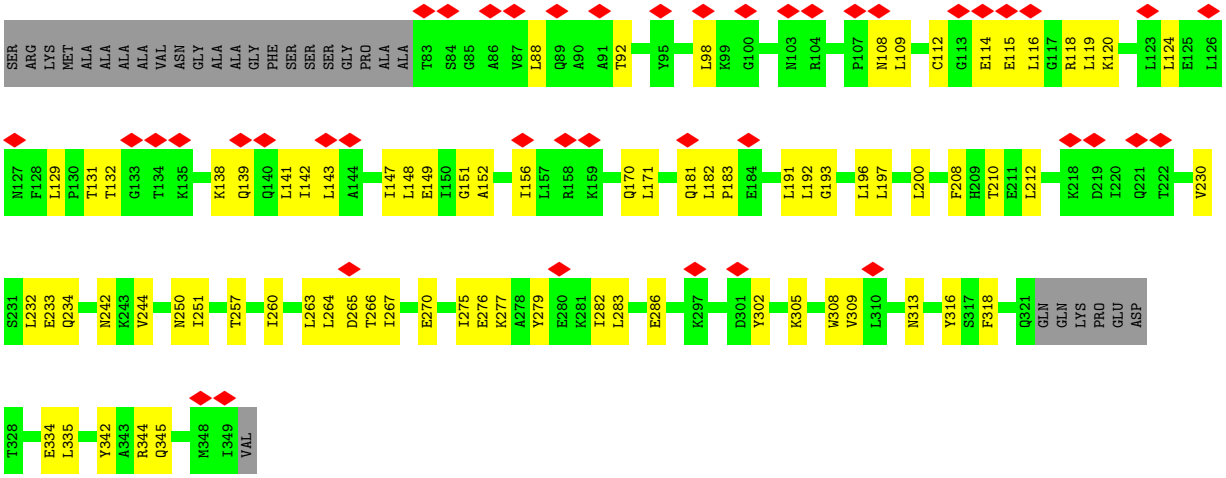
Chain c:





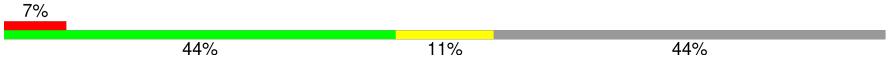
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 8

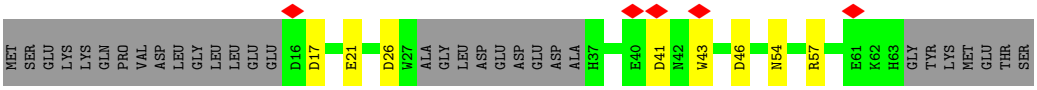
Chain d:



• Molecule 12: 26S proteasome complex subunit SEM1

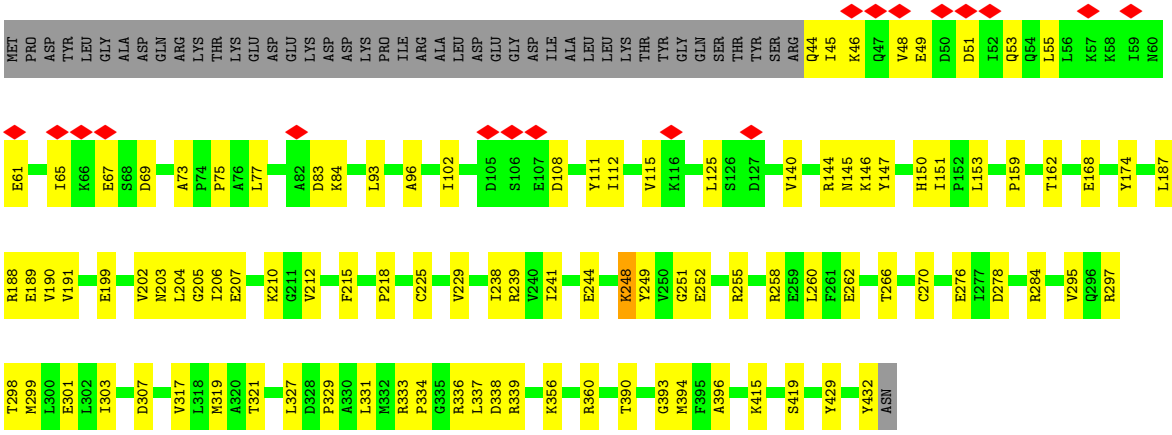
Chain e:





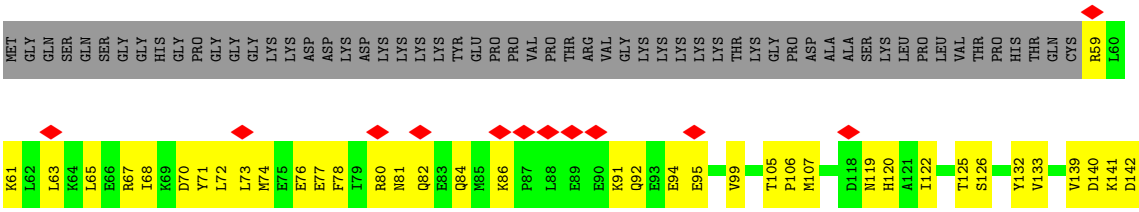
• Molecule 13: 26S proteasome regulatory subunit 7

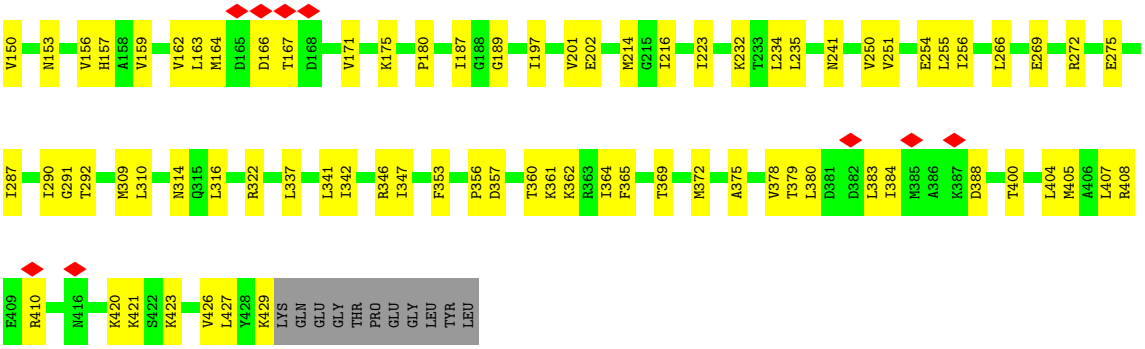
Chain A:



• Molecule 14: 26S proteasome regulatory subunit 4

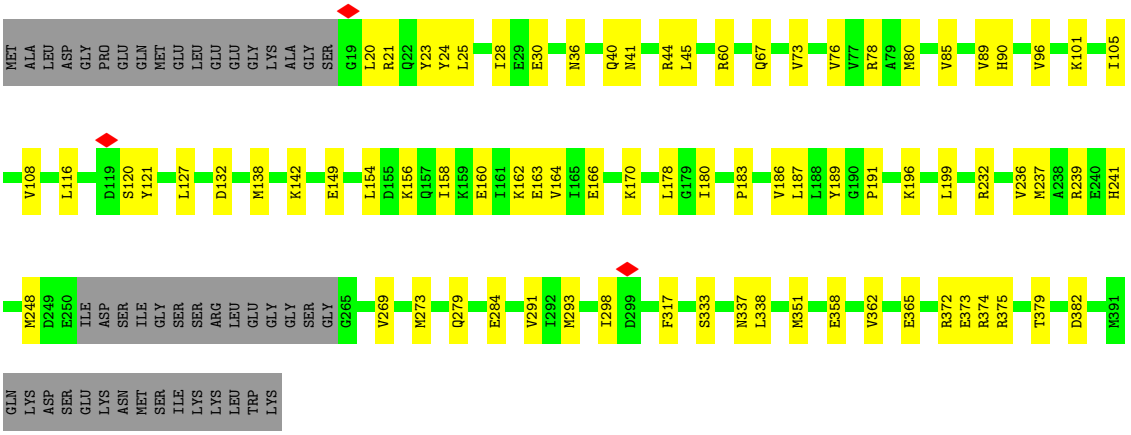
Chain B:





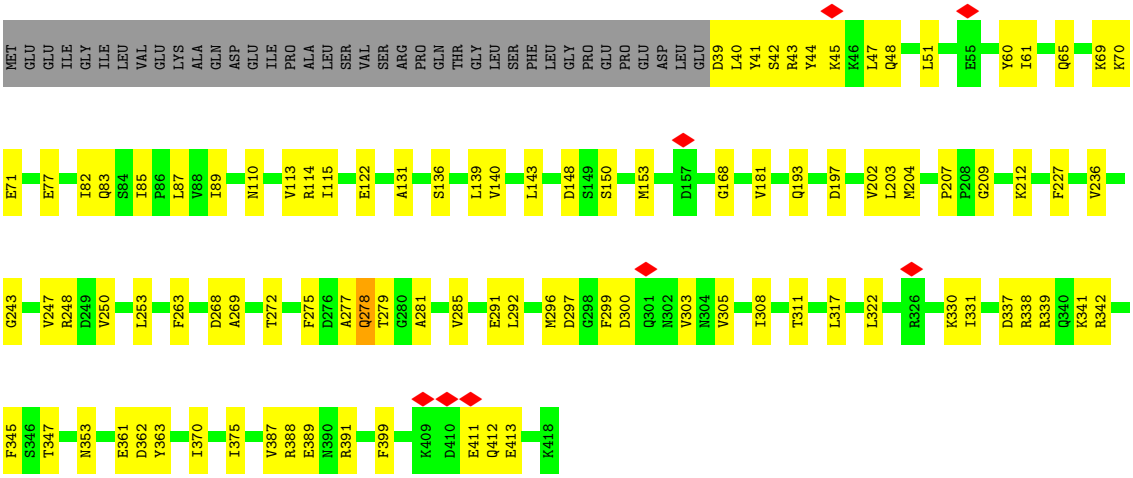
• Molecule 15: 26S protease regulatory subunit 8

Chain C:



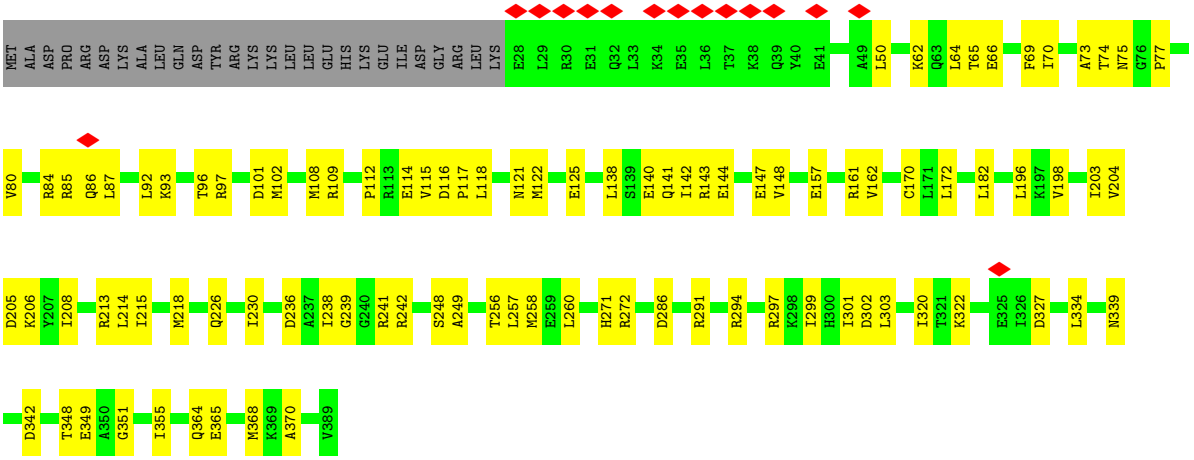
• Molecule 16: 26S proteasome regulatory subunit 6B

Chain D:



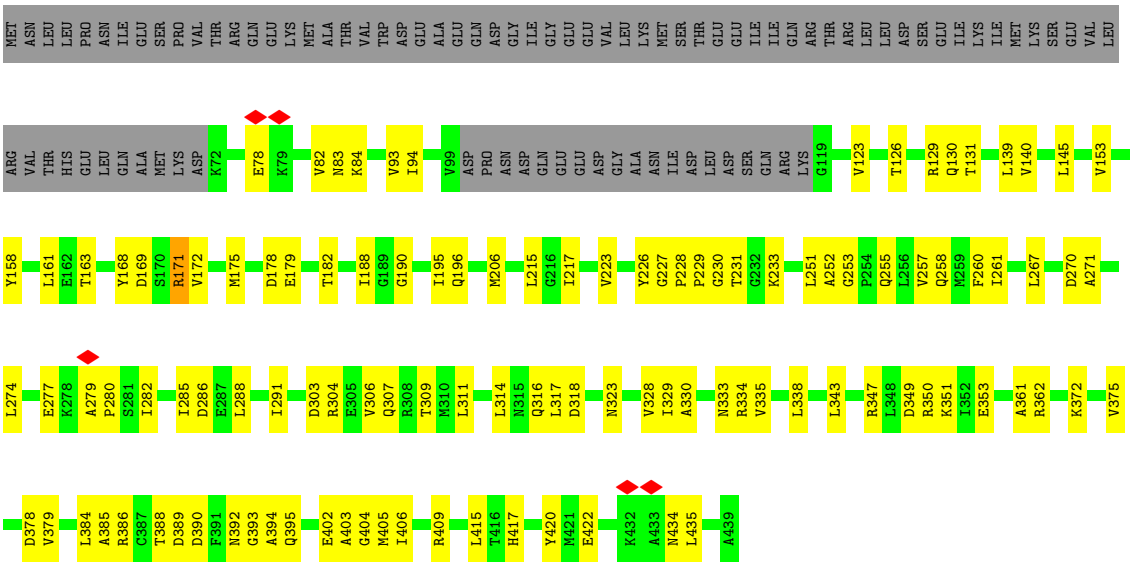
• Molecule 17: 26S protease regulatory subunit 10B

Chain E:



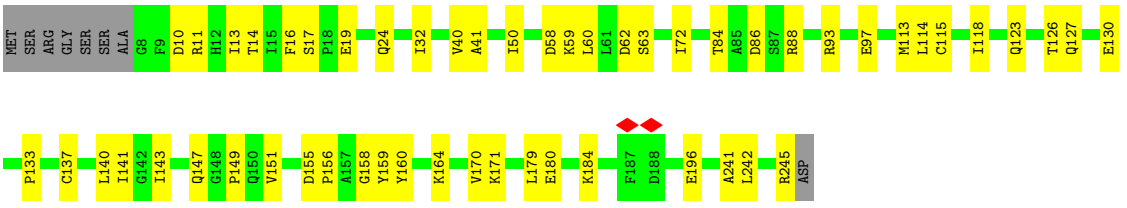
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F:



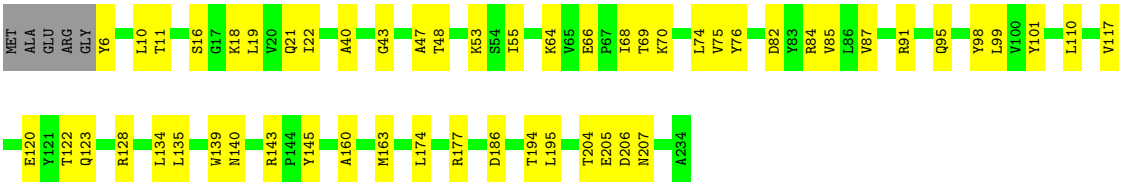
• Molecule 19: Proteasome subunit alpha type-6

Chain G:



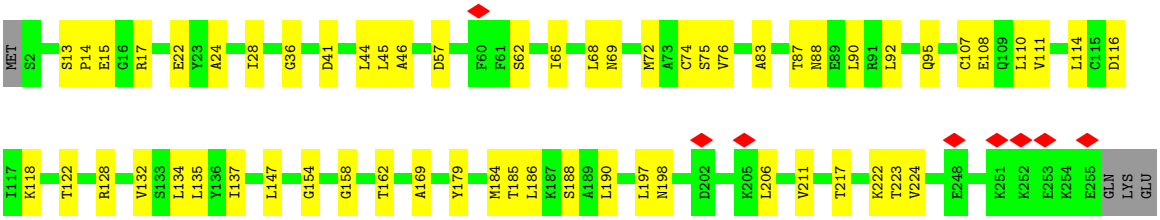
• Molecule 20: Proteasome subunit alpha type-2

Chain H:



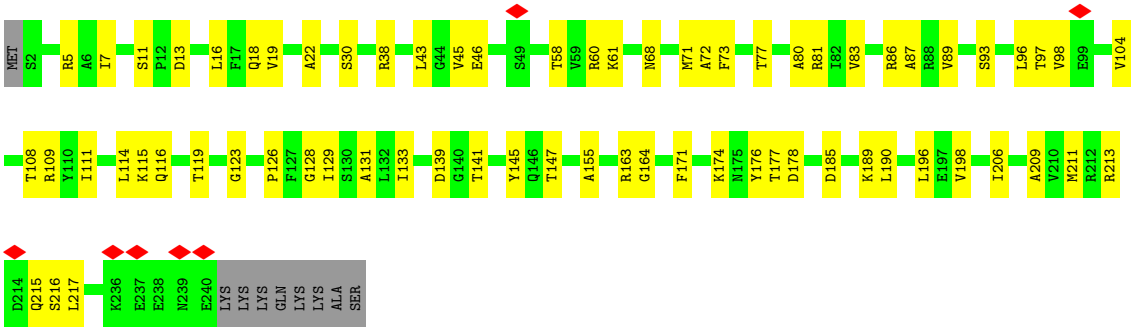
• Molecule 21: Proteasome subunit alpha type-4

Chain I:



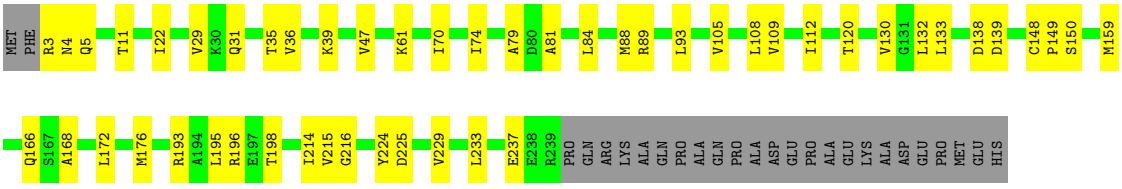
• Molecule 22: Proteasome subunit alpha type-7

Chain J:



• Molecule 23: Proteasome subunit alpha type-1

Chain L:

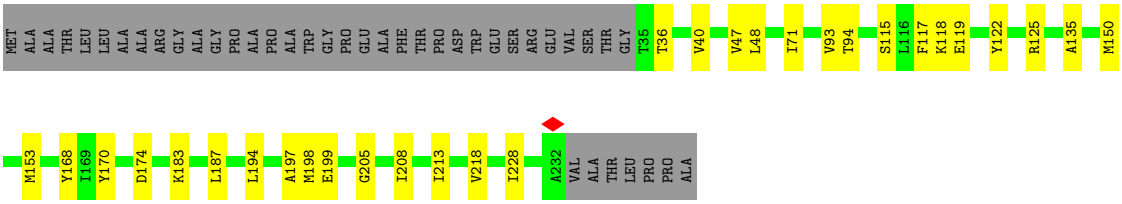


• Molecule 24: Proteasome subunit alpha type-3

Chain M:

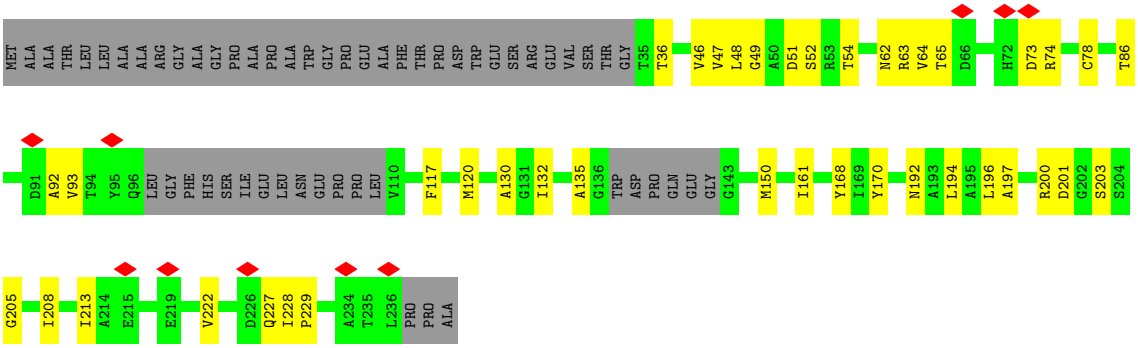
• Molecule 25: Proteasome subunit beta type-6

Chain N:



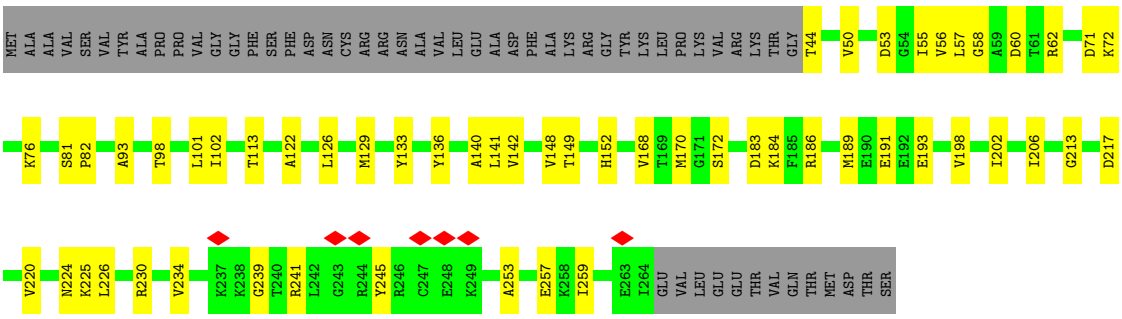
• Molecule 25: Proteasome subunit beta type-6

Chain n:



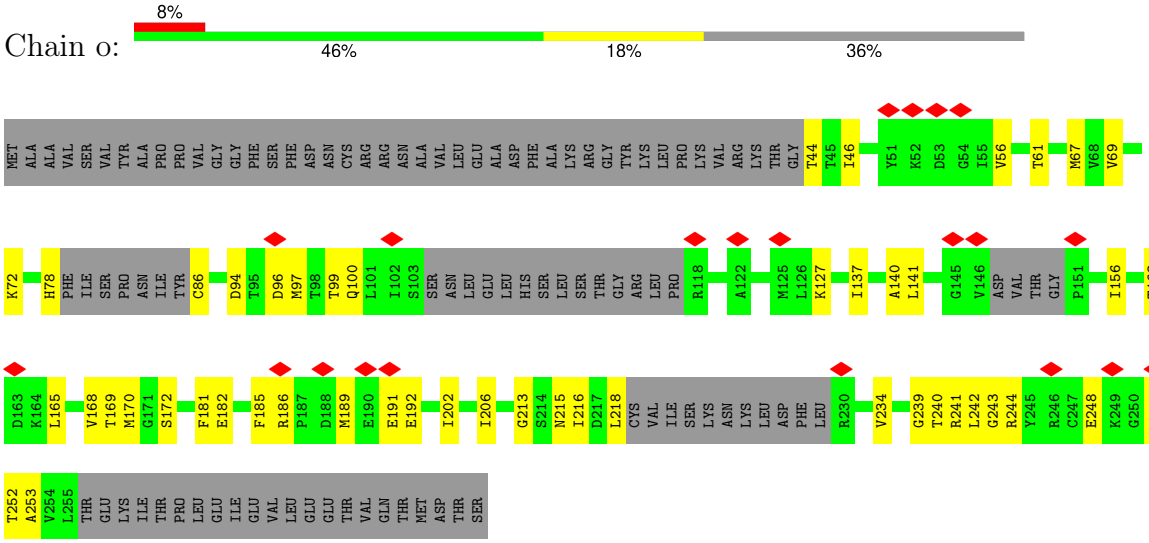
• Molecule 26: Proteasome subunit beta type-7

Chain O:



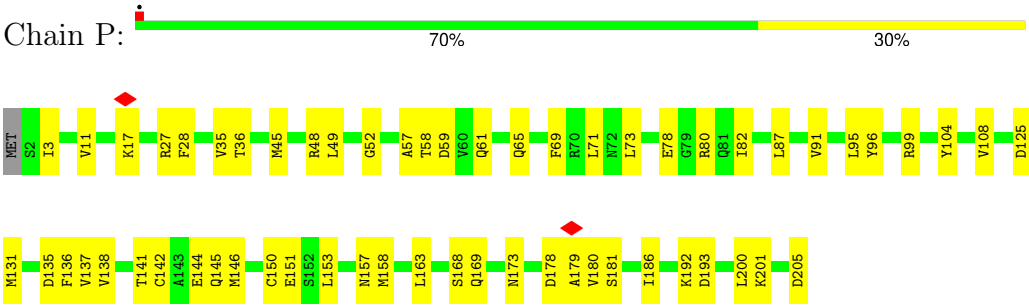
• Molecule 26: Proteasome subunit beta type-7

Chain o:



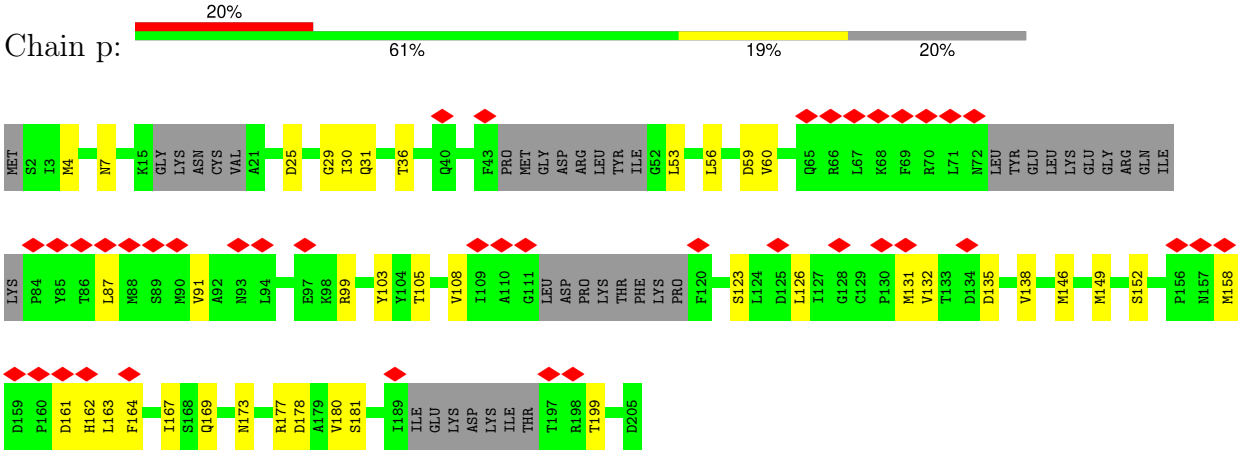
• Molecule 27: Proteasome subunit beta type-3

Chain P:



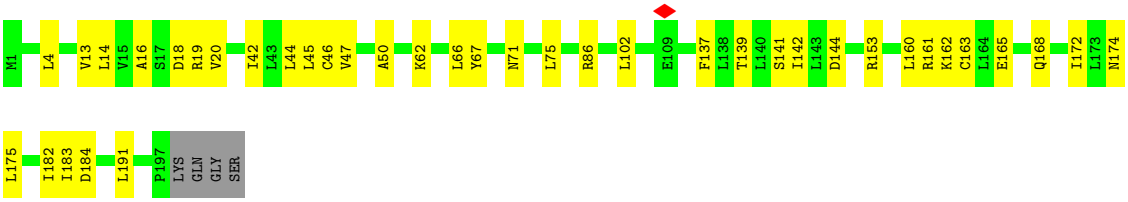
• Molecule 27: Proteasome subunit beta type-3

Chain p:

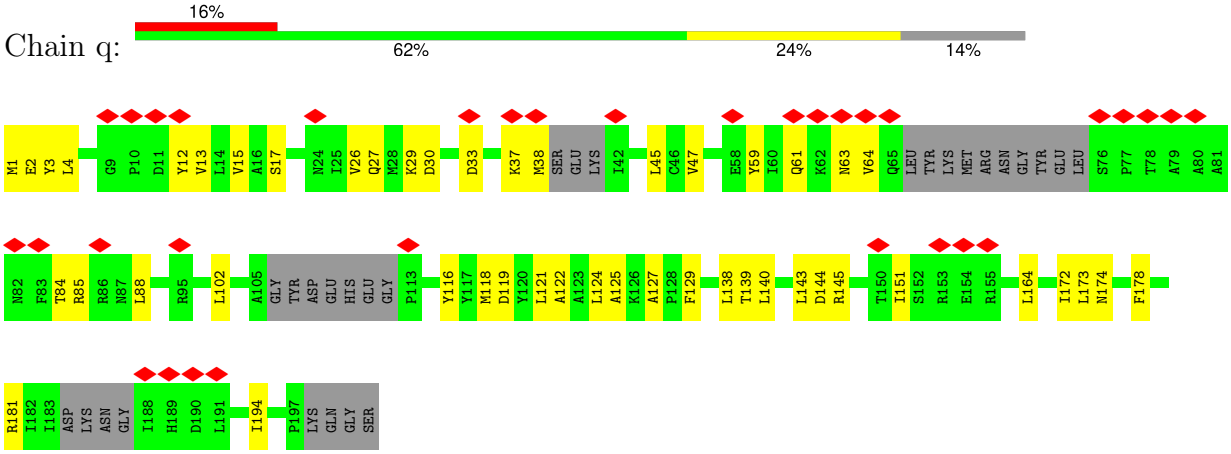


• Molecule 28: Proteasome subunit beta type-2

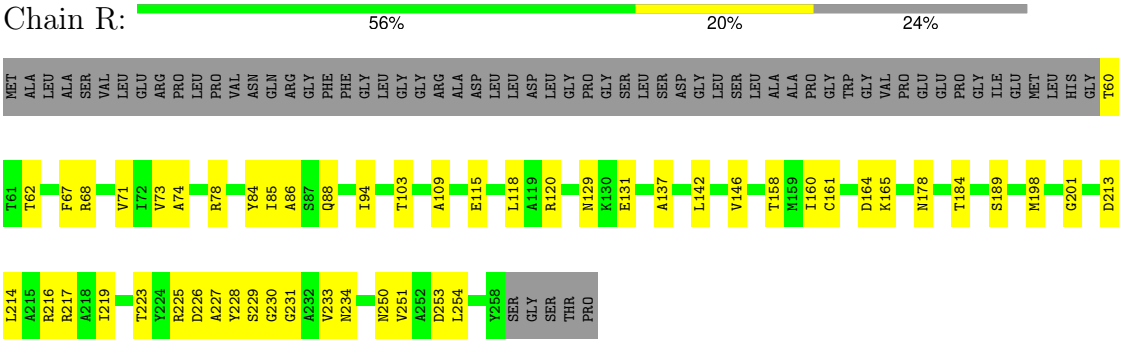
Chain Q:



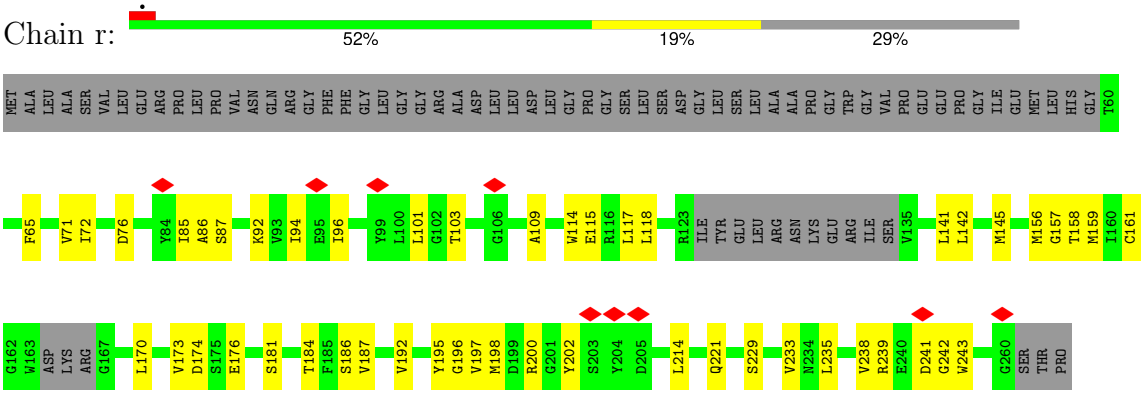
• Molecule 28: Proteasome subunit beta type-2



• Molecule 29: Proteasome subunit beta type-5

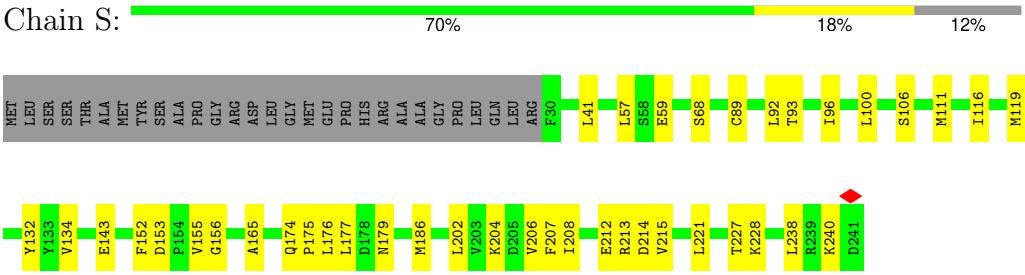


• Molecule 29: Proteasome subunit beta type-5



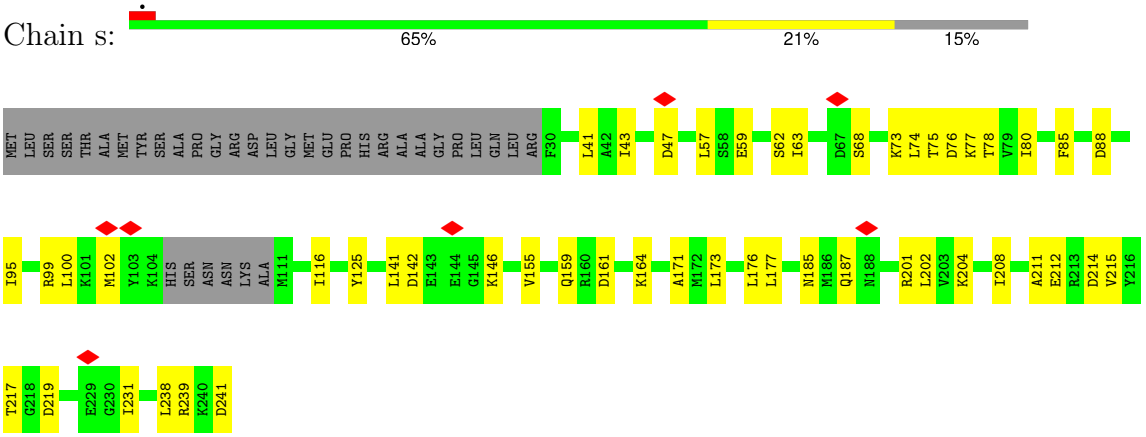
• Molecule 30: Proteasome subunit beta type-1

Chain S:



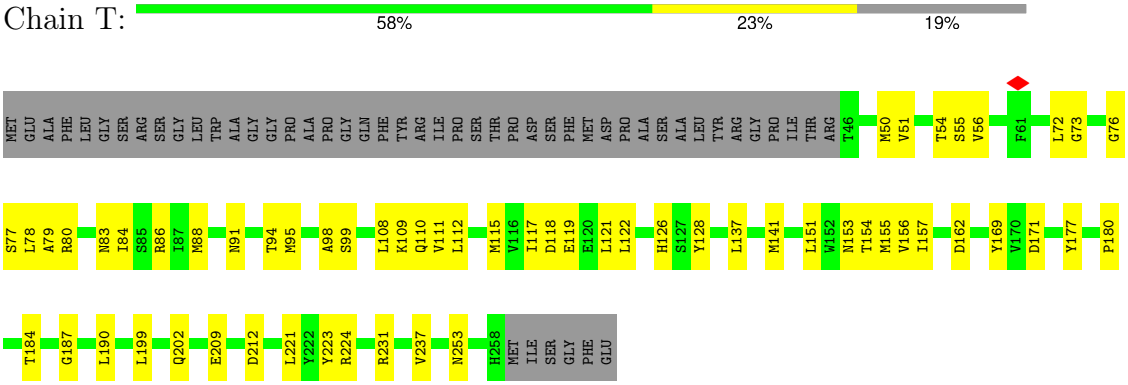
• Molecule 30: Proteasome subunit beta type-1

Chain s:



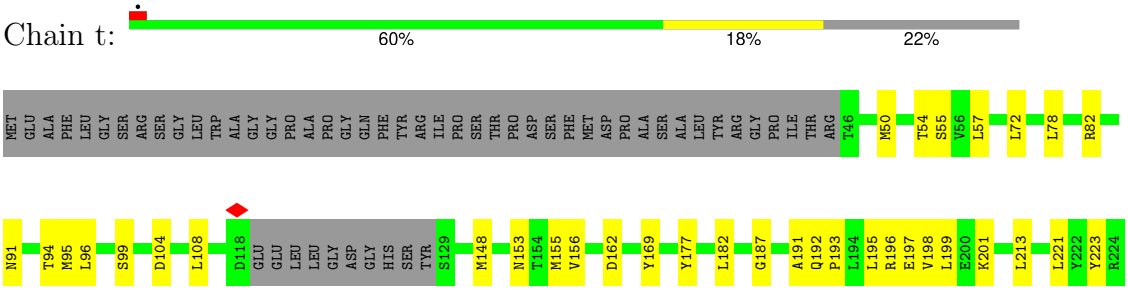
• Molecule 31: Proteasome subunit beta type-4

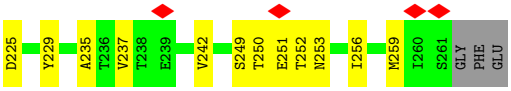
Chain T:



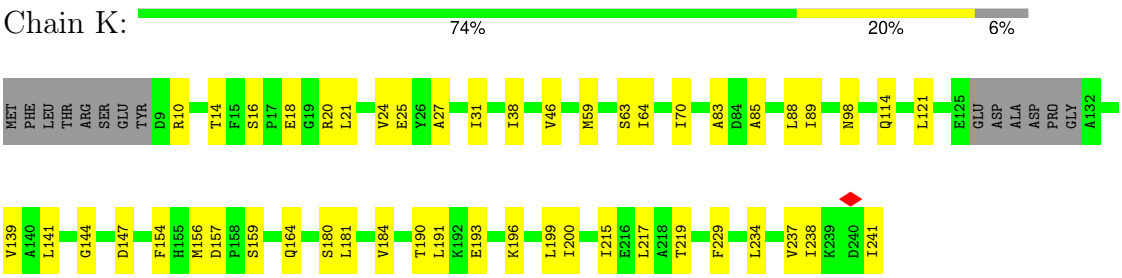
• Molecule 31: Proteasome subunit beta type-4

Chain t:

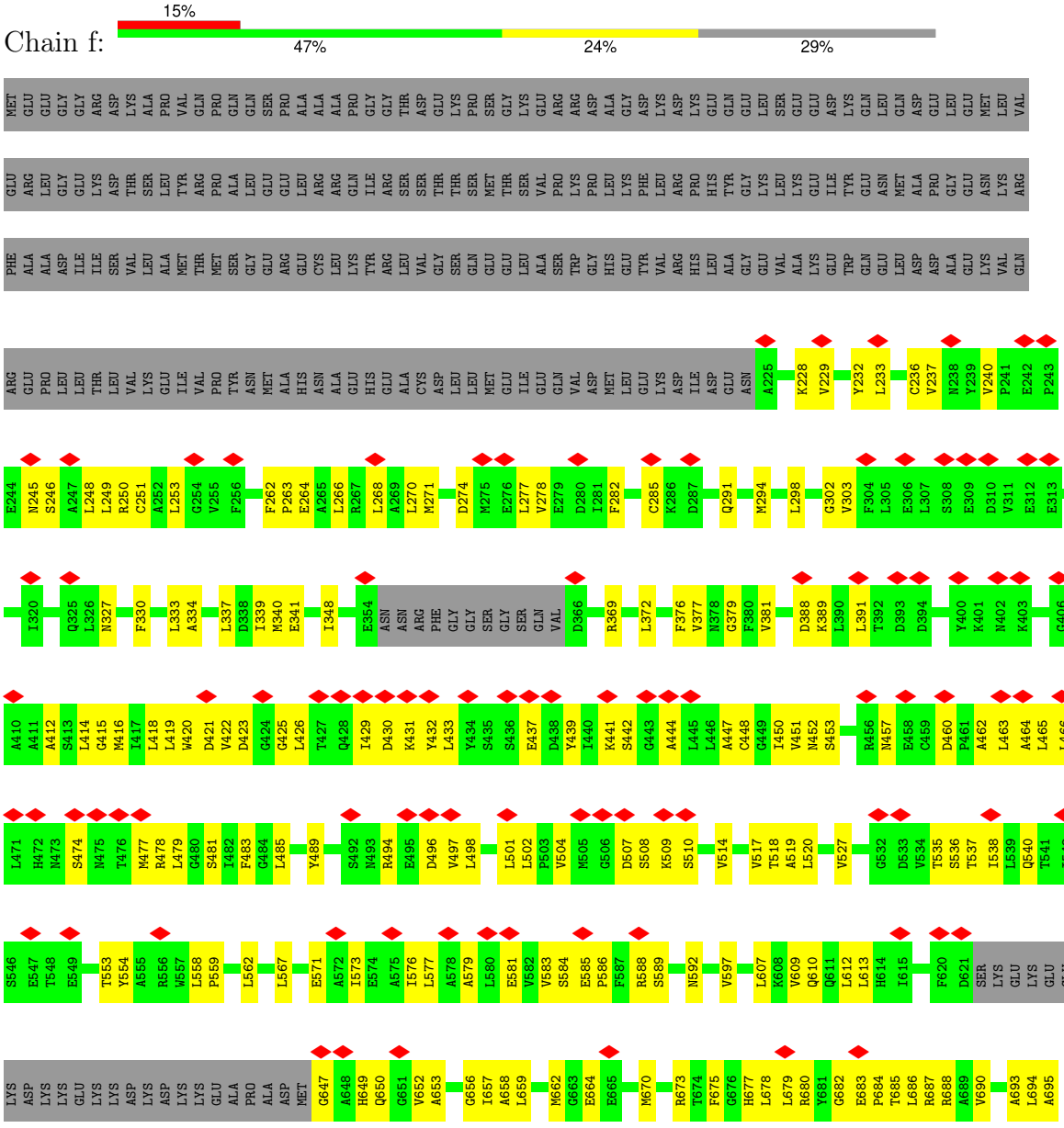


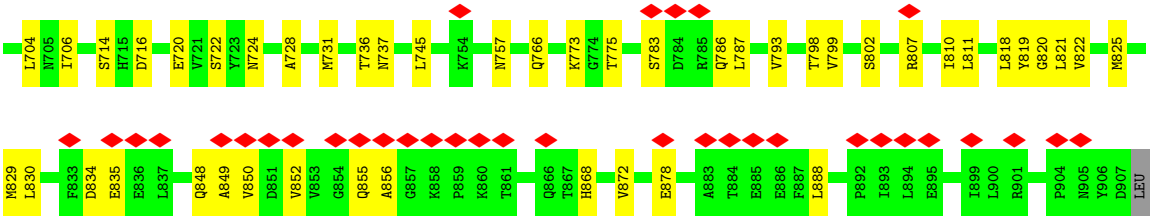


• Molecule 32: Proteasome subunit alpha type-5



• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2




L704
N705
I706
S714
H715
D716
E720
V721
S722
Y723
N724
A728
M731
T736
N737
L745
K754
N757
Q766
K773
G774
T775
S783
D784
R785
Q786
L787
V793
T798
V799
S802
R807
I810
L811
L818
Y819
G820
L821
V822
M825
M829
L830
F833
D834
E835
E836
L837
Q848
A849
V850
D851
V852
V853
G854
Q855
A856
G857
K858
P859
K860
T861
Q866
T867
H868
V872
E878
A883
T884
E885
E886
F887
L888
P892
I893
L894
E895
I899
L900
R901
P904
N905
Y906
D907
LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113946	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.310	Depositor
Minimum map value	-1.762	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

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	y	0.13	0/272	0.26	0/357
2	U	0.13	0/6446	0.32	1/8720 (0.0%)
3	V	0.14	0/3794	0.34	0/5118
4	W	0.12	0/3620	0.32	0/4869
5	X	0.13	0/3304	0.33	0/4453
6	Y	0.14	0/3193	0.31	0/4302
7	Z	0.13	0/2333	0.28	0/3162
8	a	0.17	0/3070	0.46	5/4155 (0.1%)
9	b	0.11	0/1479	0.32	0/2003
10	c	0.14	0/2302	0.36	0/3110
11	d	0.13	0/2168	0.32	0/2928
12	e	0.09	0/355	0.23	0/482
13	A	0.18	0/3108	0.38	1/4196 (0.0%)
14	B	0.17	0/2974	0.37	0/4009
15	C	0.14	0/2872	0.31	0/3866
16	D	0.17	0/3090	0.36	0/4168
17	E	0.20	0/2914	0.36	0/3927
18	F	0.19	0/2762	0.40	0/3723
19	G	0.14	0/1899	0.31	0/2567
20	H	0.13	0/1828	0.31	0/2476
21	I	0.14	0/2037	0.31	0/2740
22	J	0.14	0/1913	0.29	0/2581
23	L	0.14	0/1902	0.30	0/2569
24	M	0.13	0/1944	0.30	0/2617
25	N	0.13	0/1513	0.29	0/2047
25	n	0.11	0/1377	0.28	0/1857
26	O	0.14	0/1694	0.30	0/2293
26	o	0.11	0/1331	0.30	0/1791
27	P	0.15	0/1620	0.35	0/2184
27	p	0.13	0/1289	0.36	0/1732
28	Q	0.14	0/1611	0.30	0/2180
28	q	0.12	0/1405	0.28	0/1899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	R	0.13	0/1580	0.30	0/2134
29	r	0.12	0/1460	0.32	0/1972
30	S	0.12	0/1673	0.28	0/2254
30	s	0.12	0/1625	0.32	0/2188
31	T	0.13	0/1698	0.33	0/2299
31	t	0.12	0/1639	0.29	0/2217
32	K	0.14	0/1761	0.32	0/2376
33	f	0.14	0/5027	0.36	0/6816
All	All	0.14	0/89882	0.33	7/121337 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	233	LEU	N-CA-C	-6.58	105.39	113.41
8	a	232	TRP	N-CA-C	-6.38	97.20	110.80
8	a	231	GLN	N-CA-CB	5.67	118.71	109.69
8	a	231	GLN	N-CA-C	-5.62	102.32	110.24
13	A	252	GLU	N-CA-C	-5.33	106.91	113.41
8	a	231	GLN	CA-C-O	-5.14	115.50	121.15
2	U	400	ALA	N-CA-C	-5.05	107.77	114.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	y	273	0	309	10	0
2	U	6334	0	6368	193	0
3	V	3725	0	3781	130	0
4	W	3572	0	3689	102	0
5	X	3259	0	3371	97	0
6	Y	3135	0	3139	75	0
7	Z	2290	0	2320	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	3012	0	3029	110	0
9	b	1459	0	1499	68	0
10	c	2260	0	2276	69	0
11	d	2124	0	2155	69	0
12	e	345	0	267	7	0
13	A	3057	0	3114	76	0
14	B	2933	0	2994	107	0
15	C	2834	0	2948	63	0
16	D	3040	0	3075	97	0
17	E	2869	0	2930	88	0
18	F	2724	0	2800	114	0
19	G	1865	0	1875	46	0
20	H	1789	0	1784	47	0
21	I	2007	0	2030	48	0
22	J	1887	0	1905	46	0
23	L	1868	0	1858	42	0
24	M	1909	0	1883	57	0
25	N	1487	0	1452	21	0
25	n	1360	0	1344	35	0
26	O	1667	0	1689	43	0
26	o	1315	0	1321	38	0
27	P	1591	0	1609	56	0
27	p	1271	0	1262	36	0
28	Q	1578	0	1580	42	0
28	q	1380	0	1399	43	0
29	R	1549	0	1512	49	0
29	r	1432	0	1384	46	0
30	S	1643	0	1640	41	0
30	s	1597	0	1597	45	0
31	T	1665	0	1638	52	0
31	t	1609	0	1597	37	0
32	K	1736	0	1734	35	0
33	f	4942	0	4983	183	0
34	A	31	0	12	1	0
34	D	31	0	12	1	0
34	E	31	0	12	2	0
34	F	31	0	12	2	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	27	0	12	2	0
36	C	27	0	12	0	0
All	All	88575	0	89212	2340	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 13.

All (2340) 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)
18:F:171:ARG:HH12	18:F:267:LEU:HD21	1.11	1.09
30:S:176:LEU:HD23	30:S:206:VAL:HG12	1.34	1.06
2:U:119:PRO:O	2:U:123:LYS:NZ	1.95	0.99
33:f:450:ILE:HD11	33:f:822:VAL:HG21	1.42	0.98
4:W:385:SER:OG	4:W:388:GLU:OE1	1.81	0.98
23:L:88:MET:HE3	23:L:112:ILE:HD11	1.42	0.98
29:r:184:THR:HG23	29:r:198:MET:HE3	1.45	0.97
30:S:41:LEU:HD11	30:S:177:LEU:HD11	1.49	0.95
5:X:255:LEU:HD23	5:X:270:LEU:HD23	1.49	0.94
2:U:644:TYR:OH	15:C:60:ARG:NH1	2.02	0.93
3:V:265:ASP:OD2	3:V:269:LYS:NZ	2.02	0.93
27:P:178:ASP:OD2	27:P:181:SER:OG	1.87	0.93
18:F:171:ARG:NH1	18:F:267:LEU:HD21	1.84	0.91
27:P:179:ALA:HB2	29:r:85:ILE:HD11	1.53	0.91
13:A:339:ARG:NH1	18:F:402:GLU:OE2	2.04	0.90
16:D:204:MET:HE2	16:D:308:ILE:HG22	1.53	0.90
13:A:205:GLY:O	18:F:372:LYS:NZ	2.05	0.90
26:O:241:ARG:NH2	27:P:151:GLU:O	2.04	0.90
10:c:30:GLN:OE1	10:c:206:ASN:ND2	2.06	0.88
27:P:27:ARG:NH2	27:P:180:VAL:O	2.05	0.88
4:W:370:TYR:OH	8:a:308:GLU:OE2	1.91	0.88
13:A:284:ARG:O	18:F:334:ARG:NH1	2.07	0.88
27:p:178:ASP:OD2	27:p:181:SER:OG	1.90	0.87
33:f:339:ILE:O	33:f:773:LYS:NZ	2.07	0.87
33:f:720:GLU:OE2	33:f:807:ARG:NH2	2.07	0.87
27:P:65:GLN:OE1	28:Q:86:ARG:NH2	2.08	0.86
2:U:26:LYS:NZ	11:d:131:THR:OG1	2.08	0.86
2:U:37:GLU:OE2	3:V:266:GLN:NE2	2.08	0.86
4:W:112:VAL:O	4:W:121:LYS:NZ	2.09	0.86
18:F:362:ARG:NE	18:F:388:THR:OG1	2.09	0.85
7:Z:263:ALA:HB2	10:c:291:LEU:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:72:ILE:HG21	19:G:114:LEU:HD21	1.59	0.85
14:B:74:MET:HE2	33:f:613:LEU:HD12	1.56	0.85
2:U:70:HIS:O	3:V:236:ARG:NH1	2.10	0.84
14:B:337:LEU:HD23	14:B:342:ILE:HD11	1.59	0.84
25:N:174:ASP:OD2	25:n:200:ARG:NH2	2.10	0.84
20:H:74:LEU:HD21	20:H:134:LEU:HD22	1.59	0.84
2:U:206:MET:HE2	2:U:216:VAL:HG11	1.59	0.84
3:V:345:ARG:NH1	12:e:46:ASP:OD1	2.10	0.83
11:d:265:ASP:OD1	11:d:266:THR:N	2.11	0.83
18:F:233:LYS:NZ	18:F:333:ASN:OD1	2.11	0.83
28:Q:44:LEU:HD21	28:Q:102:LEU:HD22	1.61	0.83
2:U:187:LEU:HD21	16:D:45:LYS:HD3	1.59	0.83
4:W:316:ARG:NH1	4:W:383:ASP:OD1	2.12	0.82
23:L:148:CYS:SG	23:L:150:SER:OG	2.37	0.82
33:f:369:ARG:NH2	33:f:811:LEU:O	2.12	0.82
3:V:180:ARG:NE	3:V:183:GLU:OE2	2.12	0.82
24:M:35:SER:O	24:M:36:THR:OG1	1.98	0.81
18:F:415:LEU:HD12	18:F:417:HIS:H	1.45	0.81
26:O:245:TYR:OH	30:s:201:ARG:NH1	2.12	0.81
11:d:244:VAL:HG11	11:d:267:ILE:HD13	1.62	0.81
33:f:786:GLN:O	33:f:787:LEU:HD12	1.80	0.81
6:Y:224:VAL:HG12	6:Y:228:MET:HE2	1.61	0.80
33:f:502:LEU:HD22	33:f:537:THR:HG21	1.61	0.80
2:U:18:GLN:HG2	11:d:124:LEU:HD22	1.63	0.80
18:F:251:LEU:HD12	18:F:285:ILE:CD1	2.11	0.80
32:K:85:ALA:HB2	32:K:139:VAL:HG21	1.63	0.80
10:c:152:LYS:N	16:D:77:GLU:OE2	2.15	0.80
15:C:379:THR:OG1	15:C:382:ASP:OD1	1.98	0.80
21:I:13:SER:OG	21:I:15:GLU:O	2.00	0.79
18:F:375:VAL:HG13	18:F:415:LEU:HD21	1.64	0.79
4:W:81:ASP:OD1	4:W:123:ARG:NH2	2.16	0.79
16:D:65:GLN:OE1	16:D:69:LYS:NZ	2.14	0.79
31:T:72:LEU:HD11	31:T:79:ALA:HB1	1.64	0.79
21:I:154:GLY:O	22:J:81:ARG:NH2	2.15	0.79
10:c:46:ARG:O	17:E:85:ARG:NH2	2.16	0.78
11:d:114:GLU:OE1	11:d:118:ARG:NH1	2.15	0.78
9:b:94:HIS:NE2	9:b:134:GLU:OE1	2.16	0.78
19:G:127:GLN:NE2	20:H:128:ARG:O	2.16	0.78
17:E:92:LEU:HD12	17:E:92:LEU:O	1.84	0.78
5:X:97:LEU:HD13	5:X:132:ARG:NE	1.98	0.78
33:f:430:ASP:OD1	33:f:431:LYS:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:470:VAL:O	33:f:478:ARG:NH2	2.15	0.77
33:f:653:ALA:O	33:f:657:ILE:HD12	1.83	0.77
17:E:351:GLY:O	17:E:355:ILE:HD12	1.84	0.77
6:Y:225:TYR:OH	6:Y:281:GLU:OE2	2.02	0.77
3:V:199:ASN:OD1	3:V:201:ARG:NH2	2.18	0.77
3:V:355:ARG:NH2	12:e:26:ASP:O	2.18	0.77
4:W:296:LEU:HD23	4:W:299:ILE:HD11	1.65	0.77
9:b:115:SER:O	9:b:149:ASN:ND2	2.18	0.77
11:d:131:THR:O	11:d:132:THR:OG1	2.02	0.76
23:L:11:THR:O	24:M:23:GLN:NE2	2.18	0.76
33:f:245:ASN:OD1	33:f:246:SER:N	2.18	0.76
2:U:364:VAL:HG22	10:c:177:THR:HG21	1.66	0.76
33:f:474:SER:OG	33:f:510:SER:OG	2.04	0.76
25:n:201:ASP:OD1	25:n:203:SER:N	2.18	0.76
3:V:114:TYR:OH	3:V:137:GLU:OE1	2.01	0.76
4:W:188:GLU:OE2	4:W:191:ARG:NH2	2.19	0.76
5:X:161:ASP:O	20:H:177:ARG:NH1	2.18	0.76
22:J:87:ALA:HB2	22:J:111:ILE:HD11	1.66	0.76
27:P:48:ARG:NH1	27:P:192:LYS:O	2.18	0.76
30:S:238:LEU:O	30:S:240:LYS:NZ	2.18	0.75
14:B:119:ASN:OD1	14:B:141:LYS:NZ	2.19	0.75
26:O:140:ALA:HB1	26:O:170:MET:HE2	1.66	0.75
29:r:198:MET:HG3	29:r:214:LEU:HD21	1.67	0.75
17:E:351:GLY:HA3	18:F:217:ILE:HD12	1.67	0.75
24:M:38:ILE:HD13	24:M:198:ILE:HD13	1.68	0.75
5:X:418:ALA:O	5:X:422:THR:N	2.19	0.75
27:P:158:MET:HE2	27:P:163:LEU:HA	1.67	0.75
18:F:172:VAL:HA	18:F:175:MET:HE2	1.68	0.74
27:P:169:GLN:O	27:P:173:ASN:ND2	2.20	0.74
29:R:78:ARG:NH2	29:R:227:ALA:O	2.20	0.74
3:V:399:ARG:O	3:V:402:VAL:HG12	1.86	0.74
5:X:312:GLU:OE1	5:X:312:GLU:N	2.19	0.74
33:f:694:LEU:HD21	33:f:706:ILE:HG23	1.66	0.74
29:R:131:GLU:OE2	29:R:165:LYS:NZ	2.18	0.74
3:V:396:ILE:HG21	11:d:234:GLN:OE1	1.88	0.74
2:U:268:LEU:HD21	2:U:322:THR:HG23	1.69	0.74
5:X:97:LEU:HD13	5:X:132:ARG:CD	2.17	0.74
4:W:146:THR:OG1	4:W:169:LEU:HD11	1.87	0.74
7:Z:60:GLU:OE1	7:Z:104:ASN:ND2	2.21	0.74
22:J:46:GLU:OE2	22:J:163:ARG:NH2	2.21	0.74
29:r:76:ASP:OD2	29:r:229:SER:OG	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:7:MET:HE2	9:b:97:LEU:HD22	1.70	0.74
17:E:74:THR:OG1	18:F:131:THR:OG1	2.05	0.74
7:Z:274:ASN:OD1	10:c:281:LYS:NZ	2.20	0.73
2:U:691:SER:OG	2:U:713:TYR:OH	1.97	0.73
22:J:30:SER:OG	22:J:61:LYS:NZ	2.16	0.73
2:U:352:ILE:O	2:U:356:THR:HG23	1.87	0.73
2:U:613:ASP:OD1	2:U:616:ARG:NH2	2.20	0.73
28:Q:18:ASP:OD1	28:Q:20:VAL:N	2.22	0.73
3:V:64:GLN:OE1	3:V:65:ARG:NH1	2.20	0.73
8:a:81:LEU:HD11	8:a:117:ALA:HB2	1.71	0.73
5:X:97:LEU:HD13	5:X:132:ARG:HD2	1.70	0.73
33:f:460:ASP:OD1	33:f:489:TYR:OH	2.05	0.73
4:W:116:THR:HG22	4:W:117:ASP:H	1.53	0.73
15:C:154:LEU:HD12	15:C:154:LEU:O	1.88	0.73
9:b:140:ILE:HG21	9:b:153:LEU:HD12	1.71	0.73
33:f:477:MET:SD	33:f:479:LEU:N	2.61	0.73
4:W:166:LEU:HD12	4:W:192:LEU:HD12	1.69	0.72
7:Z:273:HIS:ND1	10:c:255:TYR:OH	2.21	0.72
2:U:410:VAL:HG23	2:U:448:LEU:HD21	1.71	0.72
3:V:235:LEU:HD13	3:V:254:LEU:HD12	1.71	0.72
8:a:134:THR:O	8:a:138:VAL:HG23	1.89	0.72
18:F:285:ILE:HG21	18:F:288:LEU:HD13	1.70	0.72
13:A:55:LEU:HD23	14:B:72:LEU:HB3	1.69	0.72
13:A:203:ASN:OD1	13:A:204:LEU:N	2.22	0.72
14:B:67:ARG:NH1	33:f:664:GLU:OE2	2.21	0.72
18:F:226:TYR:CD1	18:F:335:VAL:HG13	2.24	0.72
4:W:257:GLN:OE1	4:W:295:LYS:NZ	2.23	0.72
2:U:524:LYS:NZ	2:U:562:GLU:O	2.22	0.72
3:V:418:SER:OG	3:V:421:ASP:OD1	2.07	0.72
16:D:204:MET:HE2	16:D:308:ILE:CG2	2.19	0.72
16:D:248:ARG:NE	16:D:291:GLU:OE2	2.22	0.72
13:A:415:LYS:O	13:A:419:SER:OG	2.07	0.71
28:Q:168:GLN:NE2	28:Q:175:LEU:O	2.23	0.71
14:B:407:LEU:HB3	15:C:178:LEU:HD11	1.72	0.71
15:C:90:HIS:ND1	16:D:110:ASN:OD1	2.23	0.71
20:H:74:LEU:HD11	20:H:134:LEU:HD13	1.73	0.71
21:I:108:GLU:OE2	22:J:60:ARG:NH1	2.22	0.71
6:Y:263:LEU:HD12	6:Y:271:PHE:CE1	2.26	0.71
18:F:379:VAL:HG22	18:F:415:LEU:HD11	1.73	0.71
7:Z:75:LEU:HD11	7:Z:112:MET:HE1	1.72	0.71
3:V:168:GLN:OE1	3:V:191:LEU:HD12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:332:SER:OG	4:W:335:SER:O	2.02	0.71
6:Y:109:GLU:OE2	6:Y:143:TYR:OH	2.07	0.71
7:Z:259:VAL:HG12	10:c:291:LEU:HD13	1.71	0.71
33:f:581:GLU:OE2	33:f:592:ASN:ND2	2.24	0.70
9:b:108:ARG:NH2	9:b:139:ASP:OD2	2.24	0.70
2:U:28:ASN:OD1	2:U:66:LYS:NZ	2.22	0.70
2:U:164:GLU:HG3	2:U:204:ILE:HD11	1.73	0.70
2:U:391:GLU:OE1	2:U:391:GLU:N	2.23	0.70
6:Y:186:LEU:HD12	6:Y:213:LEU:HD13	1.71	0.70
10:c:163:ILE:HG23	10:c:174:PRO:HG3	1.74	0.70
31:t:192:GLN:OE1	31:t:196:ARG:NE	2.25	0.70
9:b:7:MET:CE	9:b:97:LEU:HD22	2.21	0.70
18:F:379:VAL:CG2	18:F:415:LEU:HD11	2.21	0.70
26:O:234:VAL:HG23	26:O:234:VAL:O	1.92	0.70
8:a:173:TYR:HE2	8:a:216:LEU:HD11	1.55	0.70
17:E:242:ARG:NH1	17:E:286:ASP:OD2	2.24	0.70
22:J:109:ARG:NH2	29:R:129:ASN:OD1	2.24	0.70
30:s:142:ASP:OD1	30:s:146:LYS:N	2.25	0.70
29:r:103:THR:O	29:r:158:THR:OG1	2.05	0.69
30:s:99:ARG:HD2	30:s:102:MET:HE2	1.74	0.69
9:b:147:GLU:OE1	9:b:147:GLU:N	2.25	0.69
14:B:356:PRO:O	14:B:361:LYS:NZ	2.21	0.69
33:f:466:LEU:O	33:f:470:VAL:HG12	1.91	0.69
7:Z:208:ILE:HG21	7:Z:230:LEU:HD11	1.73	0.69
26:o:44:THR:O	26:o:172:SER:N	2.26	0.69
6:Y:360:ASP:OD1	6:Y:363:ASN:ND2	2.25	0.69
17:E:172:LEU:CD2	17:E:299:ILE:HD11	2.23	0.69
29:R:233:VAL:HG21	29:R:254:LEU:CD1	2.23	0.69
2:U:542:GLU:OE1	10:c:32:TYR:OH	2.10	0.69
7:Z:12:HIS:ND1	7:Z:168:GLU:OE1	2.24	0.69
10:c:226:MET:O	10:c:230:THR:OG1	2.09	0.69
17:E:122:MET:HE3	17:E:198:VAL:HB	1.74	0.69
31:T:86:ARG:NH1	31:T:98:ALA:O	2.25	0.69
25:n:117:PHE:CD2	25:n:132:ILE:HD12	2.27	0.69
12:e:54:ASN:OD1	12:e:57:ARG:NH2	2.25	0.69
24:M:121:HIS:HA	24:M:124:THR:HG22	1.73	0.69
22:J:73:PHE:CE1	22:J:80:ALA:HB2	2.28	0.68
4:W:299:ILE:HD12	4:W:302:TYR:HB2	1.74	0.68
6:Y:215:ASP:OD1	6:Y:216:TYR:N	2.25	0.68
29:R:233:VAL:HG21	29:R:254:LEU:HD12	1.75	0.68
2:U:525:ASN:OD1	2:U:528:ALA:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:34:ASN:OD1	9:b:38:HIS:NE2	2.25	0.68
25:n:36:THR:HG21	25:n:197:ALA:CB	2.23	0.68
14:B:77:GLU:OE2	14:B:81:ASN:ND2	2.27	0.68
26:O:183:ASP:OD2	26:O:184:LYS:NZ	2.26	0.68
2:U:420:LEU:HD11	2:U:460:TYR:CZ	2.29	0.68
3:V:283:ASN:ND2	12:e:17:ASP:OD2	2.27	0.68
4:W:166:LEU:CD1	4:W:192:LEU:HD12	2.24	0.68
29:R:60:THR:N	29:R:228:TYR:O	2.26	0.68
5:X:318:ILE:O	5:X:318:ILE:HG22	1.94	0.68
24:M:216:TRP:CE3	24:M:228:VAL:HG22	2.29	0.68
27:p:158:MET:HE3	27:p:162:HIS:CD2	2.29	0.68
33:f:333:LEU:O	33:f:333:LEU:HD23	1.94	0.68
2:U:46:GLU:OE1	2:U:80:TYR:OH	2.06	0.68
18:F:172:VAL:HG22	18:F:175:MET:HE2	1.74	0.68
4:W:435:LEU:HD21	8:a:356:TRP:HH2	1.58	0.68
25:n:48:LEU:HD23	25:n:78:CYS:SG	2.33	0.68
6:Y:314:LEU:HD23	6:Y:319:MET:SD	2.34	0.68
5:X:240:ASP:OD2	5:X:275:LEU:HD11	1.94	0.68
10:c:184:LEU:HG	10:c:204:THR:HG22	1.74	0.68
18:F:316:GLN:O	18:F:323:ASN:ND2	2.26	0.68
14:B:166:ASP:OD1	14:B:167:THR:N	2.27	0.67
18:F:251:LEU:HD12	18:F:285:ILE:HD11	1.75	0.67
2:U:377:HIS:HB2	2:U:411:ILE:HG22	1.76	0.67
4:W:375:MET:HG2	4:W:413:ILE:HD11	1.75	0.67
6:Y:233:ARG:NH2	6:Y:264:TYR:O	2.26	0.67
2:U:633:CYS:O	2:U:637:VAL:HG22	1.95	0.67
3:V:91:PRO:O	3:V:94:VAL:HG12	1.95	0.67
8:a:80:ILE:HD13	8:a:100:THR:HG23	1.76	0.67
8:a:100:THR:O	8:a:104:VAL:HG12	1.93	0.67
2:U:637:VAL:HG21	2:U:656:LEU:HD21	1.77	0.67
4:W:62:SER:O	4:W:66:ILE:HD12	1.93	0.67
33:f:579:ALA:O	33:f:583:VAL:HG23	1.94	0.67
2:U:470:ASN:OD1	2:U:471:ASP:N	2.27	0.67
10:c:170:LEU:HD23	10:c:170:LEU:O	1.94	0.67
11:d:244:VAL:HG11	11:d:267:ILE:CD1	2.23	0.67
2:U:574:LYS:O	2:U:579:ARG:NH2	2.27	0.67
20:H:66:GLU:OE1	20:H:91:ARG:NH2	2.28	0.67
3:V:150:ARG:O	3:V:151:THR:OG1	2.08	0.67
3:V:203:LEU:HD12	3:V:206:VAL:CG2	2.25	0.67
4:W:446:ILE:HD12	7:Z:211:TYR:CG	2.29	0.67
8:a:188:LEU:HD13	8:a:192:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E:401:ATP:O3G	18:F:347:ARG:NH2	2.28	0.67
31:t:156:VAL:HG13	31:t:182:LEU:HD12	1.75	0.67
4:W:446:ILE:HD13	7:Z:226:ILE:HD13	1.77	0.67
5:X:160:MET:O	5:X:160:MET:HE3	1.94	0.67
11:d:232:LEU:HD11	11:d:244:VAL:HG13	1.77	0.67
15:C:132:ASP:OD2	15:C:241:HIS:NE2	2.28	0.67
7:Z:16:LEU:HD23	10:c:216:MET:HB3	1.76	0.66
14:B:119:ASN:O	14:B:120:HIS:ND1	2.27	0.66
16:D:203:LEU:HD22	16:D:322:LEU:HD22	1.76	0.66
7:Z:21:ASP:OD2	10:c:104:ARG:NH2	2.26	0.66
26:O:191:GLU:OE2	26:O:220:VAL:HG11	1.95	0.66
28:Q:174:ASN:N	28:q:172:ILE:O	2.27	0.66
27:p:7:ASN:ND2	27:p:29:GLY:O	2.28	0.66
13:A:207:GLU:OE1	18:F:372:LYS:NZ	2.25	0.66
29:r:114:TRP:NE1	30:s:125:TYR:OH	2.28	0.66
5:X:96:PHE:CE2	5:X:109:LEU:HD13	2.30	0.66
33:f:266:LEU:HD22	33:f:294:MET:SD	2.34	0.66
3:V:181:TYR:O	3:V:221:LEU:HD21	1.95	0.66
14:B:383:LEU:HD13	14:B:423:LYS:HE2	1.77	0.66
28:Q:18:ASP:OD1	28:Q:19:ARG:N	2.29	0.66
27:p:123:SER:OG	27:p:131:MET:SD	2.54	0.66
2:U:26:LYS:NZ	11:d:129:LEU:O	2.24	0.66
18:F:206:MET:HE1	18:F:282:ILE:HD11	1.76	0.66
14:B:269:GLU:OE1	14:B:272:ARG:NH2	2.29	0.66
19:G:14:THR:OG1	20:H:10:LEU:HD13	1.96	0.66
26:o:86:CYS:SG	26:o:141:LEU:HD12	2.35	0.66
30:s:214:ASP:OD1	30:s:215:VAL:N	2.29	0.66
4:W:281:ASN:OD1	4:W:282:GLU:N	2.29	0.66
9:b:4:GLU:N	9:b:47:ASN:OD1	2.28	0.66
17:E:97:ARG:NH1	17:E:112:PRO:O	2.28	0.66
19:G:24:GLN:NE2	24:M:13:SER:O	2.29	0.66
24:M:179:LYS:O	24:M:180:LEU:HD12	1.96	0.66
10:c:177:THR:HG23	10:c:177:THR:O	1.95	0.65
17:E:339:ASN:ND2	17:E:342:ASP:OD2	2.29	0.65
29:R:94:ILE:HD11	29:R:115:GLU:OE1	1.96	0.65
2:U:320:ASP:OD1	2:U:321:GLN:N	2.29	0.65
5:X:256:LEU:HD13	5:X:319:ILE:HG22	1.77	0.65
8:a:226:ARG:NH2	8:a:231:GLN:HE22	1.94	0.65
26:O:102:ILE:HG21	26:O:126:LEU:CD2	2.25	0.65
26:o:186:ARG:O	26:o:189:MET:HE3	1.96	0.65
33:f:694:LEU:CD2	33:f:706:ILE:HG23	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:88:LEU:HD12	24:M:134:CYS:SG	2.37	0.65
2:U:498:LYS:NZ	2:U:531:ASP:OD2	2.29	0.65
6:Y:249:VAL:O	6:Y:252:SER:OG	2.14	0.65
17:E:87:LEU:HD11	17:E:109:ARG:HA	1.78	0.65
25:n:51:ASP:OD1	25:n:52:SER:N	2.30	0.65
2:U:611:ASN:HB3	2:U:614:VAL:HG12	1.79	0.65
5:X:329:ASN:OD1	5:X:330:LEU:N	2.30	0.65
31:t:195:LEU:O	31:t:199:LEU:HD23	1.97	0.65
27:P:125:ASP:OD1	27:P:129:CYS:N	2.29	0.65
25:n:51:ASP:OD2	25:n:205:GLY:N	2.28	0.65
33:f:714:SER:O	33:f:722:SER:OG	2.11	0.65
2:U:567:ILE:HD12	2:U:586:VAL:HG23	1.79	0.65
28:q:33:ASP:OD2	28:q:181:ARG:NH2	2.29	0.65
4:W:438:LEU:HD22	7:Z:229:GLN:OE1	1.96	0.65
18:F:257:VAL:HG23	18:F:306:VAL:HG22	1.79	0.65
23:L:229:VAL:HG12	23:L:233:LEU:HD13	1.78	0.65
27:P:158:MET:HE2	27:P:163:LEU:CA	2.27	0.65
6:Y:290:PRO:O	6:Y:291:HIS:ND1	2.30	0.64
17:E:239:GLY:HA2	17:E:257:LEU:HD13	1.79	0.64
33:f:479:LEU:HD22	33:f:517:VAL:HG21	1.79	0.64
9:b:123:ASP:OD1	9:b:124:LEU:N	2.31	0.64
11:d:200:LEU:HD22	11:d:233:GLU:OE1	1.97	0.64
2:U:568:GLU:OE1	2:U:601:ARG:NH2	2.30	0.64
3:V:482:PHE:CD2	6:Y:377:LEU:HD21	2.33	0.64
13:A:333:ARG:NE	34:F:501:ATP:O3G	2.31	0.64
33:f:429:ILE:HD12	33:f:448:CYS:HB2	1.79	0.64
6:Y:300:ARG:NE	6:Y:333:GLU:OE2	2.29	0.64
15:C:191:PRO:O	15:C:196:LYS:NZ	2.31	0.64
26:O:60:ASP:OD1	26:O:76:LYS:NZ	2.29	0.64
3:V:396:ILE:HG21	11:d:234:GLN:CD	2.23	0.64
7:Z:43:TRP:CZ3	7:Z:48:LEU:HD13	2.32	0.64
30:s:159:GLN:NE2	30:s:161:ASP:OD2	2.31	0.64
7:Z:48:LEU:HD11	7:Z:92:VAL:HB	1.80	0.64
30:s:212:GLU:OE1	30:s:239:ARG:NH1	2.31	0.64
8:a:232:TRP:CZ2	8:a:255:TRP:HA	2.32	0.64
28:Q:14:LEU:HD21	28:Q:160:LEU:HD22	1.79	0.64
28:Q:182:ILE:HD11	28:Q:191:LEU:HD22	1.79	0.64
20:H:123:GLN:NE2	21:I:128:ARG:O	2.31	0.64
28:q:164:LEU:HD12	28:q:194:ILE:HG13	1.77	0.64
5:X:123:THR:OG1	20:H:186:ASP:OD2	2.11	0.63
9:b:181:ASP:OD1	9:b:182:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:74:MET:HE1	33:f:609:VAL:HG12	1.79	0.63
17:E:121:ASN:OD1	17:E:122:MET:N	2.30	0.63
25:n:93:VAL:HG21	25:n:117:PHE:CD1	2.33	0.63
2:U:520:MET:HE2	2:U:525:ASN:ND2	2.13	0.63
5:X:285:GLU:OE1	5:X:309:TYR:OH	2.08	0.63
16:D:268:ASP:OD2	16:D:311:THR:OG1	2.14	0.63
13:A:278:ASP:OD1	13:A:321:THR:OG1	2.07	0.63
14:B:309:MET:SD	14:B:341:LEU:HD22	2.38	0.63
16:D:87:LEU:CD1	16:D:131:ALA:HB1	2.28	0.63
2:U:22:PHE:HB3	11:d:124:LEU:HD11	1.79	0.63
9:b:8:VAL:HG12	9:b:110:ILE:HD11	1.79	0.63
28:q:13:VAL:O	28:q:15:VAL:HG13	1.99	0.63
2:U:415:HIS:NE2	2:U:418:GLU:OE1	2.32	0.63
2:U:194:ARG:O	2:U:198:LEU:HD23	1.98	0.63
2:U:212:ASP:OD2	2:U:215:ASN:ND2	2.32	0.63
2:U:744:VAL:HG11	2:U:783:TYR:HB3	1.80	0.63
11:d:139:GLN:OE1	11:d:142:ILE:HD13	1.99	0.63
17:E:118:LEU:O	17:E:122:MET:HG3	1.98	0.63
21:I:95:GLN:HG3	27:P:73:LEU:HD22	1.80	0.63
2:U:697:GLN:OE1	2:U:744:VAL:N	2.32	0.63
15:C:199:LEU:HD23	15:C:317:PHE:HZ	1.62	0.63
5:X:97:LEU:HD13	5:X:132:ARG:HE	1.60	0.63
8:a:201:GLY:O	8:a:205:LEU:HD23	1.99	0.63
23:L:196:ARG:NH1	23:L:237:GLU:O	2.32	0.63
30:s:75:THR:O	30:s:78:THR:N	2.31	0.63
33:f:423:ASP:O	33:f:426:LEU:HD13	1.98	0.63
33:f:437:GLU:OE1	33:f:439:TYR:N	2.31	0.63
4:W:268:LYS:O	4:W:272:LEU:HD23	1.99	0.62
8:a:35:HIS:ND1	9:b:18:ASN:OD1	2.31	0.62
16:D:148:ASP:OD2	16:D:253:LEU:HD22	1.99	0.62
17:E:203:ILE:HG23	17:E:214:LEU:HD23	1.80	0.62
18:F:279:ALA:HB1	18:F:280:PRO:HD2	1.81	0.62
33:f:348:ILE:CD1	33:f:381:VAL:HG21	2.29	0.62
33:f:496:ASP:OD1	33:f:497:VAL:N	2.31	0.62
33:f:502:LEU:CD2	33:f:537:THR:HG21	2.29	0.62
8:a:118:ILE:HG22	8:a:122:LYS:HE3	1.80	0.62
11:d:143:LEU:O	11:d:147:ILE:HG22	1.99	0.62
28:q:12:TYR:OH	28:q:151:ILE:HG23	1.99	0.62
4:W:177:MET:O	4:W:182:ARG:NH1	2.32	0.62
28:q:27:GLN:NE2	28:q:29:LYS:O	2.31	0.62
4:W:35:ALA:HB2	4:W:43:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:s:77:LYS:O	30:s:78:THR:OG1	2.17	0.62
33:f:452:ASN:HD22	33:f:462:ALA:HB2	1.63	0.62
32:K:191:LEU:HD21	32:K:219:THR:HG21	1.82	0.62
2:U:26:LYS:O	2:U:30:VAL:HG22	2.00	0.62
8:a:60:TYR:CE1	8:a:64:ILE:HG21	2.35	0.62
13:A:102:ILE:HD11	13:A:112:ILE:HD11	1.82	0.62
17:E:320:ILE:O	17:E:322:LYS:NZ	2.33	0.62
2:U:36:ALA:HB1	3:V:269:LYS:HB3	1.81	0.62
8:a:80:ILE:O	8:a:84:VAL:HG23	1.99	0.62
20:H:11:THR:HG23	20:H:21:GLN:HB3	1.82	0.62
22:J:164:GLY:HA3	22:J:198:VAL:HG21	1.81	0.62
29:R:184:THR:HB	29:R:198:MET:HE3	1.82	0.62
3:V:403:ILE:CD1	3:V:428:LEU:HD21	2.30	0.62
26:O:56:VAL:HG23	26:O:220:VAL:HG22	1.82	0.62
26:O:56:VAL:HG13	26:O:198:VAL:HG21	1.80	0.62
33:f:302:GLY:O	33:f:303:VAL:HG13	1.99	0.62
33:f:391:LEU:HD13	33:f:414:LEU:HB2	1.81	0.62
4:W:138:VAL:O	4:W:138:VAL:HG12	2.00	0.62
5:X:131:ALA:O	5:X:134:VAL:HG22	2.00	0.62
9:b:52:ILE:HD12	9:b:60:VAL:HG12	1.82	0.62
20:H:160:ALA:HB1	20:H:174:LEU:HD23	1.81	0.62
2:U:637:VAL:HG21	2:U:656:LEU:CD2	2.29	0.62
19:G:115:CYS:SG	19:G:140:LEU:HD12	2.39	0.62
26:o:243:GLY:O	26:o:244:ARG:NE	2.32	0.62
2:U:149:GLN:OE1	2:U:149:GLN:N	2.31	0.61
9:b:179:LEU:HD23	9:b:179:LEU:O	1.99	0.61
23:L:79:ALA:HB3	32:K:121:LEU:HD12	1.82	0.61
28:Q:18:ASP:OD2	28:Q:175:LEU:HD22	2.00	0.61
3:V:414:TYR:OH	3:V:425:LYS:NZ	2.23	0.61
8:a:235:ASP:OD1	8:a:236:THR:N	2.33	0.61
9:b:107:MET:HB3	9:b:136:VAL:HG23	1.81	0.61
28:q:37:LYS:O	28:q:61:GLN:NE2	2.33	0.61
2:U:105:ILE:O	2:U:109:THR:HG23	2.00	0.61
19:G:130:GLU:OE2	20:H:6:TYR:N	2.33	0.61
2:U:719:ASP:OD1	2:U:720:LYS:N	2.33	0.61
10:c:272:ILE:HG22	10:c:272:ILE:O	2.00	0.61
26:O:239:GLY:HA3	30:s:208:ILE:HD12	1.81	0.61
14:B:180:PRO:O	14:B:241:ASN:ND2	2.33	0.61
16:D:87:LEU:HD13	16:D:131:ALA:HB1	1.80	0.61
25:N:170:TYR:OH	31:T:80:ARG:O	2.19	0.61
29:r:161:CYS:SG	29:r:170:LEU:HD13	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:308:GLU:CD	8:a:312:MET:HE2	2.25	0.61
18:F:415:LEU:HD13	18:F:420:TYR:CD1	2.35	0.61
19:G:86:ASP:OD1	24:M:121:HIS:NE2	2.34	0.61
29:R:84:TYR:OH	30:S:174:GLN:OE1	2.16	0.61
3:V:116:ALA:HB1	3:V:120:PHE:HE2	1.64	0.60
4:W:314:LEU:CD2	4:W:381:LEU:HD23	2.30	0.60
29:R:60:THR:N	29:R:229:SER:HG	1.98	0.60
18:F:226:TYR:HD1	18:F:335:VAL:HG13	1.64	0.60
22:J:115:LYS:O	22:J:119:THR:HG23	2.00	0.60
6:Y:80:GLU:OE2	6:Y:83:ARG:NH2	2.34	0.60
17:E:249:ALA:HB1	18:F:261:ILE:CG2	2.30	0.60
18:F:378:ASP:OD1	18:F:378:ASP:O	2.19	0.60
18:F:415:LEU:HD22	18:F:420:TYR:CE1	2.36	0.60
2:U:38:ILE:HG21	2:U:67:VAL:HG21	1.83	0.60
28:Q:67:TYR:O	28:Q:71:ASN:ND2	2.34	0.60
31:T:169:TYR:CD1	31:T:184:THR:HG22	2.36	0.60
33:f:285:CYS:O	33:f:291:GLN:NE2	2.35	0.60
8:a:4:VAL:HG21	8:a:66:GLU:HG2	1.84	0.60
17:E:92:LEU:HA	17:E:96:THR:HG21	1.82	0.60
33:f:688:ARG:O	33:f:724:ASN:ND2	2.34	0.60
14:B:255:LEU:HD23	14:B:266:LEU:HD22	1.84	0.60
20:H:22:ILE:HD11	20:H:122:THR:HG21	1.83	0.60
33:f:463:LEU:HD23	33:f:485:LEU:HD11	1.83	0.60
19:G:93:ARG:NH1	19:G:97:GLU:OE2	2.34	0.60
32:K:199:LEU:HD12	32:K:237:VAL:HG12	1.84	0.60
30:s:57:LEU:HD13	31:t:177:TYR:CE1	2.37	0.60
4:W:59:ASP:OD2	4:W:62:SER:OG	2.15	0.60
27:P:145:GLN:OE1	30:s:171:ALA:HB1	2.01	0.60
21:I:186:LEU:O	21:I:190:LEU:HD23	2.01	0.60
23:L:74:ILE:HG22	23:L:132:LEU:CD2	2.32	0.60
2:U:697:GLN:NE2	2:U:742:HIS:O	2.35	0.59
9:b:157:VAL:HG21	9:b:170:LEU:HB2	1.82	0.59
19:G:170:VAL:HG23	19:G:171:LYS:HG2	1.84	0.59
3:V:482:PHE:CE2	3:V:486:ILE:HD11	2.37	0.59
13:A:55:LEU:HD21	14:B:73:LEU:HG	1.84	0.59
26:o:248:GLU:OE1	26:o:251:THR:N	2.35	0.59
5:X:407:MET:SD	7:Z:269:VAL:HG11	2.42	0.59
26:o:96:ASP:O	26:o:99:THR:OG1	2.19	0.59
26:o:251:THR:HG22	26:o:251:THR:O	2.02	0.59
2:U:719:ASP:OD1	2:U:721:HIS:N	2.27	0.59
20:H:174:LEU:CD1	20:H:194:THR:HG21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:7:ILE:HG22	22:J:18:GLN:OE1	2.01	0.59
6:Y:269:SER:O	6:Y:273:GLN:OE1	2.20	0.59
10:c:113:HIS:NE2	10:c:126:ASP:OD2	2.35	0.59
16:D:203:LEU:HD22	16:D:322:LEU:CD2	2.33	0.59
24:M:38:ILE:HG23	24:M:177:ILE:HD11	1.83	0.59
26:o:56:VAL:HG13	26:o:218:LEU:HD21	1.83	0.59
2:U:22:PHE:CB	11:d:124:LEU:HD11	2.32	0.59
2:U:609:ASP:OD2	2:U:614:VAL:HG11	2.03	0.59
5:X:74:ARG:NE	5:X:112:GLU:OE2	2.36	0.59
25:n:228:ILE:HG22	25:n:228:ILE:O	2.03	0.59
27:p:180:VAL:HG23	27:p:180:VAL:O	2.02	0.59
2:U:35:TRP:O	2:U:39:SER:OG	2.16	0.59
2:U:38:ILE:CG2	2:U:67:VAL:HG21	2.31	0.59
28:Q:141:SER:OG	29:r:197:VAL:HG23	2.02	0.59
1:y:388:THR:O	1:y:392:VAL:HG22	2.03	0.59
2:U:875:PHE:O	2:U:876:GLN:NE2	2.32	0.59
3:V:116:ALA:HB1	3:V:120:PHE:CE2	2.37	0.59
5:X:254:MET:HG2	5:X:270:LEU:HD21	1.83	0.59
6:Y:274:SER:O	6:Y:278:VAL:HG13	2.03	0.59
9:b:166:THR:O	9:b:169:HIS:NE2	2.36	0.59
23:L:47:VAL:HG12	23:L:195:LEU:CD1	2.32	0.59
33:f:412:ALA:HB3	33:f:819:TYR:CE2	2.37	0.59
4:W:139:GLU:OE1	17:E:161:ARG:NH1	2.36	0.59
15:C:199:LEU:HD23	15:C:317:PHE:CZ	2.38	0.59
27:p:158:MET:HE2	27:p:163:LEU:HA	1.84	0.59
30:s:176:LEU:CD2	30:s:202:LEU:HD11	2.33	0.59
33:f:731:MET:HE1	33:f:821:LEU:HD11	1.84	0.59
18:F:126:THR:HG22	18:F:130:GLN:O	2.03	0.59
4:W:272:LEU:HD11	4:W:328:LEU:HD23	1.85	0.58
7:Z:81:MET:SD	10:c:95:MET:SD	3.01	0.58
20:H:143:ARG:NH2	21:I:57:ASP:OD2	2.36	0.58
31:T:76:GLY:O	31:T:77:SER:OG	2.11	0.58
15:C:45:LEU:HB3	16:D:61:ILE:HG21	1.85	0.58
16:D:243:GLY:O	16:D:247:VAL:HG23	2.03	0.58
16:D:279:THR:HG21	17:E:248:SER:OG	2.03	0.58
2:U:364:VAL:CG2	10:c:177:THR:HG21	2.33	0.58
8:a:180:LEU:HD22	8:a:221:VAL:HG21	1.86	0.58
13:A:83:ASP:OD1	13:A:84:LYS:N	2.35	0.58
18:F:386:ARG:NH2	23:L:166:GLN:OE1	2.36	0.58
19:G:114:LEU:O	19:G:118:ILE:HD12	2.03	0.58
23:L:214:ILE:HD12	23:L:224:TYR:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:435:LEU:HD21	8:a:356:TRP:CH2	2.37	0.58
8:a:185:ILE:O	8:a:193:GLN:NE2	2.37	0.58
26:O:93:ALA:HB2	27:P:129:CYS:SG	2.42	0.58
26:O:102:ILE:HG21	26:O:126:LEU:HD22	1.85	0.58
31:T:224:ARG:NH1	26:o:182:GLU:OE1	2.36	0.58
33:f:659:LEU:HD12	33:f:662:MET:HE2	1.85	0.58
2:U:643:SER:OG	2:U:644:TYR:N	2.37	0.58
3:V:265:ASP:HB2	11:d:210:THR:HG21	1.85	0.58
2:U:679:PRO:HG3	3:V:511:ARG:CZ	2.33	0.58
2:U:884:VAL:HG13	2:U:888:GLN:O	2.04	0.58
14:B:61:LYS:O	14:B:65:LEU:HD13	2.02	0.58
18:F:385:ALA:O	18:F:388:THR:OG1	2.19	0.58
23:L:81:ALA:HB2	23:L:130:VAL:HG21	1.86	0.58
33:f:462:ALA:HB3	33:f:489:TYR:CE2	2.38	0.58
33:f:783:SER:HB3	33:f:787:LEU:HD13	1.84	0.58
2:U:137:MET:SD	2:U:140:ARG:NH1	2.76	0.58
6:Y:183:TYR:CE1	6:Y:213:LEU:HD11	2.38	0.58
8:a:35:HIS:NE2	9:b:14:GLU:O	2.37	0.58
11:d:260:ILE:O	11:d:264:LEU:HD23	2.04	0.58
17:E:172:LEU:HD22	17:E:299:ILE:HD11	1.83	0.58
16:D:389:GLU:OE1	16:D:391:ARG:NH2	2.37	0.58
17:E:114:GLU:OE2	18:F:94:ILE:HD12	2.04	0.58
33:f:270:LEU:HD11	33:f:298:LEU:CD2	2.34	0.58
2:U:105:ILE:HD11	15:C:23:TYR:CD1	2.39	0.58
3:V:125:ASN:OD1	3:V:128:ARG:NH1	2.37	0.58
3:V:306:ARG:NE	3:V:336:GLU:OE2	2.36	0.58
4:W:116:THR:HG22	4:W:117:ASP:N	2.18	0.58
27:P:69:PHE:O	27:P:73:LEU:HD23	2.04	0.58
33:f:463:LEU:HD21	33:f:497:VAL:HB	1.86	0.58
3:V:466:ILE:O	3:V:469:THR:OG1	2.20	0.57
17:E:226:GLN:NE2	17:E:271:HIS:O	2.37	0.57
23:L:47:VAL:HG12	23:L:195:LEU:HD12	1.86	0.57
24:M:216:TRP:CZ3	24:M:228:VAL:HG22	2.38	0.57
33:f:678:LEU:HB3	33:f:686:LEU:HD21	1.86	0.57
2:U:786:THR:HG23	2:U:786:THR:O	2.02	0.57
5:X:219:ALA:O	5:X:322:HIS:NE2	2.35	0.57
15:C:105:ILE:O	15:C:108:VAL:HG22	2.04	0.57
6:Y:117:LYS:NZ	6:Y:153:ASP:OD2	2.24	0.57
14:B:70:ASP:OD1	14:B:71:TYR:N	2.38	0.57
16:D:168:GLY:HA3	16:D:347:THR:HG21	1.87	0.57
18:F:93:VAL:O	18:F:93:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:214:ILE:HD12	23:L:224:TYR:CE2	2.39	0.57
25:N:150:MET:HB2	31:T:50:MET:HE1	1.87	0.57
28:q:3:TYR:CZ	28:q:139:THR:HG21	2.40	0.57
33:f:658:ALA:HB2	33:f:693:ALA:HB1	1.86	0.57
8:a:192:GLU:OE2	8:a:196:ARG:NE	2.33	0.57
8:a:258:GLN:OE1	8:a:260:ASP:N	2.37	0.57
9:b:125:VAL:HG23	9:b:159:THR:HG21	1.87	0.57
29:r:233:VAL:HG23	29:r:233:VAL:O	2.03	0.57
33:f:388:ASP:OD1	33:f:389:LYS:N	2.34	0.57
33:f:650:GLN:NE2	33:f:686:LEU:HD12	2.19	0.57
2:U:186:SER:C	2:U:187:LEU:HD23	2.29	0.57
2:U:232:ILE:O	2:U:236:LEU:HD23	2.05	0.57
7:Z:136:GLU:OE2	7:Z:157:HIS:NE2	2.38	0.57
8:a:149:THR:OG1	8:a:152:HIS:NE2	2.37	0.57
8:a:363:MET:HE2	10:c:307:VAL:HG11	1.86	0.57
16:D:42:SER:HA	16:D:45:LYS:HG3	1.86	0.57
25:N:36:THR:HG21	25:N:197:ALA:CB	2.34	0.57
25:n:194:LEU:HD12	25:n:208:ILE:HG23	1.86	0.57
33:f:433:LEU:O	33:f:441:LYS:NZ	2.35	0.57
4:W:201:ARG:HE	4:W:204:ILE:HD11	1.70	0.57
10:c:243:SER:O	10:c:247:GLU:OE1	2.22	0.57
22:J:73:PHE:CZ	22:J:80:ALA:HB2	2.39	0.57
22:J:108:THR:HG21	22:J:145:TYR:HB3	1.87	0.57
23:L:35:THR:OG1	23:L:133:LEU:HD12	2.05	0.57
29:R:253:ASP:OD1	29:R:254:LEU:N	2.38	0.57
11:d:196:LEU:HD12	11:d:208:PHE:CD2	2.40	0.57
14:B:72:LEU:O	14:B:76:GLU:OE1	2.23	0.57
21:I:44:LEU:HD22	21:I:190:LEU:HD22	1.86	0.57
28:q:3:TYR:OH	28:q:139:THR:HG21	2.04	0.57
5:X:255:LEU:HD22	5:X:267:VAL:HG13	1.87	0.57
11:d:283:LEU:HD21	11:d:286:GLU:HB3	1.87	0.57
26:O:122:ALA:O	26:O:126:LEU:HD23	2.05	0.57
33:f:535:THR:HG23	33:f:562:LEU:HD11	1.86	0.57
7:Z:263:ALA:CB	10:c:291:LEU:HD11	2.33	0.57
15:C:189:TYR:CD1	15:C:298:ILE:HG22	2.39	0.57
17:E:62:LYS:CE	17:E:70:ILE:HD12	2.35	0.57
25:N:48:LEU:HD11	25:N:135:ALA:HB3	1.87	0.57
28:Q:161:ARG:NH2	28:Q:165:GLU:OE2	2.37	0.57
29:R:233:VAL:O	29:R:233:VAL:HG12	2.05	0.57
33:f:538:ILE:HG21	33:f:562:LEU:HB2	1.87	0.57
3:V:410:ILE:HD11	3:V:425:LYS:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:139:ASP:OD1	31:T:126:HIS:NE2	2.38	0.56
31:T:169:TYR:CD2	31:T:169:TYR:O	2.58	0.56
18:F:384:LEU:O	18:F:388:THR:HG23	2.05	0.56
5:X:251:LEU:HD12	5:X:254:MET:HE2	1.87	0.56
6:Y:186:LEU:CD1	6:Y:213:LEU:HD13	2.34	0.56
6:Y:384:SER:O	6:Y:388:ASN:ND2	2.38	0.56
8:a:320:VAL:HG21	8:a:333:MET:HE1	1.87	0.56
10:c:157:ILE:HG23	10:c:205:ILE:CD1	2.34	0.56
13:A:248:LYS:HD2	13:A:249:TYR:CZ	2.41	0.56
26:O:217:ASP:OD2	26:O:230:ARG:NH1	2.38	0.56
25:n:54:THR:HG22	25:n:62:ASN:HB3	1.86	0.56
4:W:307:LYS:O	4:W:311:THR:HG23	2.05	0.56
17:E:140:GLU:O	17:E:144:GLU:HG3	2.05	0.56
22:J:139:ASP:OD1	22:J:141:THR:OG1	2.21	0.56
3:V:108:LEU:HD22	3:V:170:LEU:HD12	1.88	0.56
3:V:115:LYS:NZ	3:V:147:PHE:O	2.39	0.56
3:V:379:LEU:HD21	3:V:395:ILE:CG2	2.35	0.56
30:s:176:LEU:HD21	30:s:202:LEU:HD11	1.88	0.56
7:Z:19:VAL:HG21	7:Z:124:ILE:CD1	2.36	0.56
7:Z:19:VAL:HG21	7:Z:124:ILE:HD13	1.87	0.56
16:D:345:PHE:CE2	16:D:375:ILE:HD12	2.41	0.56
31:T:137:LEU:CD1	31:T:157:ILE:HD11	2.36	0.56
31:T:141:MET:SD	31:T:155:MET:HE1	2.46	0.56
8:a:296:ILE:HB	8:a:307:VAL:HG21	1.87	0.56
16:D:40:LEU:HD12	16:D:40:LEU:N	2.21	0.56
16:D:83:GLN:HG2	16:D:140:VAL:HG12	1.87	0.56
16:D:362:ASP:OD1	16:D:363:TYR:N	2.39	0.56
27:p:56:LEU:HD23	27:p:59:ASP:OD2	2.05	0.56
3:V:86:VAL:HG11	3:V:160:LEU:HD23	1.87	0.56
5:X:197:ALA:HB1	5:X:202:CYS:SG	2.46	0.56
6:Y:338:ILE:HD11	6:Y:345:CYS:SG	2.44	0.56
8:a:231:GLN:O	8:a:232:TRP:CB	2.53	0.56
30:S:41:LEU:CD1	30:S:177:LEU:HD11	2.29	0.56
32:K:190:THR:HG23	32:K:193:GLU:H	1.70	0.56
8:a:112:ILE:CD1	8:a:138:VAL:HG13	2.36	0.56
13:A:189:GLU:OE1	18:F:409:ARG:NH2	2.38	0.56
16:D:143:LEU:HD13	17:E:70:ILE:HD11	1.87	0.56
26:O:126:LEU:HD12	26:O:141:LEU:CD1	2.36	0.56
2:U:364:VAL:HG11	2:U:724:VAL:HG12	1.86	0.56
13:A:396:ALA:HB3	14:B:214:MET:HE3	1.88	0.56
33:f:822:VAL:HG22	33:f:825:MET:SD	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:27:LEU:HD22	2:U:38:ILE:HG12	1.87	0.55
2:U:353:LEU:HD21	2:U:376:MET:SD	2.45	0.55
9:b:51:LEU:O	9:b:52:ILE:HD13	2.04	0.55
9:b:139:ASP:CG	9:b:188:ILE:HD12	2.31	0.55
9:b:145:GLU:OE1	9:b:145:GLU:N	2.38	0.55
21:I:72:MET:SD	21:I:110:LEU:HD23	2.46	0.55
22:J:104:VAL:HG13	22:J:133:ILE:HG22	1.88	0.55
7:Z:227:ILE:HD12	8:a:346:ILE:HD12	1.88	0.55
8:a:74:LEU:O	8:a:78:GLU:OE1	2.24	0.55
16:D:202:VAL:CG1	16:D:308:ILE:HG23	2.36	0.55
19:G:17:SER:O	19:G:19:GLU:N	2.39	0.55
31:T:83:ASN:OD1	31:T:231:ARG:NH2	2.39	0.55
33:f:757:ASN:ND2	33:f:811:LEU:HD12	2.21	0.55
3:V:477:HIS:ND1	11:d:342:TYR:OH	2.23	0.55
8:a:84:VAL:HG21	8:a:97:LEU:HD21	1.86	0.55
23:L:88:MET:HE2	23:L:108:LEU:HD21	1.88	0.55
30:S:143:GLU:OE1	30:S:143:GLU:N	2.39	0.55
33:f:422:VAL:O	33:f:425:GLY:N	2.25	0.55
2:U:699:THR:HG21	2:U:810:THR:O	2.07	0.55
3:V:79:VAL:O	3:V:83:GLU:OE1	2.24	0.55
13:A:45:ILE:O	13:A:49:GLU:OE1	2.24	0.55
22:J:93:SER:O	22:J:97:THR:HG23	2.06	0.55
2:U:164:GLU:CG	2:U:204:ILE:HD11	2.35	0.55
3:V:383:GLY:O	3:V:387:GLN:NE2	2.39	0.55
13:A:96:ALA:HB2	13:A:115:VAL:HG22	1.88	0.55
14:B:235:LEU:HD12	14:B:353:PHE:CZ	2.42	0.55
16:D:300:ASP:O	16:D:303:VAL:HG12	2.07	0.55
16:D:387:VAL:CG2	17:E:162:VAL:HG21	2.36	0.55
26:O:224:ASN:OD1	26:O:225:LYS:N	2.40	0.55
33:f:333:LEU:HD23	33:f:333:LEU:C	2.32	0.55
33:f:786:GLN:C	33:f:787:LEU:HD12	2.32	0.55
6:Y:263:LEU:HD12	6:Y:271:PHE:HE1	1.68	0.55
8:a:80:ILE:HD13	8:a:100:THR:CG2	2.36	0.55
17:E:62:LYS:HE2	17:E:70:ILE:HD12	1.87	0.55
18:F:288:LEU:HD23	18:F:338:LEU:HD21	1.89	0.55
24:M:216:TRP:CZ3	24:M:228:VAL:HG13	2.41	0.55
28:Q:42:ILE:HD11	28:Q:75:LEU:O	2.06	0.55
32:K:10:ARG:O	32:K:14:THR:HG21	2.07	0.55
2:U:137:MET:HE3	15:C:20:LEU:HB3	1.87	0.55
2:U:505:ASP:HB2	2:U:508:THR:HG22	1.88	0.55
5:X:48:GLN:O	5:X:52:GLU:OE1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:144:VAL:HG23	7:Z:144:VAL:O	2.07	0.55
7:Z:208:ILE:CG2	7:Z:230:LEU:HD11	2.36	0.55
10:c:130:GLN:HB3	10:c:162:LEU:HD11	1.88	0.55
13:A:55:LEU:HD23	14:B:72:LEU:CB	2.36	0.55
23:L:61:LYS:NZ	23:L:225:ASP:OD2	2.40	0.55
23:L:89:ARG:O	23:L:93:LEU:HD23	2.07	0.55
31:T:137:LEU:HD12	31:T:157:ILE:HD11	1.88	0.55
33:f:418:LEU:HD23	33:f:425:GLY:HA3	1.89	0.55
2:U:788:VAL:HG12	2:U:884:VAL:HG21	1.87	0.55
11:d:282:ILE:O	11:d:316:TYR:N	2.39	0.55
19:G:40:VAL:HG13	19:G:179:LEU:HD11	1.88	0.55
21:I:116:ASP:OD1	22:J:81:ARG:NH1	2.35	0.55
26:o:241:ARG:NH1	27:p:152:SER:O	2.40	0.55
33:f:571:GLU:OE1	33:f:571:GLU:N	2.39	0.55
14:B:74:MET:HE3	33:f:610:GLN:HA	1.89	0.55
15:C:78:ARG:HH21	15:C:80:MET:HE1	1.71	0.55
33:f:520:LEU:HD11	33:f:798:THR:HG23	1.89	0.55
2:U:419:ALA:O	2:U:421:GLN:N	2.40	0.55
6:Y:24:PHE:CZ	6:Y:28:LEU:HD21	2.42	0.55
8:a:308:GLU:OE1	8:a:312:MET:HE2	2.07	0.55
20:H:206:ASP:OD1	20:H:207:ASN:N	2.39	0.55
22:J:5:ARG:O	22:J:123:GLY:N	2.40	0.55
27:P:35:VAL:HG12	27:P:36:THR:HG23	1.89	0.55
28:Q:161:ARG:O	28:Q:165:GLU:OE1	2.25	0.55
31:T:117:ILE:O	31:T:121:LEU:HD13	2.07	0.55
25:n:222:VAL:HG23	25:n:222:VAL:O	2.07	0.55
26:o:140:ALA:HB1	26:o:170:MET:CE	2.37	0.55
2:U:213:PHE:CD2	2:U:244:MET:HE1	2.42	0.54
2:U:410:VAL:CG2	2:U:448:LEU:HD21	2.36	0.54
19:G:141:ILE:CD1	19:G:151:VAL:HG22	2.37	0.54
21:I:44:LEU:CD2	21:I:190:LEU:HD22	2.37	0.54
23:L:84:LEU:O	23:L:88:MET:HG3	2.07	0.54
24:M:179:LYS:C	24:M:180:LEU:HD12	2.32	0.54
25:N:153:MET:SD	31:T:51:VAL:HG11	2.47	0.54
4:W:442:THR:O	4:W:446:ILE:HG12	2.08	0.54
6:Y:228:MET:HE1	6:Y:259:TYR:CE2	2.43	0.54
31:t:72:LEU:HD22	31:t:229:TYR:HB2	1.89	0.54
2:U:242:LEU:HD13	2:U:321:GLN:NE2	2.22	0.54
7:Z:35:VAL:HG22	7:Z:97:THR:OG1	2.08	0.54
26:O:98:THR:HG23	26:O:129:MET:CE	2.38	0.54
29:R:142:LEU:CD2	29:R:160:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:K:217:LEU:HD23	32:K:229:PHE:CD2	2.43	0.54
26:o:140:ALA:HB1	26:o:170:MET:HE2	1.89	0.54
3:V:411:SER:CB	3:V:447:ILE:HD12	2.38	0.54
8:a:173:TYR:CE2	8:a:216:LEU:HD11	2.40	0.54
34:A:501:ATP:O3G	14:B:346:ARG:NH1	2.36	0.54
31:T:72:LEU:HD11	31:T:79:ALA:CB	2.35	0.54
11:d:98:LEU:HD22	11:d:115:GLU:OE1	2.07	0.54
11:d:276:GLU:OE2	11:d:308:TRP:NE1	2.30	0.54
13:A:239:ARG:NH1	13:A:244:GLU:OE2	2.40	0.54
18:F:172:VAL:HG23	18:F:267:LEU:HD13	1.89	0.54
28:Q:162:LYS:HD3	29:r:200:ARG:HE	1.72	0.54
4:W:190:MET:HE3	4:W:206:SER:HB3	1.90	0.54
8:a:93:ALA:O	8:a:97:LEU:HD23	2.08	0.54
2:U:124:LYS:O	2:U:125:PRO:C	2.50	0.54
3:V:249:THR:O	3:V:253:LEU:HD23	2.07	0.54
3:V:324:PHE:O	3:V:328:VAL:HG23	2.08	0.54
14:B:105:THR:OG1	14:B:106:PRO:HD3	2.08	0.54
20:H:68:ILE:HG21	20:H:110:LEU:HD11	1.88	0.54
23:L:3:ARG:HG3	23:L:4:ASN:H	1.73	0.54
2:U:206:MET:CE	2:U:216:VAL:HG11	2.36	0.54
2:U:248:ILE:O	2:U:252:LEU:HD23	2.08	0.54
10:c:37:ALA:O	10:c:41:MET:HG3	2.08	0.54
22:J:209:ALA:HB1	22:J:217:LEU:HD11	1.90	0.54
33:f:282:PHE:O	33:f:291:GLN:NE2	2.40	0.54
2:U:12:LEU:HD22	2:U:44:LYS:HG3	1.90	0.54
2:U:22:PHE:HB2	11:d:124:LEU:HD21	1.89	0.54
18:F:227:GLY:O	18:F:233:LYS:NZ	2.36	0.54
25:N:71:ILE:O	25:N:94:THR:HG23	2.08	0.54
29:R:219:ILE:O	29:R:223:THR:HG23	2.07	0.54
4:W:316:ARG:NH2	4:W:380:GLN:O	2.41	0.54
8:a:290:GLN:OE1	8:a:290:GLN:N	2.40	0.54
18:F:392:ASN:OD1	18:F:393:GLY:N	2.38	0.54
33:f:507:ASP:OD1	33:f:508:SER:N	2.40	0.54
33:f:659:LEU:HD12	33:f:662:MET:CE	2.38	0.54
5:X:99:MET:O	5:X:99:MET:HG2	2.08	0.53
6:Y:155:ASP:OD2	6:Y:159:ARG:NH2	2.41	0.53
9:b:33:VAL:HG21	9:b:75:LEU:HD13	1.90	0.53
9:b:128:ALA:HB1	9:b:160:LEU:HG	1.90	0.53
10:c:127:ILE:HG23	10:c:162:LEU:HD13	1.89	0.53
13:A:241:ILE:HD12	14:B:314:ASN:ND2	2.23	0.53
18:F:178:ASP:OD1	18:F:179:GLU:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:135:LEU:HD13	20:H:163:MET:HE3	1.90	0.53
26:O:55:ILE:HD12	26:O:57:LEU:HD11	1.90	0.53
28:q:37:LYS:NZ	28:q:38:MET:O	2.40	0.53
2:U:410:VAL:HG23	2:U:448:LEU:CD2	2.37	0.53
5:X:78:ASN:OD1	5:X:79:SER:N	2.40	0.53
10:c:121:TRP:HZ3	10:c:123:SER:HG	1.56	0.53
17:E:69:PHE:CE2	17:E:92:LEU:HD11	2.43	0.53
32:K:16:SER:OG	32:K:18:GLU:OE1	2.22	0.53
32:K:21:LEU:HD23	32:K:24:VAL:HG23	1.90	0.53
25:n:48:LEU:HD21	25:n:135:ALA:HB3	1.89	0.53
4:W:275:ILE:HD11	4:W:306:LEU:HD12	1.90	0.53
5:X:354:ILE:HD11	5:X:361:VAL:HG12	1.90	0.53
9:b:85:THR:HG22	9:b:87:CYS:SG	2.47	0.53
33:f:447:ALA:O	33:f:451:VAL:HG23	2.09	0.53
2:U:412:HIS:CD2	2:U:422:LEU:HD21	2.43	0.53
4:W:125:ILE:HD13	4:W:145:LEU:HD11	1.91	0.53
13:A:190:VAL:HG11	13:A:212:VAL:CG2	2.38	0.53
15:C:41:ASN:OD1	15:C:44:ARG:NH1	2.34	0.53
26:o:97:MET:HA	26:o:100:GLN:HG2	1.91	0.53
28:q:164:LEU:HD13	28:q:178:PHE:CG	2.44	0.53
2:U:650:TYR:OH	2:U:770:TRP:NE1	2.34	0.53
3:V:485:ASP:OD1	11:d:345:GLN:NE2	2.41	0.53
6:Y:221:THR:HG23	6:Y:256:VAL:HG11	1.91	0.53
16:D:277:ALA:O	16:D:278:GLN:CB	2.57	0.53
18:F:188:ILE:HG21	18:F:195:ILE:HD11	1.91	0.53
25:N:168:TYR:CE1	31:t:78:LEU:HD13	2.43	0.53
5:X:256:LEU:HD13	5:X:319:ILE:CG2	2.38	0.53
14:B:375:ALA:HB3	14:B:378:VAL:HG23	1.90	0.53
34:D:501:ATP:O2G	17:E:294:ARG:NH1	2.40	0.53
18:F:126:THR:O	18:F:129:ARG:N	2.40	0.53
14:B:91:LYS:O	14:B:94:GLU:N	2.42	0.53
28:Q:174:ASN:C	28:Q:175:LEU:HD23	2.33	0.53
30:S:57:LEU:HD22	31:T:177:TYR:OH	2.08	0.53
30:s:41:LEU:HD11	30:s:177:LEU:HD11	1.91	0.53
33:f:494:ARG:O	33:f:497:VAL:HG12	2.09	0.53
4:W:314:LEU:HD12	4:W:365:ILE:HG21	1.90	0.53
13:A:75:PRO:O	33:f:680:ARG:NH1	2.42	0.53
23:L:22:ILE:HD11	23:L:120:THR:HG23	1.91	0.53
27:P:179:ALA:CB	29:r:85:ILE:HD11	2.33	0.53
26:o:78:HIS:NE2	26:o:96:ASP:OD1	2.38	0.53
26:o:94:ASP:OD2	27:p:99:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:373:ALA:O	3:V:377:GLN:OE1	2.27	0.53
4:W:72:LYS:O	4:W:76:GLU:OE1	2.27	0.53
4:W:304:ASP:O	4:W:308:LEU:HD23	2.09	0.53
6:Y:224:VAL:CG1	6:Y:228:MET:HE2	2.36	0.53
9:b:142:ASN:OD1	9:b:143:PHE:N	2.42	0.53
18:F:255:GLN:O	18:F:258:GLN:NE2	2.41	0.53
21:I:206:LEU:CD1	21:I:211:VAL:HG11	2.38	0.53
33:f:430:ASP:HA	33:f:433:LEU:HG	1.91	0.53
5:X:31:VAL:HG21	5:X:53:LEU:HD21	1.89	0.53
9:b:114:GLY:O	9:b:115:SER:OG	2.20	0.53
13:A:151:ILE:HG23	13:A:151:ILE:O	2.09	0.53
14:B:357:ASP:N	14:B:360:THR:OG1	2.42	0.53
24:M:54:VAL:O	24:M:54:VAL:HG23	2.07	0.53
27:p:199:THR:HG23	27:p:199:THR:O	2.09	0.53
33:f:333:LEU:HD12	33:f:829:MET:SD	2.49	0.53
2:U:18:GLN:CG	11:d:124:LEU:HD22	2.35	0.52
8:a:38:THR:O	8:a:42:LEU:HD13	2.09	0.52
8:a:142:LEU:HD21	8:a:152:HIS:ND1	2.24	0.52
9:b:90:ILE:HG21	9:b:131:LEU:HD11	1.91	0.52
14:B:59:ARG:O	14:B:63:LEU:HD23	2.08	0.52
18:F:251:LEU:HD12	18:F:285:ILE:HD13	1.90	0.52
18:F:317:LEU:CD2	18:F:328:VAL:HG21	2.40	0.52
31:T:119:GLU:OE1	31:T:128:TYR:CD2	2.62	0.52
25:n:36:THR:HG21	25:n:197:ALA:HB3	1.90	0.52
5:X:335:LEU:HD21	5:X:354:ILE:HD13	1.91	0.52
11:d:92:THR:HG22	11:d:143:LEU:HD21	1.90	0.52
19:G:113:MET:HE2	19:G:113:MET:HA	1.90	0.52
30:S:202:LEU:O	30:S:206:VAL:HG13	2.10	0.52
30:S:204:LYS:O	30:S:208:ILE:HG12	2.09	0.52
30:S:214:ASP:OD1	30:S:215:VAL:N	2.42	0.52
27:p:103:TYR:O	27:p:126:LEU:HD11	2.09	0.52
2:U:12:LEU:O	2:U:12:LEU:HD23	2.09	0.52
2:U:717:ILE:HG12	2:U:731:ILE:HD13	1.91	0.52
4:W:272:LEU:HD21	4:W:302:TYR:CE1	2.44	0.52
8:a:60:TYR:CZ	8:a:64:ILE:HD13	2.45	0.52
10:c:51:MET:HE3	17:E:108:MET:HE1	1.92	0.52
17:E:84:ARG:HG3	17:E:87:LEU:HD23	1.91	0.52
18:F:406:ILE:HD13	18:F:422:GLU:CB	2.39	0.52
30:s:219:ASP:O	30:s:238:LEU:N	2.38	0.52
5:X:14:SER:O	5:X:17:SER:OG	2.20	0.52
6:Y:133:ALA:HB1	15:C:149:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:213:PHE:HD1	8:a:216:LEU:HD12	1.75	0.52
9:b:27:GLN:OE1	9:b:27:GLN:N	2.42	0.52
17:E:116:ASP:OD2	17:E:213:ARG:NH2	2.40	0.52
22:J:43:LEU:HD21	22:J:72:ALA:HB2	1.91	0.52
31:T:169:TYR:O	31:T:169:TYR:CG	2.61	0.52
32:K:199:LEU:HD12	32:K:237:VAL:CG1	2.40	0.52
33:f:466:LEU:HD12	33:f:481:SER:O	2.10	0.52
3:V:353:LEU:HG	3:V:353:LEU:O	2.10	0.52
4:W:147:LYS:NZ	4:W:184:GLU:OE2	2.42	0.52
5:X:254:MET:HE3	5:X:270:LEU:HD11	1.91	0.52
20:H:75:VAL:HG22	20:H:76:TYR:H	1.74	0.52
30:S:92:LEU:HD13	30:S:134:VAL:HG11	1.92	0.52
25:n:73:ASP:OD1	25:n:74:ARG:N	2.41	0.52
25:n:227:GLN:O	25:n:228:ILE:C	2.52	0.52
29:r:141:LEU:CD2	29:r:145:MET:HE3	2.39	0.52
4:W:132:THR:HG21	4:W:138:VAL:HG11	1.92	0.52
5:X:240:ASP:CG	5:X:275:LEU:HD11	2.35	0.52
8:a:90:PRO:HB2	8:a:125:ILE:HD11	1.92	0.52
8:a:231:GLN:O	8:a:232:TRP:HB3	2.08	0.52
14:B:95:GLU:O	14:B:99:VAL:HG23	2.10	0.52
16:D:269:ALA:HA	17:E:258:MET:HE1	1.90	0.52
23:L:88:MET:CE	23:L:112:ILE:HD11	2.29	0.52
30:s:239:ARG:NH2	30:s:241:ASP:OD2	2.41	0.52
8:a:317:VAL:HG13	8:a:319:LEU:HG	1.92	0.52
9:b:123:ASP:OD1	9:b:124:LEU:HD22	2.10	0.52
14:B:223:ILE:CD1	14:B:342:ILE:HD12	2.40	0.52
25:N:183:LYS:O	25:N:187:LEU:HD23	2.09	0.52
29:R:74:ALA:HB1	29:R:219:ILE:HD12	1.91	0.52
32:K:27:ALA:O	32:K:31:ILE:HG12	2.10	0.52
33:f:737:ASN:ND2	33:f:773:LYS:O	2.43	0.52
13:A:276:GLU:HB3	14:B:310:LEU:HD21	1.92	0.52
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.91	0.52
22:J:98:VAL:HG12	29:R:137:ALA:HB1	1.91	0.52
31:T:223:TYR:OH	31:T:253:ASN:N	2.43	0.52
32:K:191:LEU:HD21	32:K:219:THR:CG2	2.40	0.52
30:s:100:LEU:HD21	30:s:116:ILE:HD13	1.91	0.52
33:f:414:LEU:C	33:f:414:LEU:HD23	2.35	0.52
33:f:460:ASP:OD2	33:f:494:ARG:NH1	2.42	0.52
33:f:683:GLU:OE1	33:f:683:GLU:N	2.43	0.52
3:V:337:LEU:HG	3:V:367:VAL:HG11	1.91	0.52
4:W:425:LEU:HD12	7:Z:252:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:275:LEU:HA	6:Y:278:VAL:HG22	1.92	0.52
8:a:77:VAL:O	8:a:81:LEU:HD23	2.09	0.52
13:A:96:ALA:C	13:A:140:VAL:HG12	2.35	0.52
14:B:360:THR:O	14:B:364:ILE:HG12	2.10	0.52
17:E:204:VAL:HG22	17:E:238:ILE:HD11	1.92	0.52
27:P:71:LEU:HD11	27:P:82:ILE:HG21	1.92	0.52
27:P:179:ALA:HB2	29:r:85:ILE:CD1	2.35	0.52
3:V:236:ARG:O	3:V:240:LEU:HD23	2.10	0.52
5:X:86:ALA:CB	5:X:125:LEU:HD22	2.40	0.52
7:Z:183:THR:OG1	16:D:70:LYS:NZ	2.37	0.52
23:L:39:LYS:NZ	24:M:60:GLU:OE2	2.28	0.52
24:M:41:ARG:NE	24:M:147:ALA:O	2.43	0.52
33:f:291:GLN:HB3	33:f:317:LEU:HD21	1.92	0.52
33:f:527:VAL:HG23	33:f:527:VAL:O	2.10	0.52
3:V:377:GLN:O	3:V:381:GLN:OE1	2.27	0.51
5:X:168:GLU:O	5:X:172:LEU:HD23	2.10	0.51
29:R:129:ASN:O	29:R:131:GLU:N	2.43	0.51
32:K:85:ALA:CB	32:K:139:VAL:HG21	2.37	0.51
10:c:113:HIS:CE1	10:c:144:VAL:HG22	2.46	0.51
18:F:406:ILE:HD13	18:F:422:GLU:HB3	1.92	0.51
29:R:74:ALA:CB	29:R:219:ILE:HD12	2.40	0.51
29:R:217:ARG:HE	28:q:145:ARG:HD2	1.76	0.51
30:s:57:LEU:HD12	30:s:68:SER:CB	2.40	0.51
33:f:377:VAL:O	33:f:381:VAL:HG23	2.10	0.51
13:A:53:GLN:OE1	13:A:53:GLN:N	2.44	0.51
13:A:67:GLU:OE1	13:A:67:GLU:N	2.43	0.51
13:A:159:PRO:HA	13:A:162:THR:HG22	1.90	0.51
18:F:349:ASP:OD1	18:F:350:ARG:N	2.43	0.51
22:J:177:THR:HG22	22:J:178:ASP:N	2.25	0.51
11:d:142:ILE:H	11:d:142:ILE:HD12	1.76	0.51
11:d:334:GLU:OE1	11:d:334:GLU:N	2.41	0.51
13:A:51:ASP:O	13:A:55:LEU:HD13	2.11	0.51
16:D:387:VAL:HG22	17:E:162:VAL:HG21	1.92	0.51
18:F:307:GLN:O	18:F:311:LEU:HD13	2.10	0.51
21:I:76:VAL:HG11	21:I:83:ALA:HB1	1.92	0.51
21:I:118:LYS:O	21:I:122:THR:HG23	2.10	0.51
28:Q:4:LEU:HD11	28:Q:47:VAL:HG13	1.93	0.51
30:s:73:LYS:HG3	30:s:231:ILE:HD13	1.93	0.51
8:a:156:TYR:HB3	8:a:179:PHE:HB2	1.92	0.51
10:c:291:LEU:HD12	10:c:292:MET:N	2.26	0.51
13:A:77:LEU:HD23	13:A:77:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:187:LEU:O	13:A:191:VAL:HG22	2.11	0.51
16:D:41:TYR:O	16:D:44:TYR:HB3	2.11	0.51
24:M:67:LEU:HD13	24:M:213:GLU:HG2	1.92	0.51
28:Q:174:ASN:O	28:Q:175:LEU:HD23	2.11	0.51
33:f:679:LEU:HG	33:f:690:VAL:HG11	1.93	0.51
2:U:105:ILE:HD11	15:C:23:TYR:CG	2.46	0.51
7:Z:242:LEU:O	7:Z:242:LEU:HD23	2.11	0.51
10:c:27:THR:HG22	10:c:27:THR:O	2.10	0.51
21:I:46:ALA:HB1	21:I:197:LEU:HD11	1.90	0.51
26:o:78:HIS:N	26:o:86:CYS:O	2.37	0.51
2:U:803:LYS:O	2:U:893:THR:N	2.40	0.51
3:V:185:GLN:NE2	3:V:218:TYR:OH	2.42	0.51
6:Y:338:ILE:HD13	6:Y:343:LEU:HB2	1.92	0.51
11:d:196:LEU:HD12	11:d:208:PHE:CE2	2.46	0.51
17:E:334:LEU:CD1	17:E:368:MET:HE1	2.41	0.51
24:M:231:ASP:OD1	24:M:231:ASP:N	2.42	0.51
31:t:250:THR:HG22	31:t:251:GLU:N	2.26	0.51
33:f:330:PHE:CE2	33:f:775:THR:HG21	2.46	0.51
2:U:46:GLU:O	2:U:50:GLU:OE1	2.29	0.51
5:X:140:THR:HG21	5:X:142:ARG:HH21	1.75	0.51
13:A:73:ALA:HB2	14:B:140:ASP:HA	1.91	0.51
16:D:202:VAL:HG21	16:D:331:ILE:HD12	1.91	0.51
17:E:64:LEU:HD11	17:E:70:ILE:HG13	1.92	0.51
21:I:68:LEU:HD21	21:I:74:CYS:SG	2.51	0.51
29:R:86:ALA:O	27:p:177:ARG:NH2	2.44	0.51
2:U:371:ILE:HG21	2:U:732:LEU:HD11	1.93	0.51
2:U:719:ASP:O	2:U:727:LYS:NZ	2.36	0.51
7:Z:130:ASP:OD1	7:Z:131:LEU:N	2.44	0.51
14:B:379:THR:HG23	14:B:379:THR:O	2.10	0.51
31:T:154:THR:HG23	31:T:171:ASP:HB3	1.92	0.51
30:s:41:LEU:HD12	30:s:173:LEU:HD23	1.93	0.51
14:B:250:VAL:HG12	14:B:251:VAL:N	2.27	0.51
29:r:239:ARG:NH2	29:r:241:ASP:OD2	2.44	0.51
33:f:426:LEU:HA	33:f:429:ILE:HG12	1.93	0.51
4:W:287:VAL:HG23	4:W:306:LEU:HD11	1.93	0.50
8:a:48:PRO:O	8:a:49:CYS:SG	2.69	0.50
14:B:150:VAL:CG1	14:B:159:VAL:HG13	2.40	0.50
16:D:82:ILE:HG23	16:D:140:VAL:HG13	1.92	0.50
22:J:96:LEU:HD11	28:Q:62:LYS:HG2	1.93	0.50
26:O:102:ILE:HG13	26:O:126:LEU:HD22	1.93	0.50
29:R:142:LEU:O	29:R:146:VAL:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:p:161:ASP:HA	27:p:164:PHE:CE2	2.46	0.50
3:V:283:ASN:OD1	3:V:284:GLU:N	2.43	0.50
4:W:137:TYR:CD2	4:W:138:VAL:HG23	2.46	0.50
7:Z:259:VAL:CG1	10:c:291:LEU:HD13	2.42	0.50
14:B:429:LYS:CB	21:I:169:ALA:HB1	2.42	0.50
24:M:40:ILE:HD12	24:M:194:VAL:HG22	1.92	0.50
31:T:137:LEU:HD22	31:T:155:MET:CE	2.41	0.50
3:V:71:THR:HG23	3:V:112:VAL:HG11	1.93	0.50
3:V:224:LEU:O	3:V:227:VAL:HG22	2.11	0.50
3:V:235:LEU:HA	3:V:250:LEU:HD13	1.92	0.50
3:V:459:GLN:NE2	3:V:460:SER:O	2.44	0.50
29:R:62:THR:OG1	29:R:103:THR:HG21	2.11	0.50
29:R:109:ALA:CB	30:S:155:VAL:HG13	2.41	0.50
30:S:176:LEU:HB2	27:p:149:MET:HE1	1.93	0.50
32:K:147:ASP:N	32:K:147:ASP:OD1	2.42	0.50
28:q:116:TYR:HB3	28:q:124:LEU:HD11	1.92	0.50
2:U:263:SER:O	2:U:267:ASN:ND2	2.45	0.50
3:V:309:MET:HE3	3:V:331:LEU:HD23	1.94	0.50
21:I:36:GLY:HA3	21:I:147:LEU:HD11	1.93	0.50
30:s:187:GLN:OE1	30:s:187:GLN:N	2.44	0.50
2:U:368:ALA:HB1	2:U:731:ILE:HB	1.92	0.50
10:c:152:LYS:O	16:D:77:GLU:CD	2.54	0.50
13:A:174:TYR:OH	13:A:229:VAL:HG22	2.12	0.50
13:A:303:ILE:HG23	13:A:336:ARG:CZ	2.41	0.50
13:A:307:ASP:O	13:A:336:ARG:NH2	2.43	0.50
14:B:256:ILE:HD11	14:B:290:ILE:HA	1.94	0.50
25:n:46:VAL:HG11	25:n:135:ALA:HB1	1.94	0.50
27:p:36:THR:HG22	28:q:127:ALA:HB2	1.94	0.50
27:p:56:LEU:O	27:p:60:VAL:HG23	2.12	0.50
3:V:242:HIS:ND1	15:C:30:GLU:OE2	2.44	0.50
5:X:82:LYS:O	5:X:85:ALA:N	2.45	0.50
6:Y:285:ASP:OD1	6:Y:286:TRP:N	2.45	0.50
8:a:36:GLN:HA	8:a:39:LEU:HD13	1.93	0.50
14:B:400:THR:O	14:B:404:LEU:HD23	2.12	0.50
16:D:197:ASP:OD1	16:D:197:ASP:O	2.30	0.50
17:E:140:GLU:OE1	17:E:143:ARG:NH1	2.45	0.50
18:F:375:VAL:HA	18:F:415:LEU:HD23	1.93	0.50
19:G:123:GLN:OE1	20:H:85:VAL:HG11	2.12	0.50
28:Q:142:ILE:HD11	29:r:196:GLY:CA	2.41	0.50
26:o:242:LEU:H	26:o:242:LEU:HD23	1.75	0.50
33:f:485:LEU:HD23	33:f:501:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:649:HIS:HA	33:f:652:VAL:HG22	1.93	0.50
3:V:98:LEU:O	3:V:101:LEU:HD23	2.11	0.50
6:Y:117:LYS:O	6:Y:121:LEU:HD13	2.12	0.50
6:Y:278:VAL:O	6:Y:282:MET:HG3	2.11	0.50
10:c:184:LEU:CG	10:c:204:THR:HG22	2.42	0.50
10:c:291:LEU:HD12	10:c:291:LEU:C	2.36	0.50
14:B:133:VAL:HG11	14:B:157:HIS:O	2.12	0.50
29:r:118:LEU:HD22	29:r:142:LEU:HD12	1.94	0.50
3:V:227:VAL:O	3:V:228:ARG:C	2.55	0.50
4:W:272:LEU:HD12	4:W:341:PHE:CE2	2.46	0.50
4:W:312:MET:HA	4:W:312:MET:HE3	1.92	0.50
6:Y:11:LEU:N	6:Y:212:GLU:OE1	2.45	0.50
25:N:36:THR:HG21	25:N:197:ALA:HB3	1.94	0.50
26:O:44:THR:N	26:O:172:SER:HG	2.10	0.50
27:P:141:THR:HG22	27:P:142:CYS:N	2.26	0.50
30:S:179:ASN:O	30:S:186:MET:HE2	2.12	0.50
32:K:85:ALA:O	32:K:89:ILE:HG12	2.12	0.50
1:y:391:LYS:HD3	33:f:464:ALA:HB1	1.94	0.50
13:A:390:THR:O	13:A:394:MET:HG2	2.12	0.50
14:B:232:LYS:NZ	36:B:501:ADP:O2B	2.35	0.50
24:M:38:ILE:CG2	24:M:177:ILE:HD11	2.42	0.50
25:N:122:TYR:O	25:N:125:ARG:HG3	2.11	0.50
30:s:211:ALA:HA	30:s:217:THR:HG23	1.93	0.50
33:f:348:ILE:HD12	33:f:381:VAL:HG21	1.94	0.50
33:f:477:MET:O	33:f:514:VAL:HG22	2.12	0.50
2:U:183:LEU:HD12	16:D:41:TYR:CE2	2.47	0.49
11:d:181:GLN:C	11:d:182:LEU:HD12	2.37	0.49
28:Q:172:ILE:O	28:q:174:ASN:N	2.44	0.49
29:R:109:ALA:HB2	30:S:155:VAL:HG13	1.94	0.49
2:U:640:LEU:HD22	16:D:60:TYR:OH	2.12	0.49
14:B:197:ILE:O	14:B:201:VAL:HG22	2.12	0.49
17:E:302:ASP:OD1	17:E:303:LEU:N	2.44	0.49
18:F:168:TYR:O	18:F:169:ASP:C	2.53	0.49
30:S:132:TYR:HB3	30:S:134:VAL:HG12	1.94	0.49
2:U:408:LEU:HD23	2:U:411:ILE:HD11	1.93	0.49
3:V:71:THR:CG2	3:V:112:VAL:HG11	2.42	0.49
3:V:379:LEU:HD21	3:V:395:ILE:HG21	1.95	0.49
8:a:308:GLU:OE2	8:a:312:MET:HE2	2.12	0.49
9:b:33:VAL:HA	9:b:36:VAL:HG12	1.93	0.49
10:c:48:GLY:HA3	10:c:53:VAL:HG11	1.95	0.49
11:d:171:LEU:HD13	11:d:191:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:80:ARG:O	14:B:81:ASN:C	2.55	0.49
14:B:80:ARG:O	14:B:84:GLN:OE1	2.31	0.49
14:B:162:VAL:HG12	14:B:163:LEU:N	2.27	0.49
16:D:299:PHE:CE2	16:D:305:VAL:HG21	2.47	0.49
19:G:62:ASP:O	19:G:63:SER:OG	2.22	0.49
21:I:158:GLY:HA3	22:J:58:THR:HG21	1.94	0.49
26:O:149:THR:O	26:O:152:HIS:NE2	2.45	0.49
32:K:20:ARG:NH1	32:K:25:GLU:OE1	2.42	0.49
26:o:206:ILE:HG23	26:o:213:GLY:HA2	1.94	0.49
27:p:164:PHE:HA	27:p:167:ILE:HG22	1.94	0.49
2:U:62:LEU:HD22	2:U:87:LEU:HD22	1.93	0.49
3:V:373:ALA:HB2	3:V:427:GLN:HG2	1.93	0.49
5:X:6:VAL:O	5:X:10:GLN:OE1	2.29	0.49
5:X:171:LEU:HD11	5:X:210:LEU:HD23	1.94	0.49
7:Z:226:ILE:O	7:Z:230:LEU:HD23	2.13	0.49
10:c:283:HIS:NE2	16:D:122:GLU:OE1	2.43	0.49
30:S:120:LEU:HD23	30:S:152:PHE:HE2	1.76	0.49
31:T:112:LEU:HD12	31:T:115:MET:HE2	1.95	0.49
33:f:450:ILE:CD1	33:f:822:VAL:HG21	2.31	0.49
33:f:571:GLU:O	33:f:573:ILE:N	2.46	0.49
2:U:894:MET:HG3	2:U:906:LEU:HD11	1.95	0.49
3:V:373:ALA:O	3:V:376:ASN:OD1	2.29	0.49
9:b:149:ASN:O	9:b:153:LEU:HD23	2.13	0.49
16:D:87:LEU:CD1	17:E:80:VAL:HG22	2.43	0.49
21:I:90:LEU:HG	21:I:114:LEU:HD13	1.95	0.49
24:M:187:CYS:SG	24:M:220:LEU:HD22	2.53	0.49
30:s:76:ASP:OD1	30:s:77:LYS:N	2.45	0.49
33:f:229:VAL:O	33:f:233:LEU:HD13	2.12	0.49
2:U:728:PHE:O	2:U:732:LEU:HD23	2.13	0.49
3:V:482:PHE:CE2	6:Y:377:LEU:HD21	2.48	0.49
5:X:171:LEU:HD13	5:X:209:THR:HG22	1.94	0.49
6:Y:285:ASP:O	6:Y:289:ALA:HB2	2.12	0.49
13:A:210:LYS:N	13:A:338:ASP:OD2	2.43	0.49
18:F:279:ALA:O	18:F:280:PRO:C	2.56	0.49
29:R:225:ARG:NH2	28:q:140:LEU:HD13	2.28	0.49
2:U:65:SER:OG	2:U:96:TYR:OH	2.30	0.49
10:c:120:CYS:SG	10:c:156:VAL:HG12	2.53	0.49
11:d:112:CYS:O	11:d:116:LEU:HD13	2.12	0.49
16:D:342:ARG:NH1	16:D:361:GLU:OE1	2.45	0.49
17:E:334:LEU:HD12	17:E:368:MET:HE1	1.95	0.49
18:F:323:ASN:O	18:F:323:ASN:OD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:406:ILE:HA	18:F:409:ARG:HD3	1.95	0.49
18:F:434:ASN:O	18:F:434:ASN:OD1	2.30	0.49
19:G:164:LYS:NZ	20:H:55:ILE:O	2.42	0.49
27:P:11:VAL:HG11	27:P:52:GLY:HA3	1.94	0.49
33:f:848:GLN:HG3	33:f:849:ALA:N	2.28	0.49
3:V:462:GLU:OE1	3:V:462:GLU:N	2.46	0.49
5:X:201:TYR:OH	16:D:339:ARG:NH1	2.46	0.49
27:P:3:ILE:HG21	27:P:104:TYR:CD2	2.47	0.49
30:S:227:THR:HG22	30:S:228:LYS:H	1.78	0.49
26:o:156:ILE:HG12	26:o:162:THR:HG22	1.94	0.49
33:f:686:LEU:O	33:f:690:VAL:HG23	2.12	0.49
22:J:196:LEU:HD12	22:J:206:ILE:HD11	1.94	0.49
25:N:115:SER:O	25:N:119:GLU:HG2	2.13	0.49
28:Q:46:CYS:SG	28:Q:102:LEU:HD21	2.53	0.49
28:q:88:LEU:HD12	28:q:118:MET:SD	2.53	0.49
2:U:457:ILE:H	2:U:457:ILE:HD12	1.78	0.49
8:a:226:ARG:CZ	8:a:231:GLN:HE22	2.25	0.49
8:a:366:LEU:HD23	8:a:366:LEU:C	2.37	0.49
9:b:119:ASP:HB2	9:b:124:LEU:HD21	1.94	0.49
18:F:78:GLU:O	18:F:82:VAL:HG23	2.13	0.49
18:F:285:ILE:HG21	18:F:288:LEU:CD1	2.41	0.49
28:q:13:VAL:O	28:q:13:VAL:HG12	2.13	0.49
8:a:109:GLU:O	8:a:112:ILE:HG22	2.13	0.48
18:F:226:TYR:HB3	18:F:353:GLU:OE1	2.13	0.48
21:I:186:LEU:HD11	21:I:217:THR:HG22	1.95	0.48
28:Q:172:ILE:HD11	28:q:26:VAL:N	2.28	0.48
4:W:201:ARG:NE	4:W:204:ILE:HD11	2.28	0.48
13:A:297:ARG:NH1	18:F:303:ASP:OD2	2.45	0.48
14:B:337:LEU:HD23	14:B:342:ILE:CD1	2.38	0.48
15:C:73:VAL:HG23	15:C:127:LEU:HD12	1.95	0.48
16:D:292:LEU:HG	16:D:296:MET:HE2	1.96	0.48
21:I:62:SER:OG	21:I:65:ILE:O	2.13	0.48
24:M:42:CYS:SG	24:M:45:GLY:N	2.86	0.48
25:n:194:LEU:CD1	25:n:208:ILE:HG23	2.42	0.48
26:o:46:ILE:O	26:o:46:ILE:HG13	2.13	0.48
31:t:57:LEU:HD22	31:t:195:LEU:HD11	1.96	0.48
1:y:388:THR:O	1:y:392:VAL:HG13	2.14	0.48
14:B:68:ILE:O	33:f:670:MET:HE1	2.13	0.48
15:C:21:ARG:O	15:C:25:LEU:HD13	2.12	0.48
16:D:45:LYS:O	16:D:48:GLN:HG3	2.13	0.48
16:D:150:SER:HB2	16:D:250:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:77:THR:O	22:J:80:ALA:HB3	2.14	0.48
22:J:89:VAL:HG22	28:Q:66:LEU:HD21	1.95	0.48
31:t:197:GLU:OE2	31:t:201:LYS:NZ	2.43	0.48
3:V:313:LEU:HD11	3:V:329:HIS:CE1	2.49	0.48
5:X:73:VAL:O	5:X:74:ARG:C	2.57	0.48
6:Y:183:TYR:CD1	6:Y:213:LEU:HD11	2.47	0.48
6:Y:338:ILE:HD12	6:Y:345:CYS:O	2.13	0.48
10:c:139:ARG:O	10:c:161:ARG:NH1	2.46	0.48
11:d:313:ASN:O	11:d:313:ASN:OD1	2.32	0.48
30:S:57:LEU:HD22	31:T:177:TYR:CE1	2.48	0.48
33:f:786:GLN:O	33:f:786:GLN:HG2	2.12	0.48
4:W:314:LEU:HD13	8:a:312:MET:SD	2.54	0.48
13:A:238:ILE:HG21	13:A:260:LEU:HD11	1.94	0.48
17:E:93:LYS:O	17:E:96:THR:HG22	2.14	0.48
18:F:182:THR:HG23	18:F:182:THR:O	2.14	0.48
24:M:216:TRP:CD1	24:M:220:LEU:HD21	2.49	0.48
2:U:545:LEU:HB3	2:U:577:ILE:HG21	1.94	0.48
2:U:701:ILE:HG21	2:U:810:THR:HG22	1.96	0.48
3:V:259:LEU:HD11	3:V:294:ARG:HD3	1.95	0.48
7:Z:19:VAL:HG22	7:Z:95:TYR:CE1	2.49	0.48
8:a:129:GLN:O	8:a:133:GLU:OE1	2.32	0.48
18:F:291:ILE:HD11	18:F:309:THR:HG22	1.95	0.48
26:O:60:ASP:HB2	26:O:213:GLY:HA3	1.96	0.48
29:R:225:ARG:HD3	28:q:144:ASP:OD2	2.14	0.48
33:f:270:LEU:HD21	33:f:298:LEU:HD23	1.93	0.48
2:U:62:LEU:HD22	2:U:87:LEU:CD2	2.44	0.48
2:U:596:ASN:OD1	16:D:51:LEU:HD22	2.14	0.48
7:Z:40:LEU:CD2	7:Z:91:ILE:HD13	2.44	0.48
11:d:265:ASP:OD1	11:d:265:ASP:C	2.56	0.48
16:D:337:ASP:OD1	16:D:338:ARG:N	2.43	0.48
18:F:228:PRO:O	18:F:230:GLY:N	2.47	0.48
27:P:193:ASP:N	27:P:193:ASP:OD1	2.46	0.48
1:y:399:LEU:HD23	1:y:399:LEU:C	2.39	0.48
2:U:418:GLU:O	2:U:422:LEU:N	2.47	0.48
2:U:650:TYR:HH	2:U:770:TRP:HE1	1.59	0.48
6:Y:157:ILE:HG21	6:Y:187:TYR:CG	2.49	0.48
8:a:225:LEU:O	8:a:231:GLN:HB2	2.14	0.48
9:b:5:SER:HA	9:b:48:ASN:OD1	2.14	0.48
9:b:138:VAL:HG12	9:b:160:LEU:HD13	1.96	0.48
18:F:223:VAL:HB	18:F:329:ILE:HG22	1.94	0.48
19:G:123:GLN:NE2	20:H:82:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:69:THR:HG22	20:H:70:LYS:N	2.29	0.48
22:J:86:ARG:HD2	22:J:114:LEU:HD22	1.96	0.48
24:M:71:ASP:HA	31:T:121:LEU:HD21	1.96	0.48
31:T:169:TYR:CE1	31:T:184:THR:HG22	2.49	0.48
25:n:93:VAL:HG21	25:n:117:PHE:HD1	1.75	0.48
28:q:59:TYR:O	28:q:63:ASN:ND2	2.47	0.48
2:U:39:SER:OG	2:U:71:LEU:HD11	2.14	0.48
3:V:121:PHE:HA	3:V:159:LEU:HD11	1.95	0.48
4:W:271:VAL:O	4:W:275:ILE:HG12	2.14	0.48
9:b:8:VAL:HG23	9:b:8:VAL:O	2.12	0.48
15:C:76:VAL:HG13	15:C:85:VAL:CG1	2.44	0.48
16:D:203:LEU:O	16:D:204:MET:C	2.56	0.48
17:E:122:MET:CE	17:E:218:MET:HE3	2.44	0.48
19:G:10:ASP:OD1	19:G:11:ARG:NH1	2.46	0.48
27:P:136:PHE:O	27:P:137:VAL:HG13	2.14	0.48
25:n:64:VAL:HG23	25:n:64:VAL:O	2.14	0.48
25:n:93:VAL:HG21	25:n:117:PHE:CE1	2.49	0.48
25:n:228:ILE:O	25:n:229:PRO:C	2.55	0.48
27:p:4:MET:HE1	27:p:126:LEU:HD13	1.95	0.48
28:q:12:TYR:OH	28:q:151:ILE:O	2.21	0.48
6:Y:11:LEU:HB3	6:Y:12:PRO:HD2	1.96	0.48
7:Z:131:LEU:HD12	7:Z:131:LEU:O	2.14	0.48
11:d:119:LEU:HD23	11:d:147:ILE:CD1	2.44	0.48
11:d:192:LEU:O	11:d:196:LEU:HD23	2.13	0.48
17:E:236:ASP:OD1	18:F:311:LEU:HD21	2.13	0.48
24:M:88:LEU:HD13	24:M:136:PHE:CE1	2.49	0.48
33:f:264:GLU:O	33:f:268:LEU:HD23	2.14	0.48
33:f:849:ALA:O	33:f:850:VAL:HG23	2.14	0.48
2:U:42:VAL:HG12	2:U:46:GLU:HG2	1.96	0.47
2:U:376:MET:HE2	2:U:738:ASP:HB2	1.96	0.47
2:U:644:TYR:OH	16:D:71:GLU:OE1	2.23	0.47
11:d:109:LEU:O	11:d:112:CYS:N	2.42	0.47
18:F:139:LEU:HD13	18:F:161:LEU:HD23	1.95	0.47
20:H:174:LEU:HD11	20:H:194:THR:HG21	1.95	0.47
21:I:17:ARG:HG3	21:I:22:GLU:OE2	2.14	0.47
25:n:192:ASN:O	25:n:196:LEU:HD23	2.14	0.47
33:f:588:ARG:O	33:f:589:SER:C	2.57	0.47
2:U:609:ASP:O	2:U:615:ARG:NH1	2.43	0.47
3:V:447:ILE:HG22	3:V:449:ALA:H	1.78	0.47
5:X:15:LEU:HD23	5:X:22:ALA:HB1	1.95	0.47
5:X:354:ILE:HD11	5:X:361:VAL:CG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:228:MET:HE1	6:Y:259:TYR:CD2	2.48	0.47
15:C:333:SER:HB2	15:C:338:LEU:HD21	1.95	0.47
15:C:351:MET:HG3	15:C:351:MET:O	2.14	0.47
19:G:113:MET:SD	26:O:113:THR:HG22	2.55	0.47
24:M:109:LEU:C	24:M:109:LEU:HD23	2.39	0.47
32:K:141:LEU:HD12	32:K:156:MET:HE2	1.96	0.47
33:f:647:GLY:HA2	33:f:685:THR:HG21	1.95	0.47
3:V:166:TYR:O	3:V:170:LEU:HD23	2.14	0.47
5:X:140:THR:O	5:X:140:THR:HG22	2.14	0.47
18:F:318:ASP:O	18:F:347:ARG:NH1	2.46	0.47
26:O:234:VAL:O	26:O:234:VAL:CG2	2.62	0.47
30:s:41:LEU:HD21	30:s:43:ILE:HD11	1.96	0.47
33:f:412:ALA:HB3	33:f:819:TYR:CD2	2.49	0.47
3:V:108:LEU:HD21	3:V:170:LEU:O	2.14	0.47
3:V:129:ASP:OD1	3:V:130:PHE:N	2.47	0.47
4:W:37:GLU:HG2	4:W:37:GLU:O	2.14	0.47
8:a:42:LEU:O	8:a:46:GLN:OE1	2.32	0.47
10:c:63:ASP:OD1	10:c:66:THR:N	2.46	0.47
13:A:319:MET:HG3	13:A:337:LEU:HD21	1.96	0.47
14:B:68:ILE:HA	33:f:670:MET:HE1	1.96	0.47
17:E:121:ASN:O	17:E:125:GLU:HG3	2.13	0.47
24:M:187:CYS:O	24:M:191:VAL:HG23	2.14	0.47
25:N:118:LYS:NZ	25:N:119:GLU:OE2	2.41	0.47
33:f:270:LEU:HD12	33:f:278:VAL:HG22	1.95	0.47
33:f:334:ALA:O	33:f:337:LEU:O	2.32	0.47
33:f:562:LEU:HD21	33:f:576:ILE:CG2	2.44	0.47
33:f:830:LEU:HG	33:f:830:LEU:O	2.14	0.47
3:V:508:ALA:HA	3:V:511:ARG:HD2	1.96	0.47
4:W:43:VAL:O	4:W:47:LEU:HD23	2.13	0.47
8:a:213:PHE:CD1	8:a:216:LEU:HD12	2.50	0.47
10:c:279:ASP:N	16:D:122:GLU:OE2	2.43	0.47
13:A:49:GLU:O	13:A:53:GLN:OE1	2.32	0.47
17:E:249:ALA:HB1	18:F:261:ILE:HG21	1.94	0.47
20:H:16:SER:OG	20:H:18:LYS:NZ	2.46	0.47
27:P:131:MET:HG3	27:P:131:MET:O	2.15	0.47
29:R:227:ALA:CB	27:p:180:VAL:HG12	2.44	0.47
29:R:250:ASN:OD1	29:R:251:VAL:N	2.45	0.47
30:S:120:LEU:HD23	30:S:152:PHE:CE2	2.50	0.47
31:T:108:LEU:HD13	31:T:155:MET:HE3	1.95	0.47
31:t:237:VAL:HG23	31:t:242:VAL:HG22	1.96	0.47
33:f:327:ASN:HB2	33:f:421:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:11:LEU:HD12	6:Y:212:GLU:OE2	2.15	0.47
15:C:78:ARG:NH2	15:C:80:MET:HE1	2.29	0.47
17:E:182:LEU:HD22	34:E:401:ATP:H2'	1.96	0.47
23:L:5:GLN:HG2	24:M:10:LEU:HD21	1.96	0.47
33:f:558:LEU:HB2	33:f:559:PRO:HD3	1.95	0.47
2:U:141:CYS:SG	15:C:20:LEU:HD11	2.54	0.47
2:U:349:ASP:OD1	2:U:817:LEU:N	2.45	0.47
2:U:638:SER:HB3	2:U:671:LEU:HD11	1.97	0.47
4:W:85:GLU:O	4:W:89:LEU:HD13	2.14	0.47
8:a:245:VAL:HG23	8:a:301:LYS:HD3	1.96	0.47
8:a:271:LYS:O	8:a:275:LEU:HD23	2.15	0.47
11:d:141:LEU:HD11	11:d:183:PRO:HD3	1.95	0.47
14:B:59:ARG:NH2	33:f:232:TYR:OH	2.47	0.47
15:C:96:VAL:HG23	15:C:96:VAL:O	2.15	0.47
15:C:248:MET:HE1	15:C:291:VAL:HG13	1.96	0.47
17:E:115:VAL:O	17:E:115:VAL:HG23	2.15	0.47
18:F:314:LEU:O	18:F:347:ARG:NH1	2.47	0.47
19:G:158:GLY:O	20:H:84:ARG:NH2	2.46	0.47
20:H:11:THR:HG22	20:H:19:LEU:HD22	1.96	0.47
24:M:24:VAL:HG22	24:M:124:THR:OG1	2.14	0.47
25:N:93:VAL:HG11	25:N:117:PHE:CE2	2.49	0.47
28:Q:13:VAL:CG1	28:Q:183:ILE:HB	2.45	0.47
29:R:201:GLY:O	29:R:214:LEU:HD22	2.15	0.47
31:T:91:ASN:OD1	31:T:94:THR:N	2.48	0.47
32:K:141:LEU:HD12	32:K:156:MET:CE	2.44	0.47
28:q:4:LEU:HD21	28:q:47:VAL:HG13	1.96	0.47
28:q:29:LYS:NZ	29:r:181:SER:O	2.43	0.47
31:t:55:SER:OG	31:t:221:LEU:HD13	2.15	0.47
2:U:233:LEU:HD11	2:U:325:MET:SD	2.55	0.47
3:V:373:ALA:C	3:V:377:GLN:OE1	2.58	0.47
5:X:8:GLU:OE1	5:X:33:ARG:NH2	2.48	0.47
11:d:251:ILE:HD13	11:d:257:THR:HG22	1.96	0.47
13:A:45:ILE:HG23	13:A:46:LYS:N	2.30	0.47
14:B:125:THR:HG22	14:B:126:SER:N	2.30	0.47
15:C:28:ILE:HD13	16:D:43:ARG:HG3	1.96	0.47
18:F:169:ASP:OD1	18:F:270:ASP:OD2	2.32	0.47
19:G:84:THR:HG23	24:M:157:VAL:HG22	1.96	0.47
21:I:41:ASP:OD2	21:I:185:THR:OG1	2.25	0.47
29:r:141:LEU:HD21	29:r:145:MET:HE3	1.97	0.47
31:t:57:LEU:HD21	31:t:191:ALA:HB3	1.96	0.47
6:Y:279:GLU:HG3	6:Y:296:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:124:ILE:HG12	7:Z:135:THR:HG22	1.97	0.47
8:a:276:CYS:SG	8:a:299:SER:OG	2.66	0.47
14:B:74:MET:HE3	33:f:610:GLN:CA	2.45	0.47
19:G:143:ILE:HD13	19:G:149:PRO:HA	1.96	0.47
24:M:224:ARG:NH2	24:M:226:GLU:OE2	2.43	0.47
26:O:206:ILE:HG23	26:O:213:GLY:O	2.15	0.47
30:S:41:LEU:HD11	30:S:177:LEU:CD1	2.33	0.47
31:T:78:LEU:O	31:T:80:ARG:HG3	2.15	0.47
31:T:162:ASP:O	31:T:162:ASP:OD1	2.33	0.47
27:p:36:THR:HG21	28:q:125:ALA:HB1	1.96	0.47
33:f:535:THR:HG21	33:f:576:ILE:CD1	2.44	0.47
24:M:40:ILE:HD12	24:M:194:VAL:CG2	2.45	0.47
28:Q:142:ILE:H	28:Q:142:ILE:HD12	1.80	0.47
25:n:48:LEU:HD11	25:n:135:ALA:HB3	1.97	0.47
5:X:259:ILE:HG23	5:X:267:VAL:HG21	1.97	0.46
17:E:86:GLN:O	17:E:87:LEU:HD22	2.15	0.46
17:E:122:MET:HE3	17:E:198:VAL:CB	2.44	0.46
17:E:241:ARG:O	18:F:304:ARG:NH1	2.44	0.46
18:F:415:LEU:HD22	18:F:420:TYR:HE1	1.78	0.46
32:K:196:LYS:O	32:K:200:ILE:HG12	2.16	0.46
33:f:553:THR:O	33:f:554:TYR:HB2	2.15	0.46
5:X:16:LEU:C	5:X:16:LEU:HD23	2.41	0.46
33:f:249:LEU:HD21	33:f:271:MET:HE3	1.97	0.46
33:f:852:VAL:O	33:f:852:VAL:HG13	2.15	0.46
1:y:382:GLN:O	1:y:386:ARG:HD3	2.15	0.46
2:U:11:LEU:HD21	11:d:170:GLN:OE1	2.14	0.46
2:U:42:VAL:HG12	2:U:46:GLU:CG	2.45	0.46
9:b:84:ILE:HD13	9:b:115:SER:HB2	1.96	0.46
32:K:157:ASP:OD2	32:K:159:SER:OG	2.28	0.46
33:f:597:VAL:HG11	33:f:656:GLY:HA3	1.98	0.46
4:W:241:LEU:HD11	4:W:286:LEU:HD12	1.98	0.46
4:W:446:ILE:HD12	7:Z:211:TYR:CD2	2.51	0.46
7:Z:50:VAL:HG23	7:Z:50:VAL:O	2.15	0.46
8:a:18:GLN:HG3	8:a:21:VAL:HB	1.97	0.46
8:a:162:TYR:CZ	8:a:166:ILE:HD11	2.51	0.46
9:b:7:MET:SD	9:b:64:LEU:HD21	2.56	0.46
10:c:168:MET:SD	10:c:169:VAL:HG13	2.56	0.46
21:I:83:ALA:O	21:I:87:THR:HG23	2.14	0.46
24:M:215:SER:HA	24:M:228:VAL:HG23	1.98	0.46
27:P:45:MET:HB3	27:P:71:LEU:HD13	1.97	0.46
28:Q:137:PHE:HB3	29:r:192:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:192:MET:HE1	3:V:211:TYR:HA	1.97	0.46
3:V:243:ASP:OD1	3:V:243:ASP:O	2.33	0.46
3:V:329:HIS:CG	3:V:353:LEU:HD11	2.50	0.46
4:W:174:TYR:O	4:W:182:ARG:NH1	2.49	0.46
7:Z:224:HIS:CD2	8:a:218:MET:HE1	2.51	0.46
11:d:265:ASP:OD1	11:d:266:THR:HG23	2.16	0.46
11:d:275:ILE:HG22	11:d:318:PHE:CZ	2.51	0.46
14:B:189:GLY:HA3	14:B:360:THR:HG22	1.96	0.46
16:D:51:LEU:HD23	16:D:51:LEU:O	2.16	0.46
16:D:281:ALA:O	16:D:285:VAL:HG23	2.15	0.46
19:G:58:ASP:O	19:G:59:LYS:HB3	2.16	0.46
19:G:147:GLN:OE1	19:G:147:GLN:N	2.48	0.46
21:I:45:LEU:HD21	21:I:75:SER:CB	2.45	0.46
26:O:253:ALA:HB3	27:P:201:LYS:NZ	2.30	0.46
27:P:168:SER:HB2	27:P:200:LEU:CD2	2.46	0.46
30:S:176:LEU:CD2	30:S:206:VAL:HG12	2.26	0.46
31:T:202:GLN:HG3	31:T:202:GLN:O	2.15	0.46
2:U:492:ASP:OD1	2:U:493:VAL:N	2.48	0.46
2:U:684:ARG:O	2:U:688:LEU:HD13	2.15	0.46
5:X:239:TYR:O	5:X:241:SER:N	2.47	0.46
7:Z:217:THR:CB	7:Z:219:LYS:HZ3	2.28	0.46
8:a:73:PRO:O	8:a:77:VAL:HG23	2.15	0.46
8:a:180:LEU:CD1	8:a:200:LEU:HD22	2.46	0.46
10:c:83:SER:OG	10:c:125:VAL:HG21	2.15	0.46
11:d:230:VAL:O	11:d:234:GLN:HG3	2.15	0.46
14:B:357:ASP:OD1	14:B:360:THR:OG1	2.21	0.46
16:D:268:ASP:OD1	17:E:258:MET:SD	2.74	0.46
18:F:279:ALA:HB1	18:F:280:PRO:CD	2.46	0.46
23:L:29:VAL:HG21	23:L:149:PRO:HD3	1.98	0.46
25:N:213:ILE:HG12	25:N:218:VAL:HG22	1.98	0.46
30:S:213:ARG:NH1	26:o:69:VAL:O	2.46	0.46
25:n:52:SER:O	25:n:65:THR:N	2.48	0.46
3:V:345:ARG:HB2	12:e:41:ASP:OD2	2.16	0.46
3:V:372:LEU:HD11	3:V:403:ILE:HG12	1.97	0.46
3:V:443:ARG:NH1	11:d:270:GLU:OE1	2.43	0.46
8:a:18:GLN:N	8:a:19:PRO:CD	2.79	0.46
8:a:104:VAL:HG22	8:a:104:VAL:O	2.15	0.46
8:a:226:ARG:NH2	8:a:231:GLN:NE2	2.62	0.46
9:b:68:THR:HG22	9:b:72:LEU:HD23	1.98	0.46
9:b:125:VAL:HG23	9:b:159:THR:CG2	2.45	0.46
14:B:163:LEU:O	14:B:164:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:404:LEU:HD22	15:C:180:ILE:HD12	1.97	0.46
14:B:427:LEU:O	14:B:429:LYS:N	2.47	0.46
19:G:180:GLU:OE2	20:H:55:ILE:HG12	2.15	0.46
20:H:68:ILE:HD11	20:H:74:LEU:HD13	1.96	0.46
23:L:3:ARG:HG3	23:L:4:ASN:N	2.31	0.46
23:L:172:LEU:O	23:L:176:MET:HG3	2.16	0.46
30:S:165:ALA:HB3	30:S:174:GLN:HG3	1.97	0.46
32:K:238:ILE:HA	32:K:241:ILE:HG12	1.97	0.46
29:r:142:LEU:HD22	29:r:173:VAL:HG11	1.98	0.46
33:f:470:VAL:HG22	33:f:478:ARG:NH2	2.30	0.46
2:U:517:GLY:HA3	2:U:551:GLY:HA2	1.98	0.46
4:W:272:LEU:HD21	4:W:302:TYR:HE1	1.80	0.46
5:X:263:THR:O	5:X:263:THR:OG1	2.34	0.46
17:E:122:MET:HE1	17:E:218:MET:HE3	1.97	0.46
18:F:172:VAL:CG2	18:F:267:LEU:HD13	2.45	0.46
18:F:215:LEU:O	18:F:215:LEU:HD23	2.16	0.46
20:H:140:ASN:OD1	20:H:145:TYR:CE1	2.69	0.46
26:O:148:VAL:HG23	26:O:149:THR:HG23	1.98	0.46
2:U:342:LEU:O	2:U:380:THR:HG22	2.15	0.46
3:V:256:ARG:NH2	12:e:21:GLU:O	2.48	0.46
10:c:32:TYR:CD2	10:c:66:THR:HG23	2.51	0.46
10:c:44:HIS:CE1	10:c:74:ALA:HB1	2.50	0.46
11:d:149:GLU:HA	11:d:171:LEU:HD11	1.98	0.46
18:F:231:THR:O	34:F:501:ATP:C8	2.69	0.46
19:G:16:PHE:O	19:G:17:SER:C	2.59	0.46
21:I:88:ASN:O	21:I:92:LEU:HD23	2.15	0.46
31:T:154:THR:HG23	31:T:171:ASP:CB	2.45	0.46
28:q:138:LEU:H	28:q:138:LEU:HD12	1.81	0.46
33:f:248:LEU:HA	33:f:251:CYS:SG	2.55	0.46
2:U:38:ILE:HD12	2:U:38:ILE:H	1.80	0.46
2:U:247:GLN:N	2:U:913:ILE:HD12	2.31	0.46
2:U:368:ALA:HB2	2:U:728:PHE:CD2	2.51	0.46
2:U:638:SER:CB	2:U:671:LEU:HD21	2.46	0.46
4:W:132:THR:CG2	4:W:138:VAL:HG11	2.45	0.46
6:Y:157:ILE:HG21	6:Y:187:TYR:CD1	2.51	0.46
7:Z:52:ASN:OD1	7:Z:53:SER:N	2.44	0.46
7:Z:86:ASN:OD1	7:Z:87:ALA:N	2.49	0.46
9:b:97:LEU:HD11	9:b:108:ARG:H	1.81	0.46
9:b:97:LEU:HD12	9:b:107:MET:HG2	1.96	0.46
9:b:156:PHE:CE2	9:b:160:LEU:HD11	2.51	0.46
11:d:88:LEU:O	11:d:92:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:144:ARG:HA	13:A:147:TYR:CE1	2.51	0.46
14:B:142:ASP:OD1	14:B:143:LEU:N	2.47	0.46
33:f:584:SER:O	33:f:588:ARG:HB2	2.15	0.46
2:U:229:VAL:HG11	2:U:260:PHE:CZ	2.51	0.45
2:U:673:GLU:HB3	2:U:674:PRO:HD3	1.98	0.45
3:V:85:ALA:HB2	3:V:93:PHE:HB2	1.97	0.45
4:W:183:VAL:HG21	4:W:213:PHE:CE2	2.51	0.45
8:a:102:GLU:O	8:a:105:LYS:NZ	2.43	0.45
9:b:140:ILE:HG21	9:b:153:LEU:CD1	2.43	0.45
18:F:253:GLY:N	18:F:286:ASP:O	2.50	0.45
22:J:108:THR:HG23	22:J:147:THR:CG2	2.46	0.45
26:O:62:ARG:CB	26:O:213:GLY:HA2	2.47	0.45
27:P:17:LYS:HD2	27:P:157:ASN:OD1	2.17	0.45
28:Q:13:VAL:HG22	28:Q:13:VAL:O	2.16	0.45
30:S:96:ILE:O	30:S:100:LEU:HD13	2.16	0.45
31:T:187:GLY:CA	31:T:221:LEU:HD21	2.45	0.45
26:o:202:ILE:HG21	26:o:216:ILE:HG23	1.98	0.45
29:r:86:ALA:O	30:s:164:LYS:NZ	2.43	0.45
33:f:274:ASP:O	33:f:277:LEU:N	2.50	0.45
2:U:524:LYS:HE3	2:U:562:GLU:HG2	1.98	0.45
3:V:309:MET:HE1	3:V:331:LEU:C	2.42	0.45
19:G:13:ILE:H	19:G:13:ILE:HD12	1.80	0.45
30:S:41:LEU:HD13	30:S:165:ALA:HB2	1.98	0.45
32:K:88:LEU:HD12	32:K:139:VAL:CG1	2.46	0.45
28:q:88:LEU:HB3	28:q:122:ALA:HB2	1.97	0.45
3:V:435:GLU:OE2	11:d:279:TYR:OH	2.05	0.45
6:Y:139:ASP:OD1	6:Y:176:ARG:NH2	2.50	0.45
8:a:8:LEU:HD12	8:a:9:GLN:N	2.30	0.45
8:a:245:VAL:O	8:a:249:GLN:OE1	2.33	0.45
8:a:363:MET:HG2	10:c:304:LEU:HD22	1.98	0.45
16:D:204:MET:HE1	16:D:263:PHE:HE1	1.81	0.45
19:G:155:ASP:HB2	19:G:156:PRO:HD2	1.98	0.45
20:H:91:ARG:O	20:H:95:GLN:HG2	2.16	0.45
20:H:160:ALA:CB	20:H:174:LEU:HD23	2.47	0.45
20:H:204:THR:HG22	20:H:205:GLU:N	2.31	0.45
24:M:38:ILE:HD13	24:M:198:ILE:CD1	2.42	0.45
24:M:50:VAL:CG2	24:M:67:LEU:HD11	2.45	0.45
25:N:208:ILE:HD12	25:N:228:ILE:HG12	1.97	0.45
27:p:4:MET:CE	27:p:126:LEU:HD13	2.47	0.45
2:U:27:LEU:HD22	2:U:38:ILE:CG1	2.46	0.45
3:V:108:LEU:HD11	3:V:113:LEU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:208:ALA:HB1	3:V:249:THR:HG21	1.97	0.45
6:Y:42:MET:HE3	6:Y:63:TRP:HZ3	1.82	0.45
6:Y:200:LEU:O	6:Y:204:THR:HG22	2.16	0.45
6:Y:250:LEU:O	6:Y:253:LEU:O	2.35	0.45
8:a:198:PHE:HB2	8:a:230:ARG:HD3	1.98	0.45
9:b:97:LEU:HD21	9:b:109:ILE:HG12	1.98	0.45
10:c:241:ASN:O	10:c:245:VAL:HG23	2.16	0.45
11:d:283:LEU:HD23	11:d:283:LEU:H	1.81	0.45
14:B:150:VAL:HG13	14:B:159:VAL:HG13	1.99	0.45
17:E:50:LEU:HD21	18:F:83:ASN:CB	2.46	0.45
19:G:50:ILE:HG23	19:G:141:ILE:HG13	1.99	0.45
21:I:107:CYS:O	21:I:111:VAL:HG23	2.16	0.45
24:M:136:PHE:CE2	24:M:152:ILE:HD12	2.51	0.45
25:N:40:VAL:HG13	25:N:47:VAL:HG22	1.97	0.45
29:R:223:THR:HG22	29:R:229:SER:O	2.17	0.45
30:S:68:SER:OG	30:S:68:SER:O	2.31	0.45
31:T:95:MET:HE2	31:T:237:VAL:HG12	1.99	0.45
29:r:109:ALA:CB	30:s:155:VAL:HG23	2.47	0.45
33:f:498:LEU:O	33:f:502:LEU:HG	2.16	0.45
2:U:78:LEU:O	2:U:82:LEU:HD23	2.17	0.45
2:U:727:LYS:O	2:U:731:ILE:HG12	2.17	0.45
4:W:115:ILE:HG22	4:W:116:THR:O	2.16	0.45
4:W:440:ASN:O	4:W:443:THR:HG22	2.17	0.45
5:X:15:LEU:HD23	5:X:22:ALA:CB	2.47	0.45
8:a:80:ILE:HG23	8:a:96:PHE:CZ	2.52	0.45
8:a:307:VAL:O	8:a:311:VAL:HG23	2.16	0.45
10:c:148:ILE:HG23	16:D:85:ILE:HD13	1.97	0.45
15:C:164:VAL:HG11	15:C:186:VAL:HG22	1.97	0.45
15:C:358:GLU:O	15:C:362:VAL:HG23	2.17	0.45
21:I:15:GLU:O	21:I:17:ARG:N	2.47	0.45
26:O:71:ASP:OD1	26:O:72:LYS:N	2.49	0.45
26:O:186:ARG:NH2	26:O:193:GLU:OE1	2.49	0.45
29:R:226:ASP:OD1	29:R:228:TYR:N	2.50	0.45
28:q:26:VAL:HG21	29:r:195:TYR:HD2	1.81	0.45
30:s:47:ASP:OD1	30:s:47:ASP:O	2.34	0.45
33:f:520:LEU:HD11	33:f:798:THR:CG2	2.45	0.45
33:f:682:GLY:HA3	33:f:686:LEU:HD22	1.99	0.45
2:U:524:LYS:HZ3	2:U:556:MET:HE3	1.82	0.45
5:X:259:ILE:CG2	5:X:267:VAL:HG21	2.46	0.45
8:a:148:VAL:HG13	8:a:148:VAL:O	2.17	0.45
10:c:304:LEU:O	10:c:308:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:91:LYS:O	14:B:92:GLN:C	2.60	0.45
17:E:348:THR:HA	18:F:217:ILE:HD11	1.97	0.45
18:F:435:LEU:HD13	23:L:31:GLN:OE1	2.15	0.45
22:J:155:ALA:HB3	32:K:63:SER:HB2	1.98	0.45
23:L:138:ASP:OD1	23:L:138:ASP:N	2.47	0.45
26:o:185:PHE:CG	26:o:185:PHE:O	2.69	0.45
33:f:430:ASP:OD1	33:f:430:ASP:C	2.60	0.45
2:U:141:CYS:O	2:U:144:ASP:O	2.34	0.45
3:V:248:ALA:O	3:V:252:ASN:ND2	2.44	0.45
11:d:116:LEU:HD21	11:d:151:GLY:HA2	1.99	0.45
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.49	0.45
16:D:153:MET:HE2	16:D:227:PHE:HD1	1.82	0.45
27:P:168:SER:HB2	27:P:200:LEU:HD22	1.99	0.45
26:o:169:THR:HG21	26:o:181:PHE:CD2	2.52	0.45
30:s:241:ASP:C	30:s:241:ASP:OD1	2.60	0.45
33:f:485:LEU:HD21	33:f:497:VAL:HG23	1.98	0.45
5:X:97:LEU:HB3	5:X:132:ARG:HE	1.82	0.45
6:Y:334:LEU:O	6:Y:338:ILE:HG12	2.16	0.45
6:Y:334:LEU:HD23	6:Y:347:ILE:HG21	1.97	0.45
8:a:60:TYR:CE2	8:a:64:ILE:HD13	2.52	0.45
14:B:162:VAL:HG12	14:B:163:LEU:H	1.82	0.45
24:M:109:LEU:HD12	24:M:140:SER:CB	2.47	0.45
29:R:118:LEU:CD1	29:R:142:LEU:HB2	2.47	0.45
31:T:190:LEU:HD23	31:T:190:LEU:H	1.81	0.45
33:f:253:LEU:CD2	33:f:277:LEU:HD13	2.47	0.45
33:f:868:HIS:HB3	33:f:872:VAL:HG22	1.98	0.45
5:X:408:SER:HA	6:Y:376:LEU:HD13	1.98	0.45
7:Z:36:VAL:HG22	7:Z:96:HIS:CB	2.47	0.45
11:d:148:LEU:CB	11:d:171:LEU:HD21	2.46	0.45
13:A:207:GLU:CD	18:F:372:LYS:HZ1	2.18	0.45
13:A:393:GLY:HA3	14:B:216:ILE:HD13	1.99	0.45
15:C:337:ASN:OD1	16:D:193:GLN:O	2.35	0.45
18:F:172:VAL:CG1	18:F:271:ALA:HA	2.46	0.45
20:H:22:ILE:HD11	20:H:122:THR:CG2	2.46	0.45
23:L:74:ILE:HG22	23:L:132:LEU:HD23	1.99	0.45
27:p:87:LEU:O	27:p:91:VAL:HG23	2.17	0.45
31:t:96:LEU:HD11	31:t:155:MET:HB3	1.99	0.45
31:t:153:ASN:HB3	31:t:155:MET:SD	2.57	0.45
33:f:282:PHE:CZ	33:f:317:LEU:HD23	2.52	0.45
33:f:341:GLU:OE1	33:f:341:GLU:N	2.44	0.45
2:U:515:ALA:O	2:U:519:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:314:LEU:HD21	4:W:381:LEU:HD23	1.99	0.45
5:X:70:LEU:HD21	5:X:92:LEU:HB3	1.99	0.45
6:Y:241:ILE:HG22	6:Y:241:ILE:O	2.16	0.45
7:Z:235:ASN:C	7:Z:235:ASN:OD1	2.60	0.45
9:b:136:VAL:HG13	9:b:136:VAL:O	2.17	0.45
10:c:29:GLU:OE2	10:c:139:ARG:NH2	2.43	0.45
13:A:356:LYS:O	13:A:360:ARG:HG3	2.16	0.45
14:B:429:LYS:HB2	21:I:169:ALA:HB1	1.99	0.45
15:C:154:LEU:HD12	15:C:158:ILE:HG13	1.99	0.45
17:E:157:GLU:OE1	17:E:157:GLU:N	2.43	0.45
22:J:119:THR:HG22	22:J:126:PRO:HB3	1.99	0.45
26:O:93:ALA:N	27:P:129:CYS:SG	2.90	0.45
2:U:179:TYR:O	2:U:183:LEU:HD23	2.17	0.44
5:X:147:LEU:HG	5:X:176:THR:HG21	1.99	0.44
16:D:42:SER:O	16:D:45:LYS:HB2	2.17	0.44
19:G:196:GLU:OE1	19:G:242:LEU:HB2	2.17	0.44
25:N:198:MET:HE3	25:N:205:GLY:C	2.42	0.44
27:P:17:LYS:HZ3	27:P:158:MET:HA	1.82	0.44
28:Q:139:THR:HB	28:Q:163:CYS:SG	2.56	0.44
31:T:78:LEU:HD13	25:n:168:TYR:CE1	2.52	0.44
28:q:30:ASP:OD1	28:q:30:ASP:O	2.35	0.44
29:r:142:LEU:HD21	29:r:156:MET:HE1	1.98	0.44
2:U:525:ASN:OD1	2:U:525:ASN:O	2.34	0.44
3:V:108:LEU:HD22	3:V:170:LEU:CD1	2.46	0.44
5:X:215:GLY:O	5:X:218:HIS:O	2.36	0.44
7:Z:256:GLN:NE2	10:c:298:GLN:OE1	2.50	0.44
10:c:32:TYR:CE2	10:c:66:THR:HG23	2.51	0.44
11:d:138:LYS:HG2	11:d:139:GLN:N	2.31	0.44
16:D:44:TYR:O	16:D:47:LEU:HB3	2.17	0.44
17:E:339:ASN:OD1	17:E:342:ASP:N	2.46	0.44
18:F:386:ARG:NE	23:L:166:GLN:OE1	2.47	0.44
19:G:155:ASP:OD1	19:G:159:TYR:N	2.51	0.44
21:I:184:MET:HA	21:I:188:SER:OG	2.17	0.44
24:M:54:VAL:CG2	24:M:209:ALA:HB1	2.47	0.44
28:Q:182:ILE:CD1	28:Q:191:LEU:HD22	2.47	0.44
29:R:71:VAL:HG11	29:R:161:CYS:HB3	1.99	0.44
29:R:142:LEU:HD22	29:R:160:ILE:HD11	1.99	0.44
29:R:231:GLY:O	29:R:251:VAL:HG23	2.16	0.44
25:n:150:MET:O	31:t:50:MET:HE2	2.17	0.44
2:U:184:CYS:HA	2:U:188:MET:HG2	1.99	0.44
2:U:637:VAL:HG21	2:U:656:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:118:LEU:C	4:W:118:LEU:HD23	2.42	0.44
5:X:75:PRO:O	5:X:78:ASN:OD1	2.36	0.44
5:X:205:LYS:N	5:X:243:ASP:OD2	2.50	0.44
11:d:250:ASN:O	11:d:251:ILE:C	2.61	0.44
13:A:251:GLY:O	13:A:255:ARG:HB2	2.18	0.44
15:C:36:ASN:O	15:C:40:GLN:OE1	2.36	0.44
15:C:166:GLU:OE2	15:C:170:LYS:HG3	2.17	0.44
17:E:148:VAL:HG11	17:E:170:CYS:SG	2.57	0.44
18:F:153:VAL:CG1	18:F:158:TYR:HA	2.48	0.44
24:M:76:MET:HA	24:M:137:MET:O	2.17	0.44
29:R:142:LEU:HD23	29:R:160:ILE:HD11	1.98	0.44
29:r:238:VAL:HG23	29:r:238:VAL:O	2.17	0.44
3:V:114:TYR:HA	3:V:135:LEU:HD21	1.99	0.44
3:V:183:GLU:O	3:V:187:ILE:HG12	2.17	0.44
5:X:93:LEU:HD11	5:X:113:CYS:SG	2.58	0.44
8:a:198:PHE:CD1	8:a:233:LEU:HD13	2.53	0.44
10:c:130:GLN:OE1	10:c:162:LEU:HG	2.17	0.44
14:B:287:ILE:HD12	14:B:290:ILE:HD12	1.98	0.44
14:B:365:PHE:O	14:B:369:THR:HG23	2.18	0.44
16:D:204:MET:HE1	16:D:263:PHE:CE1	2.53	0.44
17:E:73:ALA:HB3	17:E:75:ASN:OD1	2.17	0.44
18:F:405:MET:O	18:F:409:ARG:HD2	2.18	0.44
19:G:141:ILE:HD12	19:G:151:VAL:HG22	1.99	0.44
27:P:205:ASP:N	27:P:205:ASP:OD1	2.50	0.44
29:R:115:GLU:OE2	29:R:158:THR:OG1	2.32	0.44
29:R:213:ASP:OD1	29:R:216:ARG:NH2	2.51	0.44
32:K:180:SER:O	32:K:184:VAL:HG12	2.17	0.44
33:f:270:LEU:HD11	33:f:298:LEU:HD21	2.00	0.44
33:f:810:ILE:HD12	33:f:818:LEU:HG	2.00	0.44
2:U:450:HIS:CD2	2:U:457:ILE:HD13	2.52	0.44
2:U:501:LEU:HD21	2:U:535:TYR:CD1	2.53	0.44
3:V:302:TYR:HB3	3:V:339:LEU:HG	2.00	0.44
7:Z:176:LEU:HD11	10:c:217:LEU:C	2.42	0.44
9:b:60:VAL:HG23	9:b:60:VAL:O	2.16	0.44
13:A:225:CYS:O	13:A:229:VAL:HG23	2.17	0.44
18:F:171:ARG:HH12	18:F:267:LEU:CD2	2.02	0.44
18:F:195:ILE:O	18:F:196:GLN:C	2.61	0.44
18:F:335:VAL:HA	18:F:338:LEU:HD13	1.99	0.44
21:I:179:TYR:HA	21:I:184:MET:HE1	1.99	0.44
22:J:176:TYR:HD2	22:J:190:LEU:HD21	1.83	0.44
26:O:53:ASP:OD1	26:O:53:ASP:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:141:THR:HG22	27:P:142:CYS:H	1.83	0.44
28:Q:4:LEU:HD13	28:Q:45:LEU:HB3	1.99	0.44
28:Q:50:ALA:HB1	29:R:178:ASN:OD1	2.17	0.44
32:K:70:ILE:HD11	32:K:89:ILE:HD12	1.98	0.44
30:s:214:ASP:HB3	30:s:217:THR:HG22	2.00	0.44
31:t:54:THR:OG1	31:t:225:ASP:OD2	2.35	0.44
2:U:42:VAL:O	2:U:45:ILE:HG22	2.18	0.44
2:U:636:VAL:O	2:U:640:LEU:HD23	2.17	0.44
2:U:898:CYS:SG	2:U:899:ARG:N	2.90	0.44
3:V:477:HIS:CG	11:d:342:TYR:HH	2.25	0.44
8:a:112:ILE:HD11	8:a:138:VAL:O	2.17	0.44
8:a:179:PHE:CE1	8:a:183:VAL:HG11	2.53	0.44
14:B:201:VAL:HG23	14:B:202:GLU:N	2.32	0.44
14:B:342:ILE:O	14:B:342:ILE:HG22	2.17	0.44
15:C:120:SER:O	15:C:121:TYR:C	2.60	0.44
16:D:268:ASP:HB3	16:D:317:LEU:HD21	2.00	0.44
20:H:48:THR:HG21	20:H:64:LYS:HG3	1.99	0.44
22:J:68:ASN:HA	22:J:211:MET:HE1	1.99	0.44
22:J:83:VAL:HG21	22:J:129:ILE:HD11	1.99	0.44
22:J:116:GLN:HE21	32:K:83:ALA:HB3	1.83	0.44
23:L:47:VAL:HG12	23:L:195:LEU:HD11	2.00	0.44
24:M:204:GLU:O	24:M:208:LYS:N	2.51	0.44
28:Q:45:LEU:HD12	28:Q:45:LEU:N	2.32	0.44
30:S:106:SER:O	32:K:114:GLN:NE2	2.48	0.44
31:t:104:ASP:O	31:t:108:LEU:HD23	2.17	0.44
31:t:198:VAL:HG21	31:t:213:LEU:HD13	1.98	0.44
33:f:423:ASP:OD2	33:f:457:ASN:ND2	2.50	0.44
33:f:834:ASP:OD1	33:f:835:GLU:N	2.46	0.44
4:W:122:LEU:HD21	4:W:152:ILE:HG21	1.99	0.44
6:Y:51:ALA:HB3	6:Y:52:PRO:HD3	1.99	0.44
7:Z:42:SER:OG	7:Z:43:TRP:N	2.51	0.44
15:C:273:MET:SD	15:C:293:MET:SD	3.16	0.44
16:D:363:TYR:CE2	16:D:399:PHE:HB3	2.53	0.44
17:E:138:LEU:O	17:E:142:ILE:HD12	2.18	0.44
17:E:365:GLU:OE2	24:M:179:LYS:NZ	2.32	0.44
20:H:75:VAL:HG22	20:H:76:TYR:N	2.33	0.44
32:K:46:VAL:HG11	32:K:144:GLY:HA3	1.99	0.44
30:s:57:LEU:HD13	31:t:177:TYR:HE1	1.82	0.44
33:f:236:CYS:HB2	33:f:248:LEU:HD21	2.00	0.44
33:f:442:SER:HB3	33:f:477:MET:HE1	2.00	0.44
2:U:637:VAL:HG21	2:U:656:LEU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:219:GLU:HA	3:V:224:LEU:HD11	2.00	0.44
5:X:187:ARG:HD2	5:X:217:ILE:HG21	2.00	0.44
5:X:190:LEU:HD21	5:X:214:SER:HA	1.99	0.44
7:Z:122:VAL:HG23	7:Z:122:VAL:O	2.16	0.44
8:a:217:LEU:HD23	8:a:237:LEU:HD23	1.99	0.44
19:G:180:GLU:OE2	19:G:184:LYS:HE3	2.17	0.44
21:I:114:LEU:O	21:I:118:LYS:HG2	2.18	0.44
27:P:91:VAL:O	27:P:95:LEU:HD23	2.17	0.44
28:Q:13:VAL:HG12	28:Q:183:ILE:HB	1.99	0.44
26:o:67:MET:HG3	26:o:67:MET:O	2.16	0.44
27:p:138:VAL:HG11	27:p:146:MET:HG3	2.00	0.44
33:f:687:ARG:NH2	33:f:716:ASP:OD2	2.51	0.44
2:U:345:ASN:O	2:U:743:ASN:ND2	2.50	0.44
2:U:423:MET:HG3	2:U:446:LEU:HD21	2.00	0.44
5:X:335:LEU:O	5:X:339:ILE:HG12	2.17	0.44
6:Y:104:MET:HE2	6:Y:127:THR:HA	2.00	0.44
6:Y:253:LEU:HB3	6:Y:256:VAL:HG22	1.99	0.44
10:c:51:MET:SD	10:c:81:GLY:N	2.83	0.44
11:d:309:VAL:HG22	11:d:309:VAL:O	2.18	0.44
13:A:299:MET:O	13:A:303:ILE:HG12	2.17	0.44
13:A:334:PRO:HG3	18:F:395:GLN:HG2	2.00	0.44
15:C:24:TYR:CB	16:D:40:LEU:HD23	2.48	0.44
15:C:365:GLU:OE2	15:C:372:ARG:NH2	2.46	0.44
20:H:139:TRP:CD1	20:H:139:TRP:O	2.71	0.44
32:K:59:MET:SD	32:K:64:ILE:HD11	2.58	0.44
25:n:46:VAL:HG12	25:n:47:VAL:N	2.31	0.44
29:r:65:PHE:HZ	29:r:202:TYR:CE1	2.36	0.44
33:f:334:ALA:O	33:f:337:LEU:C	2.61	0.44
33:f:501:LEU:O	33:f:504:VAL:HG22	2.17	0.44
33:f:519:ALA:CB	33:f:558:LEU:HD23	2.48	0.44
33:f:675:PHE:HA	33:f:678:LEU:HD12	2.00	0.44
4:W:19:ASP:OD1	4:W:19:ASP:N	2.51	0.43
5:X:93:LEU:HD11	5:X:113:CYS:CB	2.47	0.43
5:X:132:ARG:O	5:X:132:ARG:HD3	2.18	0.43
8:a:147:GLY:O	8:a:152:HIS:NE2	2.48	0.43
14:B:275:GLU:OE2	14:B:322:ARG:NE	2.50	0.43
14:B:405:MET:HG2	14:B:421:LYS:HE3	2.00	0.43
20:H:117:VAL:O	20:H:120:GLU:HG2	2.18	0.43
27:P:127:ILE:O	27:P:127:ILE:HG22	2.18	0.43
25:n:49:GLY:HA3	25:n:194:LEU:HD11	2.00	0.43
26:o:140:ALA:C	26:o:141:LEU:HD22	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:431:LYS:HZ1	33:f:432:TYR:HE1	1.63	0.43
2:U:168:LEU:HD21	2:U:204:ILE:HD12	2.00	0.43
3:V:395:ILE:O	3:V:398:LEU:HB2	2.18	0.43
5:X:178:HIS:ND1	5:X:183:LEU:HD21	2.33	0.43
6:Y:387:ILE:O	7:Z:279:LYS:NZ	2.46	0.43
9:b:155:ALA:O	9:b:159:THR:HG23	2.18	0.43
13:A:327:LEU:HD22	13:A:331:LEU:HD23	2.00	0.43
15:C:101:LYS:HG3	15:C:101:LYS:O	2.18	0.43
15:C:248:MET:HB3	15:C:269:VAL:HG13	1.99	0.43
15:C:279:GLN:NE2	15:C:284:GLU:OE1	2.45	0.43
16:D:39:ASP:O	16:D:42:SER:HB2	2.18	0.43
20:H:19:LEU:HD13	20:H:22:ILE:HD12	2.00	0.43
22:J:185:ASP:O	22:J:189:LYS:HG2	2.18	0.43
28:Q:144:ASP:OD2	29:r:221:GLN:NE2	2.42	0.43
26:o:61:THR:OG1	26:o:215:ASN:N	2.51	0.43
26:o:252:THR:HG23	26:o:252:THR:O	2.19	0.43
29:r:173:VAL:HG22	29:r:174:ASP:N	2.32	0.43
30:s:95:ILE:O	30:s:99:ARG:HG2	2.18	0.43
2:U:38:ILE:O	2:U:42:VAL:HG23	2.17	0.43
2:U:268:LEU:HD22	2:U:326:ILE:HD11	2.00	0.43
2:U:348:THR:HG22	2:U:349:ASP:N	2.32	0.43
3:V:333:ILE:HG23	3:V:343:PRO:HG2	2.00	0.43
5:X:15:LEU:HD22	5:X:26:ILE:HD12	1.99	0.43
8:a:218:MET:CE	8:a:340:VAL:HG11	2.48	0.43
8:a:347:LYS:O	8:a:351:ASP:OD1	2.37	0.43
8:a:353:LEU:HD23	8:a:353:LEU:O	2.18	0.43
9:b:169:HIS:HB2	9:b:188:ILE:HD11	2.01	0.43
17:E:297:ARG:HG2	17:E:299:ILE:HG23	2.00	0.43
18:F:343:LEU:O	18:F:351:LYS:NZ	2.42	0.43
19:G:180:GLU:O	19:G:184:LYS:HG2	2.18	0.43
22:J:73:PHE:CE1	22:J:129:ILE:HB	2.53	0.43
24:M:40:ILE:HG23	24:M:182:MET:SD	2.57	0.43
29:R:164:ASP:OD1	29:R:164:ASP:N	2.51	0.43
26:o:252:THR:O	26:o:253:ALA:C	2.61	0.43
27:p:135:ASP:OD1	27:p:135:ASP:N	2.45	0.43
28:q:129:PHE:CZ	28:q:144:ASP:OD1	2.71	0.43
29:r:71:VAL:HB	29:r:238:VAL:HG22	2.01	0.43
31:t:54:THR:O	31:t:99:SER:OG	2.34	0.43
33:f:264:GLU:OE1	33:f:264:GLU:N	2.48	0.43
4:W:66:ILE:O	4:W:70:VAL:HG23	2.18	0.43
7:Z:70:LEU:HD23	7:Z:111:LEU:HD22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:181:ASP:CG	16:D:70:LYS:HZ1	2.26	0.43
11:d:131:THR:O	11:d:131:THR:HG22	2.18	0.43
14:B:316:LEU:HD13	14:B:347:ILE:HD11	2.00	0.43
16:D:85:ILE:H	16:D:85:ILE:HD12	1.84	0.43
17:E:92:LEU:CA	17:E:96:THR:HG21	2.47	0.43
18:F:288:LEU:HD22	18:F:330:ALA:HB1	2.00	0.43
20:H:40:ALA:N	20:H:43:GLY:O	2.44	0.43
22:J:11:SER:OG	22:J:13:ASP:OD1	2.34	0.43
26:o:239:GLY:O	26:o:240:THR:OG1	2.35	0.43
27:p:132:VAL:O	27:p:132:VAL:HG13	2.18	0.43
30:s:77:LYS:NZ	30:s:141:LEU:HB2	2.33	0.43
31:t:91:ASN:OD1	31:t:94:THR:N	2.51	0.43
33:f:731:MET:HE1	33:f:821:LEU:CD1	2.47	0.43
33:f:888:LEU:HD23	33:f:888:LEU:H	1.84	0.43
2:U:252:LEU:HD12	2:U:260:PHE:HE1	1.83	0.43
2:U:603:LEU:O	2:U:607:VAL:HG23	2.17	0.43
3:V:283:ASN:OD1	3:V:284:GLU:OE2	2.37	0.43
4:W:112:VAL:HG21	4:W:125:ILE:CD1	2.49	0.43
4:W:405:LYS:HB2	4:W:414:ASN:OD1	2.19	0.43
5:X:154:LEU:HD11	5:X:173:GLU:OE1	2.19	0.43
9:b:140:ILE:HD13	9:b:153:LEU:HD12	2.01	0.43
11:d:141:LEU:HD11	11:d:183:PRO:CD	2.48	0.43
11:d:193:GLY:O	11:d:197:LEU:HD23	2.19	0.43
16:D:207:PRO:O	16:D:212:LYS:NZ	2.52	0.43
16:D:279:THR:O	16:D:279:THR:HG22	2.17	0.43
17:E:205:ASP:OD1	17:E:206:LYS:N	2.51	0.43
18:F:257:VAL:HG13	18:F:257:VAL:O	2.18	0.43
19:G:11:ARG:HE	24:M:7:GLY:HA2	1.83	0.43
23:L:70:ILE:HD13	23:L:108:LEU:HD23	1.99	0.43
29:r:241:ASP:OD1	29:r:242:GLY:N	2.51	0.43
30:s:76:ASP:OD1	30:s:77:LYS:HG3	2.18	0.43
33:f:474:SER:O	33:f:509:LYS:NZ	2.52	0.43
3:V:64:GLN:NE2	3:V:68:ASP:OD1	2.51	0.43
3:V:183:GLU:OE1	3:V:183:GLU:N	2.40	0.43
4:W:260:SER:HA	4:W:263:TRP:CD1	2.54	0.43
5:X:91:SER:O	5:X:95:LEU:HG	2.19	0.43
5:X:317:PRO:HG2	5:X:319:ILE:HG12	2.01	0.43
7:Z:216:ALA:HA	8:a:343:LEU:HD11	1.99	0.43
7:Z:266:ILE:HG21	10:c:284:LEU:HG	2.01	0.43
15:C:24:TYR:HB2	16:D:40:LEU:HD23	2.00	0.43
15:C:162:LYS:O	15:C:163:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:239:ARG:NH1	15:C:284:GLU:OE2	2.48	0.43
15:C:373:GLU:O	15:C:374:ARG:C	2.61	0.43
16:D:341:LYS:NZ	16:D:370:ILE:O	2.52	0.43
18:F:384:LEU:HD21	18:F:420:TYR:HB3	1.99	0.43
20:H:99:LEU:HD21	26:O:101:LEU:HA	2.01	0.43
21:I:69:ASN:OD1	21:I:72:MET:HB3	2.18	0.43
31:T:54:THR:OG1	31:T:55:SER:N	2.51	0.43
28:q:4:LEU:HD23	28:q:17:SER:HB2	2.01	0.43
28:q:172:ILE:HG13	28:q:173:LEU:HD22	2.00	0.43
30:s:62:SER:O	30:s:63:ILE:C	2.60	0.43
33:f:736:THR:O	33:f:737:ASN:C	2.62	0.43
2:U:880:ASN:HB3	2:U:881:PRO:CD	2.48	0.43
3:V:113:LEU:HD12	3:V:171:VAL:HG22	2.01	0.43
3:V:368:ARG:NH1	12:e:43:TRP:O	2.51	0.43
4:W:306:LEU:O	4:W:310:THR:HG22	2.19	0.43
9:b:123:ASP:OD1	9:b:123:ASP:C	2.62	0.43
14:B:235:LEU:HD12	14:B:353:PHE:HZ	1.81	0.43
14:B:291:GLY:O	14:B:292:THR:C	2.61	0.43
17:E:121:ASN:OD1	17:E:121:ASN:C	2.61	0.43
29:R:68:ARG:O	29:R:68:ARG:HD3	2.18	0.43
30:S:111:MET:HG2	30:S:116:ILE:HG13	1.99	0.43
30:S:175:PRO:HB2	27:p:149:MET:HE3	2.01	0.43
25:n:92:ALA:HB3	25:n:120:MET:HE1	2.01	0.43
29:r:76:ASP:OD1	29:r:92:LYS:NZ	2.52	0.43
4:W:307:LYS:HA	4:W:310:THR:HG22	2.01	0.43
6:Y:245:GLU:O	6:Y:249:VAL:HG23	2.18	0.43
6:Y:301:ILE:HD13	6:Y:342:ARG:HE	1.84	0.43
8:a:374:ILE:HG21	11:d:344:ARG:HA	2.00	0.43
9:b:86:PHE:CD2	9:b:113:VAL:HG21	2.54	0.43
10:c:266:THR:N	10:c:267:PRO:CD	2.82	0.43
10:c:303:MET:CE	11:d:335:LEU:HB3	2.48	0.43
13:A:188:ARG:O	13:A:189:GLU:C	2.61	0.43
14:B:234:LEU:HD22	36:B:501:ADP:C8	2.54	0.43
17:E:86:GLN:O	17:E:86:GLN:HG3	2.19	0.43
18:F:140:VAL:HG21	18:F:163:THR:HG23	2.00	0.43
21:I:135:LEU:HD21	21:I:162:THR:HG23	2.01	0.43
23:L:215:VAL:HG22	23:L:216:GLY:N	2.34	0.43
27:P:49:LEU:HD21	27:P:87:LEU:HD22	2.01	0.43
26:o:127:LYS:HD2	26:o:162:THR:HG21	2.00	0.43
29:r:174:ASP:OD1	29:r:176:GLU:N	2.51	0.43
33:f:704:LEU:HD12	33:f:704:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:400:GLN:O	1:y:404:LEU:HD13	2.19	0.43
2:U:119:PRO:O	2:U:123:LYS:CE	2.66	0.43
2:U:669:ILE:HG12	2:U:695:MET:SD	2.59	0.43
4:W:24:VAL:HG12	4:W:50:LEU:HD21	2.01	0.43
8:a:198:PHE:CB	8:a:230:ARG:HD3	2.49	0.43
11:d:108:ASN:HB2	11:d:112:CYS:SG	2.59	0.43
13:A:93:LEU:O	14:B:132:TYR:N	2.48	0.43
13:A:145:ASN:O	13:A:146:LYS:HB2	2.19	0.43
14:B:82:GLN:O	14:B:86:LYS:HG2	2.18	0.43
14:B:388:ASP:OD2	14:B:429:LYS:NZ	2.50	0.43
16:D:209:GLY:CA	17:E:291:ARG:HD2	2.49	0.43
16:D:272:THR:O	16:D:275:PHE:CZ	2.72	0.43
22:J:86:ARG:CD	22:J:114:LEU:HD13	2.49	0.43
28:Q:44:LEU:HD23	28:Q:44:LEU:C	2.44	0.43
26:o:137:ILE:HG13	26:o:137:ILE:O	2.19	0.43
33:f:447:ALA:HA	33:f:450:ILE:HG22	2.00	0.43
33:f:483:PHE:HE1	33:f:820:GLY:CA	2.32	0.43
2:U:109:THR:HG22	2:U:157:THR:OG1	2.19	0.43
3:V:72:LEU:O	3:V:76:LYS:HG2	2.18	0.43
3:V:225:ASP:OD1	3:V:226:VAL:N	2.51	0.43
3:V:341:GLU:OE1	3:V:341:GLU:N	2.48	0.43
4:W:305:LEU:HD22	4:W:328:LEU:HD21	2.00	0.43
9:b:88:THR:O	9:b:89:GLY:C	2.62	0.43
13:A:61:GLU:HA	13:A:65:ILE:HD11	2.01	0.43
13:A:168:GLU:HG2	13:A:168:GLU:O	2.18	0.43
13:A:206:ILE:HD13	18:F:404:GLY:HA3	2.01	0.43
14:B:420:LYS:O	14:B:423:LYS:HB2	2.19	0.43
18:F:190:GLY:HA3	18:F:361:ALA:HB1	2.00	0.43
19:G:13:ILE:HD11	19:G:133:PRO:HD3	2.01	0.43
20:H:48:THR:HG21	20:H:64:LYS:CG	2.49	0.43
22:J:22:ALA:HB1	22:J:128:GLY:HA2	2.01	0.43
22:J:215:GLN:CG	22:J:216:SER:N	2.81	0.43
27:P:96:TYR:CE2	27:P:99:ARG:HD2	2.54	0.43
25:n:86:THR:HG22	25:n:130:ALA:HB1	1.99	0.43
30:s:85:PHE:HD2	30:s:88:ASP:OD2	2.01	0.43
31:t:197:GLU:OE1	31:t:198:VAL:N	2.51	0.43
2:U:732:LEU:O	2:U:736:ILE:HG12	2.19	0.42
3:V:91:PRO:O	3:V:94:VAL:N	2.41	0.42
6:Y:263:LEU:HD23	6:Y:263:LEU:C	2.44	0.42
14:B:426:VAL:HG13	14:B:427:LEU:N	2.33	0.42
15:C:67:GLN:HA	16:D:136:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:388:ARG:NE	17:E:147:GLU:OE2	2.52	0.42
18:F:435:LEU:HD21	32:K:20:ARG:HG3	2.01	0.42
19:G:84:THR:HG21	24:M:157:VAL:HG13	2.00	0.42
27:P:28:PHE:O	27:P:28:PHE:CG	2.72	0.42
27:P:135:ASP:OD1	27:P:135:ASP:N	2.46	0.42
28:q:1:MET:HE3	28:q:2:GLU:H	1.84	0.42
29:r:233:VAL:O	29:r:233:VAL:CG2	2.67	0.42
31:t:148:MET:HG3	31:t:148:MET:O	2.19	0.42
33:f:237:VAL:HG23	33:f:248:LEU:HD23	2.01	0.42
2:U:153:ILE:HG13	15:C:24:TYR:OH	2.19	0.42
2:U:170:SER:CB	2:U:176:MET:HG3	2.50	0.42
2:U:375:PHE:O	2:U:378:CYS:SG	2.76	0.42
2:U:638:SER:HB2	2:U:671:LEU:HD21	2.00	0.42
3:V:213:TYR:O	3:V:217:VAL:HG23	2.20	0.42
4:W:116:THR:CG2	4:W:117:ASP:H	2.28	0.42
8:a:226:ARG:HH21	8:a:231:GLN:HE22	1.65	0.42
9:b:93:ALA:O	9:b:97:LEU:HD23	2.20	0.42
10:c:102:THR:O	10:c:102:THR:HG23	2.19	0.42
14:B:357:ASP:N	14:B:357:ASP:OD1	2.45	0.42
15:C:138:MET:HA	15:C:138:MET:HE3	2.00	0.42
19:G:241:ALA:HB1	19:G:245:ARG:HH21	1.84	0.42
24:M:210:PHE:CD1	24:M:211:GLU:N	2.87	0.42
27:P:57:ALA:O	27:P:61:GLN:HG3	2.19	0.42
31:T:110:GLN:HG3	31:T:111:VAL:N	2.34	0.42
27:p:30:ILE:HG13	27:p:31:GLN:H	1.83	0.42
33:f:233:LEU:O	33:f:237:VAL:HG23	2.19	0.42
33:f:236:CYS:O	33:f:240:VAL:HB	2.19	0.42
33:f:419:LEU:HD23	33:f:420:TRP:CG	2.54	0.42
33:f:683:GLU:HB3	33:f:684:PRO:HD2	2.01	0.42
2:U:157:THR:HG22	2:U:157:THR:O	2.18	0.42
2:U:555:VAL:O	2:U:555:VAL:HG22	2.19	0.42
2:U:609:ASP:OD1	2:U:610:VAL:N	2.50	0.42
3:V:265:ASP:CG	3:V:269:LYS:HZ2	2.23	0.42
4:W:20:TYR:HA	4:W:23:THR:HG22	2.00	0.42
4:W:51:GLU:HA	4:W:54:THR:HG22	2.01	0.42
4:W:296:LEU:CD2	4:W:299:ILE:HD11	2.42	0.42
5:X:335:LEU:CD2	5:X:354:ILE:HD13	2.50	0.42
7:Z:165:GLU:HG2	7:Z:166:GLU:N	2.34	0.42
8:a:33:LEU:O	8:a:34:TRP:HB2	2.19	0.42
9:b:51:LEU:C	9:b:52:ILE:HD13	2.44	0.42
13:A:44:GLN:O	13:A:48:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:140:VAL:CG2	13:A:150:HIS:CD2	3.03	0.42
13:A:153:LEU:HD21	14:B:122:ILE:HD11	2.00	0.42
13:A:258:ARG:NH1	13:A:301:GLU:OE1	2.50	0.42
14:B:380:LEU:HD23	14:B:380:LEU:H	1.83	0.42
21:I:132:VAL:HG12	21:I:134:LEU:HD22	2.01	0.42
21:I:206:LEU:HD11	21:I:211:VAL:HG11	2.02	0.42
22:J:45:VAL:CG2	22:J:61:LYS:HZ3	2.32	0.42
24:M:70:VAL:HG21	24:M:76:MET:HE3	2.01	0.42
27:P:180:VAL:O	27:P:180:VAL:HG22	2.18	0.42
28:Q:153:ARG:NH1	28:Q:184:ASP:OD2	2.49	0.42
28:Q:182:ILE:HD13	28:Q:191:LEU:HD13	2.01	0.42
28:q:140:LEU:HD23	28:q:143:LEU:HD12	2.00	0.42
30:s:74:LEU:CD1	30:s:80:ILE:HD13	2.50	0.42
31:t:95:MET:HE1	31:t:235:ALA:O	2.18	0.42
31:t:197:GLU:OE1	31:t:198:VAL:HG23	2.19	0.42
33:f:585:GLU:OE2	33:f:588:ARG:NH1	2.52	0.42
3:V:391:THR:O	3:V:392:TYR:C	2.62	0.42
3:V:443:ARG:HA	11:d:277:LYS:HG2	2.02	0.42
5:X:66:LEU:HG	5:X:96:PHE:CE1	2.54	0.42
5:X:132:ARG:NH1	5:X:136:LEU:HG	2.34	0.42
7:Z:38:VAL:HG21	7:Z:75:LEU:HG	2.01	0.42
7:Z:242:LEU:O	7:Z:243:GLN:HB3	2.20	0.42
9:b:11:ASP:OD1	9:b:11:ASP:O	2.37	0.42
13:A:329:PRO:HB2	18:F:229:PRO:HG2	2.00	0.42
16:D:44:TYR:CE1	16:D:47:LEU:HD23	2.54	0.42
17:E:141:GLN:HG2	17:E:301:ILE:HD13	2.02	0.42
21:I:92:LEU:HD22	27:P:73:LEU:HD11	2.00	0.42
24:M:51:GLU:OE2	24:M:202:HIS:ND1	2.44	0.42
25:N:47:VAL:HG11	25:N:187:LEU:HD22	2.01	0.42
27:P:141:THR:O	27:P:142:CYS:SG	2.74	0.42
30:S:59:GLU:O	30:S:59:GLU:HG3	2.19	0.42
32:K:215:ILE:HD11	32:K:234:LEU:HD22	2.01	0.42
33:f:415:GLY:O	33:f:451:VAL:HG22	2.19	0.42
33:f:416:MET:HB2	33:f:450:ILE:HD13	2.00	0.42
2:U:486:MET:HE1	2:U:781:LEU:HD21	2.02	0.42
2:U:880:ASN:C	2:U:880:ASN:OD1	2.62	0.42
4:W:109:CYS:HA	4:W:112:VAL:HG12	2.01	0.42
5:X:97:LEU:HD22	5:X:136:LEU:HD21	2.02	0.42
5:X:407:MET:HE3	7:Z:266:ILE:HD13	2.01	0.42
8:a:225:LEU:CD1	8:a:230:ARG:HB3	2.49	0.42
8:a:269:LEU:O	8:a:272:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:b:120:ASN:ND2	9:b:122:LYS:HB3	2.34	0.42
10:c:266:THR:N	10:c:267:PRO:HD3	2.35	0.42
14:B:107:MET:HB2	15:C:96:VAL:HG22	2.02	0.42
16:D:305:VAL:HG23	16:D:305:VAL:O	2.19	0.42
20:H:47:ALA:HB1	20:H:195:LEU:HD11	2.01	0.42
31:T:118:ASP:O	31:T:122:LEU:HD23	2.19	0.42
25:n:48:LEU:HD13	25:n:213:ILE:CD1	2.50	0.42
25:n:63:ARG:NH1	26:o:182:GLU:OE2	2.39	0.42
31:t:187:GLY:HA2	31:t:221:LEU:HD21	2.01	0.42
31:t:250:THR:CG2	31:t:252:THR:HG23	2.49	0.42
33:f:477:MET:SD	33:f:479:LEU:HB2	2.59	0.42
2:U:151:ILE:O	2:U:155:LEU:HD23	2.18	0.42
2:U:745:THR:HG22	2:U:786:THR:HB	2.02	0.42
2:U:906:LEU:HD23	2:U:912:ILE:HD13	2.01	0.42
3:V:411:SER:HB3	3:V:447:ILE:HD12	2.00	0.42
4:W:251:TYR:CE1	4:W:267:LEU:HB2	2.55	0.42
4:W:439:VAL:O	4:W:442:THR:HG22	2.19	0.42
7:Z:215:VAL:CG1	7:Z:222:ILE:HD13	2.49	0.42
8:a:354:GLU:O	8:a:358:THR:HG23	2.19	0.42
11:d:116:LEU:O	11:d:120:LYS:HD3	2.19	0.42
13:A:69:ASP:OD1	13:A:69:ASP:N	2.53	0.42
18:F:139:LEU:HD12	18:F:139:LEU:N	2.34	0.42
21:I:44:LEU:C	21:I:44:LEU:HD12	2.44	0.42
23:L:159:MET:HE3	24:M:59:TYR:HE1	1.84	0.42
28:Q:13:VAL:O	28:Q:14:LEU:C	2.62	0.42
28:Q:16:ALA:HB2	28:Q:160:LEU:HD21	2.01	0.42
29:R:120:ARG:NE	32:K:98:ASN:OD1	2.45	0.42
33:f:282:PHE:HZ	33:f:317:LEU:HD23	1.84	0.42
33:f:607:LEU:H	33:f:607:LEU:HD12	1.84	0.42
33:f:612:LEU:HB3	33:f:657:ILE:HD11	2.02	0.42
33:f:745:LEU:HD13	33:f:766:GLN:HA	2.02	0.42
3:V:121:PHE:O	3:V:128:ARG:CZ	2.67	0.42
4:W:241:LEU:CD1	4:W:286:LEU:HD12	2.50	0.42
5:X:183:LEU:N	5:X:184:PRO:CD	2.82	0.42
9:b:86:PHE:C	9:b:86:PHE:CD1	2.97	0.42
10:c:220:LEU:HD23	10:c:221:HIS:ND1	2.34	0.42
14:B:372:MET:HA	15:C:178:LEU:O	2.19	0.42
16:D:40:LEU:HA	16:D:43:ARG:HG2	2.01	0.42
19:G:13:ILE:HG21	19:G:126:THR:O	2.19	0.42
27:P:138:VAL:HB	27:P:146:MET:HE3	2.01	0.42
27:P:186:ILE:O	27:P:186:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:85:ILE:O	29:R:85:ILE:HG13	2.19	0.42
30:S:119:MET:O	30:S:122:THR:OG1	2.33	0.42
31:T:78:LEU:O	31:T:78:LEU:HG	2.19	0.42
27:p:53:LEU:CB	27:p:60:VAL:HG13	2.49	0.42
28:q:4:LEU:HD22	28:q:45:LEU:HB3	2.02	0.42
2:U:250:PHE:HE1	2:U:328:ILE:HD12	1.83	0.42
2:U:889:LEU:HD21	2:U:906:LEU:O	2.20	0.42
3:V:128:ARG:HA	3:V:132:LEU:HD23	2.02	0.42
4:W:271:VAL:O	4:W:274:VAL:HG12	2.20	0.42
4:W:414:ASN:OD1	4:W:414:ASN:O	2.37	0.42
5:X:86:ALA:HB1	5:X:125:LEU:HD22	2.01	0.42
8:a:173:TYR:HB2	8:a:203:ALA:HB1	2.02	0.42
8:a:279:GLU:O	8:a:283:THR:HG23	2.19	0.42
9:b:58:CYS:SG	9:b:89:GLY:N	2.93	0.42
14:B:189:GLY:CA	14:B:360:THR:HG22	2.50	0.42
14:B:362:LYS:HA	14:B:384:ILE:HD11	2.00	0.42
18:F:169:ASP:C	18:F:171:ARG:H	2.28	0.42
21:I:24:ALA:O	21:I:28:ILE:HG12	2.20	0.42
21:I:137:ILE:HG13	21:I:137:ILE:O	2.19	0.42
27:P:58:THR:HG23	27:P:59:ASP:N	2.34	0.42
31:T:156:VAL:HG23	31:T:184:THR:HG23	2.00	0.42
31:T:169:TYR:HD2	31:T:177:TYR:HD2	1.68	0.42
30:s:142:ASP:OD1	30:s:142:ASP:N	2.50	0.42
4:W:409:LEU:HD22	5:X:346:GLN:NE2	2.35	0.42
6:Y:31:HIS:ND1	6:Y:34:ASP:OD2	2.53	0.42
10:c:86:ALA:O	10:c:87:VAL:C	2.61	0.42
15:C:89:VAL:HG12	15:C:116:LEU:CD1	2.50	0.42
16:D:202:VAL:CG2	16:D:331:ILE:HD12	2.50	0.42
18:F:84:LYS:HG2	18:F:84:LYS:O	2.20	0.42
22:J:83:VAL:CG1	22:J:111:ILE:HD12	2.50	0.42
26:O:50:VAL:O	26:O:50:VAL:HG13	2.19	0.42
28:Q:137:PHE:HB3	29:r:192:VAL:HG21	2.01	0.42
30:S:202:LEU:HD12	30:S:206:VAL:HG13	2.01	0.42
31:T:56:VAL:HG23	31:T:99:SER:HB3	2.02	0.42
33:f:536:SER:O	33:f:540:GLN:OE1	2.37	0.42
33:f:799:VAL:O	33:f:802:SER:OG	2.32	0.42
2:U:137:MET:CE	15:C:20:LEU:N	2.83	0.42
2:U:183:LEU:HD12	16:D:41:TYR:CD2	2.55	0.42
2:U:756:HIS:ND1	2:U:759:SER:OG	2.49	0.42
3:V:203:LEU:HD12	3:V:206:VAL:HG21	2.01	0.42
5:X:99:MET:O	5:X:100:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:248:ILE:HG23	5:X:249:THR:N	2.35	0.42
6:Y:148:GLY:C	6:Y:157:ILE:HD11	2.45	0.42
8:a:87:MET:SD	8:a:88:THR:O	2.77	0.42
10:c:177:THR:O	10:c:177:THR:CG2	2.66	0.42
14:B:139:VAL:HG12	14:B:141:LYS:H	1.85	0.42
15:C:142:LYS:NZ	16:D:297:ASP:OD1	2.48	0.42
17:E:84:ARG:HG3	17:E:87:LEU:CD2	2.50	0.42
17:E:327:ASP:H	17:E:364:GLN:HE21	1.66	0.42
18:F:172:VAL:HG22	18:F:175:MET:CE	2.44	0.42
24:M:91:ILE:O	24:M:95:GLU:HG2	2.20	0.42
24:M:191:VAL:HG21	24:M:216:TRP:CZ3	2.55	0.42
28:Q:182:ILE:CD1	28:Q:191:LEU:HD13	2.49	0.42
29:R:60:THR:O	29:R:189:SER:N	2.53	0.42
30:S:153:ASP:OD1	30:S:156:GLY:N	2.48	0.42
28:q:164:LEU:HD13	28:q:178:PHE:CD2	2.54	0.42
31:t:223:TYR:OH	31:t:253:ASN:N	2.42	0.42
33:f:799:VAL:HG21	33:f:821:LEU:HB2	2.01	0.42
3:V:318:GLN:OE1	3:V:318:GLN:N	2.48	0.41
5:X:58:ALA:HA	5:X:99:MET:SD	2.60	0.41
5:X:246:LYS:O	5:X:249:THR:HG22	2.20	0.41
5:X:315:ASP:C	5:X:317:PRO:HD3	2.45	0.41
6:Y:310:SER:O	6:Y:310:SER:OG	2.35	0.41
8:a:29:TYR:O	8:a:32:LYS:NZ	2.35	0.41
8:a:112:ILE:HD11	8:a:138:VAL:HG13	2.00	0.41
13:A:218:PRO:HD3	13:A:429:TYR:CB	2.50	0.41
17:E:117:PRO:HD3	18:F:94:ILE:HB	2.01	0.41
17:E:196:LEU:HD12	17:E:230:ILE:HG12	2.02	0.41
17:E:272:ARG:HG2	17:E:272:ARG:HH11	1.85	0.41
23:L:148:CYS:HG	23:L:150:SER:HG	1.55	0.41
27:p:25:ASP:HB2	27:p:181:SER:O	2.20	0.41
28:q:38:MET:HB3	28:q:64:VAL:HG11	2.02	0.41
29:r:71:VAL:HB	29:r:238:VAL:CG2	2.50	0.41
29:r:72:ILE:HD11	29:r:235:LEU:HD21	2.02	0.41
31:t:192:GLN:HG3	31:t:193:PRO:HD3	2.02	0.41
2:U:37:GLU:OE2	3:V:266:GLN:CD	2.62	0.41
2:U:524:LYS:O	2:U:524:LYS:HG2	2.20	0.41
3:V:169:LEU:HD12	3:V:210:CYS:SG	2.59	0.41
4:W:55:ARG:HD3	4:W:96:GLN:HA	2.01	0.41
6:Y:351:ASN:OD1	6:Y:351:ASN:N	2.53	0.41
7:Z:224:HIS:NE2	8:a:218:MET:HE1	2.35	0.41
8:a:87:MET:SD	8:a:88:THR:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:287:ILE:CD1	14:B:290:ILE:HD12	2.49	0.41
18:F:123:VAL:O	18:F:123:VAL:HG12	2.19	0.41
18:F:227:GLY:O	18:F:333:ASN:HA	2.20	0.41
20:H:98:TYR:O	20:H:101:TYR:O	2.38	0.41
23:L:36:VAL:O	23:L:36:VAL:HG23	2.19	0.41
25:N:194:LEU:O	25:N:198:MET:HG3	2.19	0.41
27:P:108:VAL:O	27:P:108:VAL:HG23	2.19	0.41
27:P:136:PHE:CD1	27:P:150:CYS:HB3	2.55	0.41
29:R:78:ARG:HE	29:R:230:GLY:H	1.68	0.41
33:f:270:LEU:HD12	33:f:278:VAL:CG2	2.49	0.41
3:V:168:GLN:NE2	3:V:187:ILE:HB	2.35	0.41
3:V:379:LEU:HD21	3:V:395:ILE:HG22	2.00	0.41
9:b:7:MET:SD	9:b:64:LEU:HD11	2.61	0.41
9:b:100:ARG:NH2	9:b:103:LYS:O	2.53	0.41
14:B:187:ILE:HD13	14:B:235:LEU:HD23	2.03	0.41
16:D:411:GLU:O	16:D:413:GLU:OE1	2.38	0.41
17:E:62:LYS:HE3	17:E:70:ILE:HD12	2.02	0.41
20:H:84:ARG:O	20:H:87:VAL:HG12	2.20	0.41
29:R:73:VAL:O	29:R:73:VAL:HG23	2.20	0.41
30:s:204:LYS:O	30:s:208:ILE:HG12	2.21	0.41
33:f:379:GLY:C	33:f:416:MET:HE3	2.45	0.41
33:f:450:ILE:O	33:f:453:SER:OG	2.24	0.41
2:U:205:TYR:HB3	2:U:216:VAL:CG2	2.51	0.41
4:W:99:GLN:HB3	4:W:103:LYS:NZ	2.36	0.41
9:b:11:ASP:OD1	9:b:16:MET:HE3	2.21	0.41
16:D:153:MET:HE2	16:D:227:PHE:CD1	2.55	0.41
16:D:236:VAL:HG12	17:E:208:ILE:HG22	2.03	0.41
17:E:65:THR:O	17:E:66:GLU:HB2	2.20	0.41
17:E:70:ILE:HG12	17:E:80:VAL:HG12	2.02	0.41
22:J:38:ARG:O	22:J:213:ARG:NH2	2.53	0.41
24:M:171:GLN:O	24:M:175:THR:HG23	2.21	0.41
27:P:158:MET:CE	27:P:163:LEU:HA	2.46	0.41
31:T:156:VAL:CG2	31:T:184:THR:HG23	2.49	0.41
27:p:158:MET:HE3	27:p:162:HIS:HD2	1.82	0.41
29:r:142:LEU:HD23	29:r:142:LEU:C	2.45	0.41
2:U:252:LEU:HD12	2:U:260:PHE:CE1	2.56	0.41
2:U:483:LEU:O	2:U:486:MET:HE3	2.20	0.41
5:X:24:ILE:HG22	5:X:28:HIS:CE1	2.56	0.41
5:X:86:ALA:HB2	5:X:125:LEU:HD22	2.03	0.41
5:X:251:LEU:O	5:X:255:LEU:HG	2.21	0.41
5:X:310:ARG:NH1	5:X:310:ARG:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:360:ASP:OD1	6:Y:360:ASP:N	2.53	0.41
11:d:152:ALA:O	11:d:156:ILE:HG12	2.20	0.41
11:d:302:TYR:O	11:d:305:LYS:HB2	2.20	0.41
14:B:254:GLU:OE2	15:C:232:ARG:NH2	2.53	0.41
21:I:198:ASN:OD1	21:I:206:LEU:CB	2.69	0.41
22:J:171:PHE:O	22:J:174:LYS:O	2.38	0.41
23:L:74:ILE:HG21	23:L:81:ALA:HB1	2.02	0.41
23:L:193:ARG:NH1	23:L:237:GLU:OE1	2.53	0.41
24:M:180:LEU:HD21	24:M:193:GLU:HB3	2.03	0.41
27:P:3:ILE:HD13	27:P:104:TYR:CE2	2.56	0.41
30:S:89:CYS:O	30:S:93:THR:HG23	2.21	0.41
32:K:38:ILE:HG23	32:K:181:LEU:HD11	2.02	0.41
26:o:215:ASN:OD1	26:o:234:VAL:HG13	2.20	0.41
30:s:41:LEU:CD1	30:s:177:LEU:HD11	2.51	0.41
31:t:192:GLN:OE1	31:t:196:ARG:CZ	2.69	0.41
2:U:677:ASN:ND2	3:V:508:ALA:HB1	2.36	0.41
4:W:335:SER:O	4:W:336:PRO:C	2.63	0.41
13:A:238:ILE:HD12	13:A:270:CYS:SG	2.60	0.41
14:B:76:GLU:HB3	14:B:80:ARG:NH1	2.35	0.41
14:B:426:VAL:HG13	14:B:427:LEU:H	1.85	0.41
14:B:427:LEU:O	14:B:427:LEU:HG	2.20	0.41
16:D:51:LEU:HD23	16:D:51:LEU:C	2.46	0.41
21:I:13:SER:O	21:I:14:PRO:C	2.64	0.41
22:J:16:LEU:O	22:J:19:VAL:HG12	2.20	0.41
26:O:82:PRO:O	26:O:226:LEU:HD13	2.20	0.41
29:R:233:VAL:O	29:R:234:ASN:C	2.64	0.41
30:S:176:LEU:N	27:p:149:MET:HE1	2.36	0.41
31:T:209:GLU:O	31:T:212:ASP:OD1	2.38	0.41
28:q:84:THR:HG21	28:q:102:LEU:HD13	2.02	0.41
28:q:88:LEU:CB	28:q:122:ALA:HB2	2.50	0.41
30:s:59:GLU:O	30:s:62:SER:OG	2.34	0.41
33:f:514:VAL:O	33:f:518:THR:HG23	2.19	0.41
2:U:58:GLN:OE1	2:U:58:GLN:N	2.54	0.41
2:U:356:THR:O	2:U:360:VAL:HG23	2.20	0.41
2:U:697:GLN:NE2	2:U:883:ARG:HE	2.19	0.41
2:U:900:TYR:HB3	2:U:914:LEU:HD12	2.02	0.41
3:V:408:ARG:HA	3:V:447:ILE:HD11	2.02	0.41
3:V:436:PHE:HD2	11:d:242:ASN:OD1	2.03	0.41
4:W:74:CYS:HB3	4:W:83:LEU:HD13	2.02	0.41
5:X:89:VAL:HG21	5:X:116:TRP:CZ3	2.55	0.41
5:X:331:LEU:HD23	5:X:331:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:81:MET:CE	10:c:94:LYS:HE3	2.51	0.41
8:a:198:PHE:HB2	8:a:230:ARG:CD	2.51	0.41
10:c:26:ASP:OD1	10:c:27:THR:N	2.54	0.41
13:A:108:ASP:O	13:A:108:ASP:OD1	2.38	0.41
14:B:78:PHE:CE2	33:f:678:LEU:HD23	2.55	0.41
16:D:113:VAL:HG22	16:D:114:ARG:N	2.35	0.41
16:D:413:GLU:O	20:H:53:LYS:HE2	2.21	0.41
18:F:394:ALA:O	18:F:395:GLN:C	2.64	0.41
19:G:32:ILE:HD13	19:G:137:CYS:HB2	2.03	0.41
21:I:222:LYS:HG2	21:I:223:THR:N	2.35	0.41
24:M:28:MET:O	24:M:32:GLU:OE1	2.39	0.41
24:M:50:VAL:HG23	24:M:67:LEU:HD11	2.03	0.41
26:O:81:SER:OG	26:O:82:PRO:HD2	2.21	0.41
27:P:173:ASN:OD1	30:s:185:ASN:ND2	2.42	0.41
30:S:120:LEU:O	30:S:124:LEU:HD13	2.20	0.41
30:S:207:PHE:CG	30:S:221:LEU:HD13	2.56	0.41
28:q:4:LEU:HD11	28:q:47:VAL:HG13	2.03	0.41
29:r:96:ILE:HD11	29:r:115:GLU:OE1	2.21	0.41
31:t:249:SER:OG	31:t:250:THR:N	2.53	0.41
33:f:228:LYS:HA	33:f:856:ALA:HB3	2.02	0.41
33:f:848:GLN:HA	33:f:878:GLU:HA	2.03	0.41
1:y:384:GLU:O	1:y:388:THR:HG23	2.20	0.41
2:U:756:HIS:CD2	2:U:758:PRO:HD2	2.55	0.41
3:V:108:LEU:HD23	3:V:173:ILE:HG23	2.02	0.41
7:Z:32:GLN:O	7:Z:33:LYS:HB3	2.21	0.41
7:Z:181:ASP:OD1	16:D:70:LYS:NZ	2.53	0.41
13:A:241:ILE:HD12	14:B:314:ASN:HD21	1.86	0.41
14:B:369:THR:HG22	14:B:372:MET:CE	2.50	0.41
16:D:87:LEU:HD11	16:D:131:ALA:HB1	1.99	0.41
17:E:348:THR:O	18:F:217:ILE:HD11	2.21	0.41
23:L:105:VAL:O	23:L:109:VAL:HG23	2.21	0.41
26:O:133:TYR:O	26:O:136:TYR:N	2.48	0.41
26:O:186:ARG:HG2	26:O:189:MET:HE3	2.03	0.41
31:T:73:GLY:CA	31:T:84:ILE:HD11	2.50	0.41
32:K:16:SER:HB3	32:K:20:ARG:HB3	2.02	0.41
27:p:30:ILE:HG13	27:p:31:GLN:N	2.36	0.41
31:t:169:TYR:HB2	31:t:182:LEU:HD13	2.02	0.41
33:f:433:LEU:HB3	33:f:444:ALA:HB3	2.02	0.41
33:f:662:MET:HG3	33:f:662:MET:O	2.21	0.41
2:U:742:HIS:O	2:U:742:HIS:CG	2.73	0.41
4:W:105:VAL:O	4:W:109:CYS:SG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:163:LYS:HB2	5:X:200:ILE:HG21	2.02	0.41
5:X:415:TYR:HE1	6:Y:383:LEU:HB2	1.86	0.41
6:Y:104:MET:HE2	6:Y:127:THR:CA	2.51	0.41
6:Y:204:THR:HG23	6:Y:219:PHE:HZ	1.85	0.41
6:Y:245:GLU:HG2	6:Y:246:ILE:HD12	2.03	0.41
6:Y:261:PHE:O	6:Y:265:GLU:HG2	2.20	0.41
7:Z:94:TRP:CD1	7:Z:112:MET:HG3	2.55	0.41
8:a:18:GLN:CG	8:a:21:VAL:HB	2.50	0.41
8:a:60:TYR:HH	8:a:96:PHE:HE1	1.65	0.41
8:a:131:THR:HA	8:a:134:THR:HG22	2.01	0.41
8:a:292:THR:OG1	8:a:295:GLU:HG3	2.21	0.41
13:A:83:ASP:OD1	13:A:83:ASP:C	2.64	0.41
14:B:153:ASN:OD1	14:B:156:VAL:HG22	2.21	0.41
14:B:380:LEU:HG	14:B:380:LEU:O	2.21	0.41
14:B:408:ARG:O	14:B:410:ARG:NH1	2.54	0.41
14:B:429:LYS:HB3	21:I:169:ALA:HB1	2.03	0.41
15:C:154:LEU:HD13	15:C:199:LEU:HD22	2.03	0.41
15:C:156:LYS:O	15:C:160:GLU:HG3	2.21	0.41
15:C:162:LYS:O	15:C:166:GLU:HB3	2.20	0.41
15:C:164:VAL:HG13	15:C:183:PRO:HB2	2.02	0.41
16:D:115:ILE:HG22	16:D:139:LEU:HB3	2.01	0.41
16:D:279:THR:HG21	17:E:248:SER:CB	2.50	0.41
17:E:215:ILE:HD12	17:E:256:THR:CG2	2.51	0.41
18:F:389:ASP:O	18:F:390:ASP:CB	2.69	0.41
19:G:58:ASP:C	19:G:60:LEU:H	2.27	0.41
20:H:69:THR:HG22	20:H:70:LYS:H	1.86	0.41
21:I:72:MET:CE	21:I:107:CYS:HA	2.51	0.41
22:J:71:MET:HE3	22:J:131:ALA:CB	2.51	0.41
23:L:3:ARG:O	23:L:4:ASN:ND2	2.54	0.41
24:M:40:ILE:HG21	24:M:190:ILE:HD12	2.02	0.41
25:N:199:GLU:OE2	31:t:82:ARG:NH1	2.54	0.41
26:O:142:VAL:HG13	26:O:168:VAL:CG2	2.51	0.41
26:O:257:GLU:OE1	26:O:259:ILE:HD11	2.20	0.41
27:P:144:GLU:CD	30:s:171:ALA:HB3	2.46	0.41
27:P:153:LEU:O	27:P:153:LEU:HD23	2.20	0.41
31:T:88:MET:SD	31:T:109:LYS:HG3	2.61	0.41
31:T:151:LEU:O	31:T:153:ASN:N	2.53	0.41
31:T:162:ASP:OD1	31:T:162:ASP:C	2.64	0.41
31:T:180:PRO:HB2	31:T:199:LEU:HD13	2.01	0.41
31:T:187:GLY:HA2	31:T:221:LEU:HD21	2.03	0.41
27:p:169:GLN:O	27:p:173:ASN:ND2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:119:ASP:OD1	28:q:119:ASP:C	2.63	0.41
29:r:94:ILE:HD12	29:r:115:GLU:HG3	2.03	0.41
30:s:75:THR:HG1	30:s:78:THR:HG1	1.57	0.41
31:t:256:ILE:HG22	31:t:259:MET:HE2	2.03	0.41
33:f:372:LEU:HD11	33:f:376:PHE:HE1	1.86	0.41
33:f:567:LEU:HD21	33:f:793:VAL:CG1	2.51	0.41
33:f:577:LEU:HD22	33:f:592:ASN:OD1	2.21	0.41
3:V:435:GLU:OE2	3:V:451:ILE:HG21	2.20	0.41
4:W:436:MET:O	4:W:439:VAL:HG22	2.21	0.41
6:Y:112:CYS:SG	6:Y:124:PHE:HE2	2.44	0.41
7:Z:217:THR:OG1	7:Z:219:LYS:NZ	2.52	0.41
8:a:228:THR:HG22	8:a:230:ARG:H	1.86	0.41
10:c:175:ARG:NH1	10:c:201:TYR:CD1	2.89	0.41
11:d:232:LEU:HD21	11:d:263:LEU:HD23	2.03	0.41
14:B:171:VAL:HG12	14:B:175:LYS:CD	2.51	0.41
14:B:383:LEU:CD1	14:B:423:LYS:HE2	2.50	0.41
16:D:181:VAL:HG21	16:D:308:ILE:HD11	2.02	0.41
16:D:353:ASN:OD1	16:D:353:ASN:O	2.39	0.41
19:G:160:TYR:CD2	19:G:160:TYR:O	2.73	0.41
26:O:58:GLY:O	26:O:202:ILE:HD11	2.21	0.41
26:O:62:ARG:HB3	26:O:213:GLY:HA2	2.02	0.41
27:p:60:VAL:HG22	27:p:105:THR:OG1	2.21	0.41
27:p:108:VAL:HG12	27:p:123:SER:CB	2.52	0.41
29:r:85:ILE:HG22	29:r:87:SER:N	2.36	0.41
33:f:585:GLU:HB3	33:f:586:PRO:HD3	2.03	0.41
1:y:391:LYS:NZ	33:f:465:LEU:HA	2.36	0.40
1:y:392:VAL:HG11	33:f:465:LEU:HD11	2.02	0.40
2:U:761:VAL:O	2:U:765:VAL:HG23	2.21	0.40
4:W:164:SER:O	4:W:168:GLU:HG2	2.21	0.40
4:W:239:SER:O	4:W:243:ILE:HD12	2.21	0.40
4:W:285:ASP:O	4:W:289:ARG:HG2	2.19	0.40
4:W:344:THR:O	4:W:347:GLY:N	2.53	0.40
4:W:439:VAL:HA	4:W:442:THR:HG22	2.03	0.40
8:a:89:ASP:O	8:a:92:VAL:HG12	2.21	0.40
9:b:43:SER:O	9:b:44:ASN:C	2.64	0.40
9:b:97:LEU:HB3	9:b:107:MET:HG2	2.03	0.40
13:A:429:TYR:HA	13:A:432:TYR:HB2	2.03	0.40
16:D:89:ILE:HD11	17:E:70:ILE:HG12	2.02	0.40
16:D:203:LEU:HD23	16:D:330:LYS:HG2	2.04	0.40
18:F:93:VAL:HG11	18:F:145:LEU:HB3	2.02	0.40
18:F:251:LEU:O	18:F:252:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:168:ALA:HB2	23:L:198:THR:CG2	2.51	0.40
30:S:165:ALA:O	30:S:174:GLN:NE2	2.54	0.40
30:S:212:GLU:OE2	26:o:72:LYS:NZ	2.43	0.40
31:T:223:TYR:HB3	26:o:182:GLU:OE2	2.21	0.40
32:K:154:PHE:HA	32:K:164:GLN:HA	2.03	0.40
26:o:191:GLU:HG2	26:o:192:GLU:N	2.36	0.40
28:q:121:LEU:O	28:q:122:ALA:HB3	2.21	0.40
29:r:117:LEU:HG	29:r:145:MET:HE1	2.02	0.40
29:r:159:MET:CE	29:r:187:VAL:HG13	2.51	0.40
29:r:186:SER:HB3	29:r:195:TYR:CE1	2.56	0.40
31:t:162:ASP:N	31:t:162:ASP:OD1	2.54	0.40
33:f:673:ARG:O	33:f:677:HIS:ND1	2.55	0.40
33:f:848:GLN:CG	33:f:849:ALA:N	2.84	0.40
2:U:186:SER:O	2:U:187:LEU:HD23	2.20	0.40
2:U:599:ILE:HD11	2:U:625:ILE:CG2	2.51	0.40
3:V:403:ILE:HD12	3:V:428:LEU:HD21	2.01	0.40
5:X:82:LYS:C	5:X:84:LYS:N	2.77	0.40
5:X:160:MET:O	5:X:160:MET:CE	2.67	0.40
6:Y:278:VAL:HA	6:Y:281:GLU:HG2	2.03	0.40
8:a:84:VAL:HG21	8:a:97:LEU:CD2	2.52	0.40
10:c:165:ALA:HA	10:c:168:MET:HG3	2.03	0.40
14:B:235:LEU:HD12	14:B:353:PHE:CE2	2.56	0.40
15:C:375:ARG:NH2	15:C:382:ASP:OD2	2.54	0.40
16:D:411:GLU:O	16:D:412:GLN:HB2	2.22	0.40
21:I:186:LEU:HD11	21:I:217:THR:CG2	2.51	0.40
21:I:224:VAL:O	21:I:224:VAL:HG23	2.21	0.40
25:n:161:ILE:HD11	25:n:170:TYR:CD1	2.56	0.40
26:o:165:LEU:HD12	26:o:168:VAL:HG12	2.03	0.40
28:q:85:ARG:NH1	28:q:122:ALA:O	2.47	0.40
29:r:159:MET:HE3	29:r:187:VAL:HG22	2.02	0.40
33:f:246:SER:O	33:f:250:ARG:HG2	2.20	0.40
33:f:262:PHE:N	33:f:263:PRO:HD2	2.36	0.40
1:y:396:GLN:O	1:y:400:GLN:HG2	2.22	0.40
4:W:441:LYS:O	4:W:445:LEU:HG	2.21	0.40
6:Y:347:ILE:HG22	6:Y:354:VAL:HG22	2.02	0.40
13:A:111:TYR:CE2	13:A:125:LEU:HG	2.55	0.40
13:A:215:PHE:HA	13:A:321:THR:O	2.22	0.40
13:A:317:VAL:HG11	13:A:319:MET:HE2	2.02	0.40
15:C:236:VAL:HG23	15:C:237:MET:N	2.37	0.40
17:E:101:ASP:OD1	17:E:102:MET:N	2.54	0.40
17:E:349:GLU:HB2	17:E:370:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:274:LEU:O	18:F:277:GLU:HG2	2.21	0.40
18:F:403:ALA:HB2	18:F:420:TYR:HA	2.03	0.40
19:G:41:ALA:HB2	19:G:50:ILE:HG22	2.04	0.40
19:G:141:ILE:HD13	19:G:151:VAL:HG22	2.02	0.40
29:r:156:MET:HG2	29:r:157:GLY:N	2.36	0.40
30:s:77:LYS:C	30:s:78:THR:OG1	2.65	0.40
2:U:808:PRO:HB3	2:U:876:GLN:CD	2.47	0.40
3:V:81:GLN:HA	3:V:84:LYS:HG2	2.04	0.40
3:V:393:THR:HG22	11:d:212:LEU:HD22	2.04	0.40
4:W:67:LEU:CD2	4:W:90:LEU:HD22	2.51	0.40
4:W:163:ALA:O	4:W:167:GLN:OE1	2.39	0.40
4:W:353:ASP:O	4:W:357:ARG:HG2	2.21	0.40
4:W:373:ILE:HD12	8:a:326:GLU:HB3	2.02	0.40
7:Z:81:MET:HE1	10:c:94:LYS:HG2	2.03	0.40
7:Z:262:LEU:O	7:Z:266:ILE:HG12	2.22	0.40
13:A:199:GLU:HA	13:A:202:VAL:HG22	2.03	0.40
13:A:295:VAL:HA	13:A:298:THR:HG22	2.03	0.40
14:B:74:MET:HE1	33:f:609:VAL:CG1	2.47	0.40
14:B:365:PHE:CZ	14:B:383:LEU:HB3	2.56	0.40
18:F:260:PHE:O	18:F:261:ILE:C	2.64	0.40
19:G:88:ARG:NH2	24:M:114:ASP:OD1	2.54	0.40
24:M:109:LEU:HD12	24:M:140:SER:HB3	2.04	0.40
30:S:175:PRO:HB2	27:p:149:MET:CE	2.52	0.40
25:n:150:MET:HB2	31:t:50:MET:HE2	2.03	0.40
33:f:334:ALA:HB3	33:f:340:MET:HE3	2.03	0.40
33:f:452:ASN:OD1	33:f:452:ASN:O	2.39	0.40
2:U:206:MET:SD	2:U:213:PHE:CE1	3.14	0.40
2:U:437:TYR:HA	2:U:472:ILE:HG21	2.04	0.40
3:V:191:LEU:O	3:V:191:LEU:HD23	2.20	0.40
3:V:235:LEU:C	3:V:235:LEU:HD23	2.47	0.40
3:V:338:LEU:HD21	3:V:397:ARG:HB2	2.03	0.40
3:V:376:ASN:OD1	3:V:377:GLN:N	2.55	0.40
3:V:387:GLN:NE2	3:V:392:TYR:CE1	2.90	0.40
5:X:114:ILE:HD12	5:X:133:LEU:HD22	2.03	0.40
5:X:124:PHE:CE2	20:H:186:ASP:OD1	2.74	0.40
5:X:377:ILE:HD11	6:Y:312:ARG:HA	2.02	0.40
6:Y:282:MET:HE3	6:Y:288:PHE:CD1	2.57	0.40
6:Y:381:GLN:HE22	6:Y:385:ARG:NH1	2.19	0.40
9:b:56:ASN:OD1	9:b:57:ASP:N	2.54	0.40
9:b:68:THR:CG2	9:b:72:LEU:HD23	2.51	0.40
9:b:120:ASN:O	9:b:123:ASP:OD1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:262:GLU:O	13:A:266:THR:HG23	2.21	0.40
15:C:187:LEU:HD22	15:C:189:TYR:CE1	2.57	0.40
17:E:75:ASN:OD1	17:E:77:PRO:HD2	2.22	0.40
17:E:204:VAL:CG2	17:E:238:ILE:HD11	2.52	0.40
17:E:215:ILE:HD13	17:E:260:LEU:HB2	2.02	0.40
27:P:17:LYS:N	27:P:158:MET:O	2.47	0.40
27:P:78:GLU:O	27:P:80:ARG:N	2.54	0.40
27:P:136:PHE:CE1	27:P:150:CYS:HB3	2.57	0.40
29:R:67:PHE:CD2	29:R:67:PHE:O	2.73	0.40
29:R:78:ARG:HD3	29:R:88:GLN:OE1	2.21	0.40
29:r:101:LEU:HD21	29:r:243:TRP:CG	2.56	0.40
31:t:250:THR:CG2	31:t:251:GLU:N	2.85	0.40
33:f:695:ALA:HB2	33:f:728:ALA:HB1	2.04	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	y	29/567 (5%)	29 (100%)	0	0	100	100
2	U	804/953 (84%)	745 (93%)	59 (7%)	0	100	100
3	V	453/534 (85%)	416 (92%)	37 (8%)	0	100	100
4	W	436/456 (96%)	406 (93%)	30 (7%)	0	100	100
5	X	409/422 (97%)	375 (92%)	34 (8%)	0	100	100
6	Y	379/389 (97%)	366 (97%)	13 (3%)	0	100	100
7	Z	285/324 (88%)	278 (98%)	7 (2%)	0	100	100
8	a	373/376 (99%)	347 (93%)	25 (7%)	1 (0%)	37	66
9	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
10	c	285/310 (92%)	258 (90%)	27 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	d	257/350 (73%)	226 (88%)	31 (12%)	0	100	100
12	e	35/70 (50%)	34 (97%)	1 (3%)	0	100	100
13	A	387/433 (89%)	353 (91%)	34 (9%)	0	100	100
14	B	369/440 (84%)	348 (94%)	21 (6%)	0	100	100
15	C	355/406 (87%)	333 (94%)	22 (6%)	0	100	100
16	D	378/418 (90%)	353 (93%)	24 (6%)	1 (0%)	37	66
17	E	360/389 (92%)	337 (94%)	23 (6%)	0	100	100
18	F	345/439 (79%)	306 (89%)	39 (11%)	0	100	100
19	G	236/246 (96%)	218 (92%)	18 (8%)	0	100	100
20	H	227/234 (97%)	213 (94%)	14 (6%)	0	100	100
21	I	252/261 (97%)	237 (94%)	15 (6%)	0	100	100
22	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
23	L	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
24	M	241/255 (94%)	229 (95%)	11 (5%)	1 (0%)	30	60
25	N	196/239 (82%)	182 (93%)	14 (7%)	0	100	100
25	n	177/239 (74%)	166 (94%)	11 (6%)	0	100	100
26	O	219/277 (79%)	203 (93%)	16 (7%)	0	100	100
26	o	166/277 (60%)	157 (95%)	9 (5%)	0	100	100
27	P	202/205 (98%)	179 (89%)	23 (11%)	0	100	100
27	p	153/205 (75%)	137 (90%)	16 (10%)	0	100	100
28	Q	195/201 (97%)	186 (95%)	9 (5%)	0	100	100
28	q	163/201 (81%)	153 (94%)	10 (6%)	0	100	100
29	R	197/263 (75%)	186 (94%)	11 (6%)	0	100	100
29	r	181/263 (69%)	176 (97%)	5 (3%)	0	100	100
30	S	210/241 (87%)	199 (95%)	11 (5%)	0	100	100
30	s	202/241 (84%)	188 (93%)	14 (7%)	0	100	100
31	T	211/264 (80%)	195 (92%)	16 (8%)	0	100	100
31	t	202/264 (76%)	186 (92%)	16 (8%)	0	100	100
32	K	223/241 (92%)	213 (96%)	10 (4%)	0	100	100
33	f	641/908 (71%)	560 (87%)	80 (12%)	1 (0%)	44	73
All	All	11094/13689 (81%)	10294 (93%)	796 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	a	232	TRP
16	D	278	GLN
24	M	208	LYS
33	f	855	GLN

5.3.2 Protein sidechains (i)

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	y	29/459 (6%)	29 (100%)	0	100	100
2	U	691/816 (85%)	691 (100%)	0	100	100
3	V	402/460 (87%)	402 (100%)	0	100	100
4	W	403/416 (97%)	403 (100%)	0	100	100
5	X	353/362 (98%)	353 (100%)	0	100	100
6	Y	336/344 (98%)	336 (100%)	0	100	100
7	Z	258/295 (88%)	258 (100%)	0	100	100
8	a	335/336 (100%)	334 (100%)	1 (0%)	91	97
9	b	167/312 (54%)	167 (100%)	0	100	100
10	c	252/268 (94%)	252 (100%)	0	100	100
11	d	230/294 (78%)	230 (100%)	0	100	100
12	e	37/63 (59%)	37 (100%)	0	100	100
13	A	334/372 (90%)	333 (100%)	1 (0%)	91	97
14	B	329/385 (86%)	329 (100%)	0	100	100
15	C	311/352 (88%)	311 (100%)	0	100	100
16	D	333/366 (91%)	333 (100%)	0	100	100
17	E	317/341 (93%)	317 (100%)	0	100	100
18	F	296/379 (78%)	295 (100%)	1 (0%)	91	97
19	G	204/210 (97%)	204 (100%)	0	100	100
20	H	188/191 (98%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	I	214/221 (97%)	214 (100%)	0	100	100
22	J	203/211 (96%)	203 (100%)	0	100	100
23	L	203/224 (91%)	203 (100%)	0	100	100
24	M	201/212 (95%)	201 (100%)	0	100	100
25	N	154/181 (85%)	154 (100%)	0	100	100
25	n	140/181 (77%)	140 (100%)	0	100	100
26	O	182/228 (80%)	182 (100%)	0	100	100
26	o	139/228 (61%)	139 (100%)	0	100	100
27	P	173/174 (99%)	173 (100%)	0	100	100
27	p	137/174 (79%)	137 (100%)	0	100	100
28	Q	168/171 (98%)	168 (100%)	0	100	100
28	q	148/171 (86%)	148 (100%)	0	100	100
29	R	155/202 (77%)	155 (100%)	0	100	100
29	r	142/202 (70%)	142 (100%)	0	100	100
30	S	177/199 (89%)	177 (100%)	0	100	100
30	s	172/199 (86%)	172 (100%)	0	100	100
31	T	176/215 (82%)	176 (100%)	0	100	100
31	t	171/215 (80%)	171 (100%)	0	100	100
32	K	191/203 (94%)	191 (100%)	0	100	100
33	f	537/763 (70%)	537 (100%)	0	100	100
All	All	9588/11595 (83%)	9585 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	a	232	TRP
13	A	248	LYS
18	F	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
2	U	32	ASN
2	U	338	HIS

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Mol	Chain	Res	Type
2	U	450	HIS
2	U	467	ASN
2	U	677	ASN
2	U	742	HIS
3	V	109	ASN
3	V	110	HIS
3	V	266	GLN
5	X	207	GLN
6	Y	178	ASN
6	Y	280	GLN
7	Z	193	ASN
7	Z	194	GLN
7	Z	231	GLN
7	Z	235	ASN
7	Z	243	GLN
8	a	12	GLN
8	a	194	GLN
8	a	212	ASN
8	a	231	GLN
8	a	264	ASN
8	a	370	GLN
8	a	372	HIS
10	c	44	HIS
10	c	254	ASN
11	d	108	ASN
11	d	127	ASN
13	A	88	GLN
13	A	117	GLN
13	A	247	GLN
13	A	414	ASN
14	B	157	HIS
15	C	53	ASN
15	C	332	HIS
15	C	337	ASN
16	D	57	GLN
16	D	278	GLN
16	D	294	ASN
17	E	32	GLN
17	E	141	GLN
17	E	155	ASN
17	E	263	GLN
18	F	130	GLN

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Mol	Chain	Res	Type
18	F	321	GLN
18	F	374	ASN
20	H	140	ASN
20	H	166	ASN
21	I	102	GLN
22	J	92	GLN
22	J	205	ASN
23	L	4	ASN
24	M	102	ASN
25	N	41	GLN
25	N	140	GLN
25	N	227	GLN
26	O	105	ASN
27	P	33	GLN
28	Q	8	GLN
28	Q	186	ASN
29	R	210	GLN
30	S	136	ASN
30	S	185	ASN
32	K	23	GLN
32	K	97	GLN
32	K	164	GLN
32	K	221	GLN
25	n	111	HIS
26	o	236	ASN
27	p	162	HIS
28	q	101	ASN
33	f	396	ASN
33	f	405	HIS
33	f	452	ASN
33	f	493	ASN
33	f	614	HIS
33	f	650	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	ATP	E	401	35	28,33,33	0.67	0	34,52,52	0.91	1 (2%)
34	ATP	A	501	35	28,33,33	0.69	0	34,52,52	0.93	2 (5%)
36	ADP	C	501	-	24,29,29	0.87	0	29,45,45	1.25	2 (6%)
34	ATP	D	501	35	28,33,33	0.74	0	34,52,52	0.95	1 (2%)
36	ADP	B	501	35	24,29,29	0.88	0	29,45,45	1.27	2 (6%)
34	ATP	F	501	35	28,33,33	0.71	0	34,52,52	0.89	1 (2%)

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	ATP	E	401	35	-	4/18/38/38	0/3/3/3
34	ATP	A	501	35	-	5/18/38/38	0/3/3/3
36	ADP	C	501	-	-	3/12/32/32	0/3/3/3
34	ATP	D	501	35	-	3/18/38/38	0/3/3/3
36	ADP	B	501	35	-	2/12/32/32	0/3/3/3
34	ATP	F	501	35	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	501	ADP	N3-C2-N1	-4.16	123.03	128.67
36	B	501	ADP	N3-C2-N1	-4.04	123.19	128.67
36	B	501	ADP	C4-C5-N7	-2.44	106.76	109.34
34	F	501	ATP	C5-C6-N6	2.42	123.99	120.31
36	C	501	ADP	C4-C5-N7	-2.36	106.84	109.34
34	D	501	ATP	C5-C6-N6	2.34	123.87	120.31
34	E	401	ATP	C5-C6-N6	2.28	123.79	120.31
34	A	501	ATP	C5-C6-N6	2.28	123.78	120.31
34	A	501	ATP	O2'-C2'-C3'	-2.00	105.40	111.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	PB-O3B-PG-O3G
34	A	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	PB-O3B-PG-O2G
34	F	501	ATP	C5'-O5'-PA-O2A
34	F	501	ATP	C5'-O5'-PA-O3A
36	B	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O3A
34	F	501	ATP	O4'-C4'-C5'-O5'
34	F	501	ATP	C3'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
34	E	401	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	PG-O3B-PB-O1B
34	A	501	ATP	C5'-O5'-PA-O3A
36	C	501	ADP	C5'-O5'-PA-O2A
36	B	501	ADP	PA-O3A-PB-O2B
34	A	501	ATP	PG-O3B-PB-O1B
34	A	501	ATP	PG-O3B-PB-O2B
34	D	501	ATP	PG-O3B-PB-O2B
34	E	401	ATP	PA-O3A-PB-O2B

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	401	ATP	2	0

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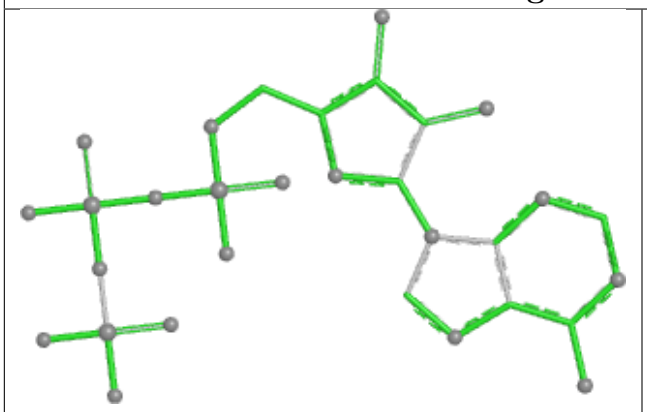
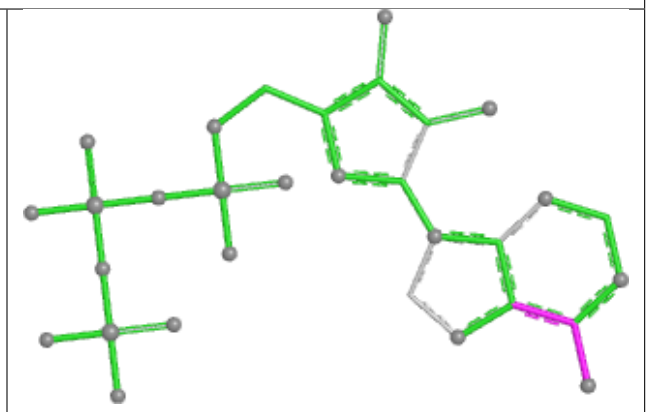
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	501	ATP	1	0
34	D	501	ATP	1	0
36	B	501	ADP	2	0
34	F	501	ATP	2	0

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

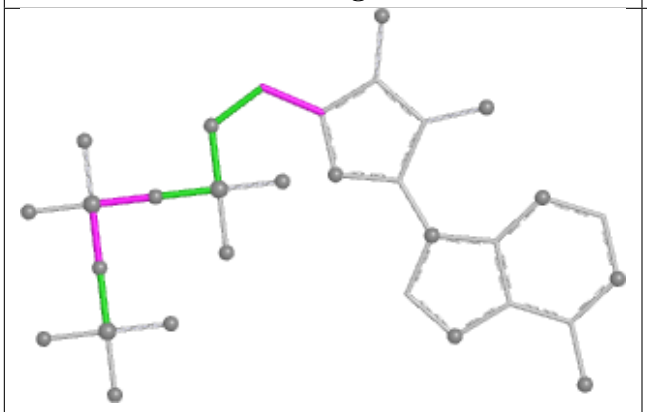
Ligand ATP E 401



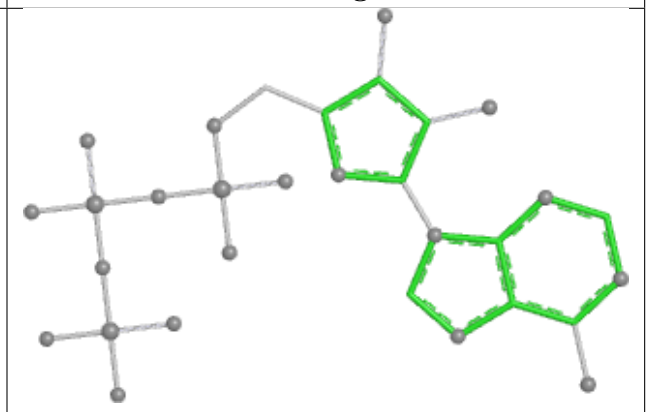
Bond lengths



Bond angles

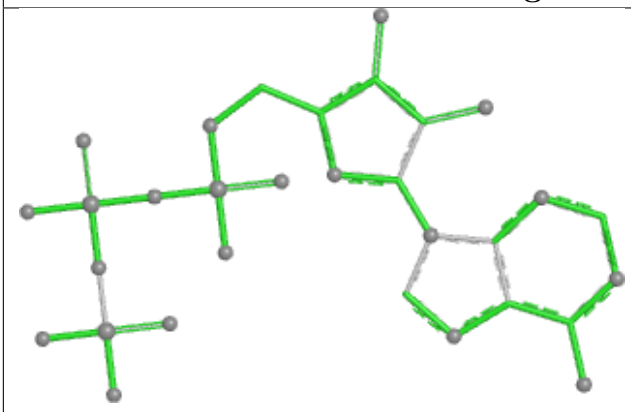


Torsions

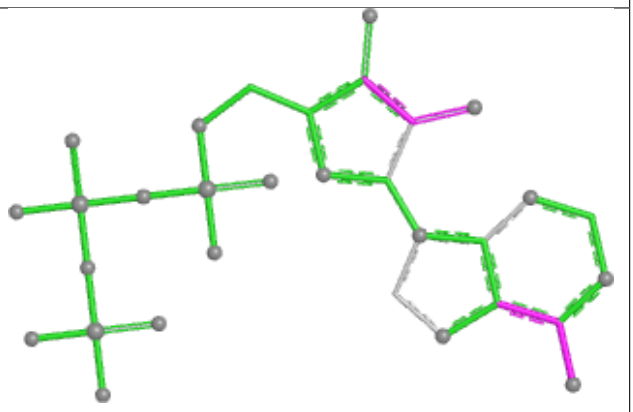


Rings

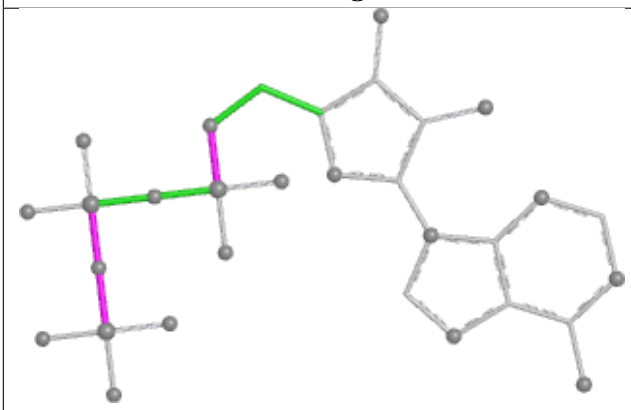
Ligand ATP A 501



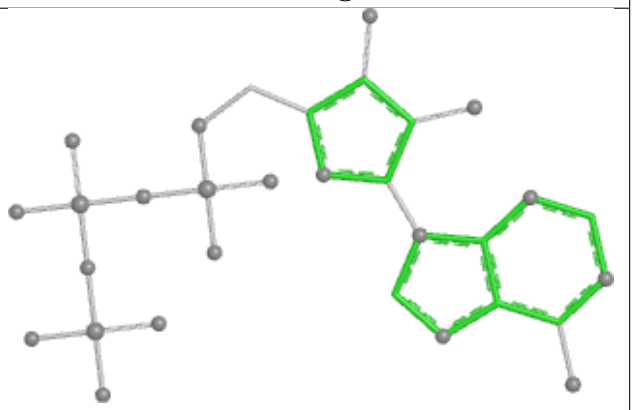
Bond lengths



Bond angles

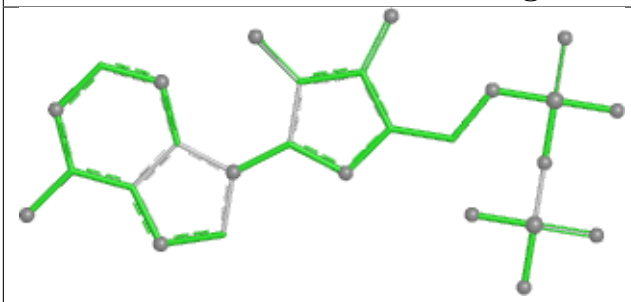


Torsions

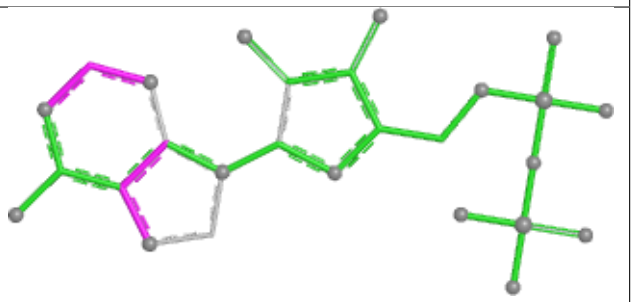


Rings

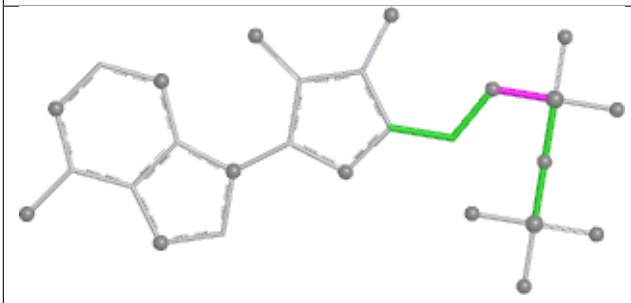
Ligand ADP C 501



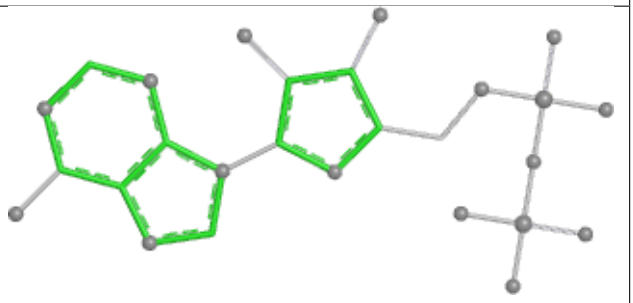
Bond lengths



Bond angles

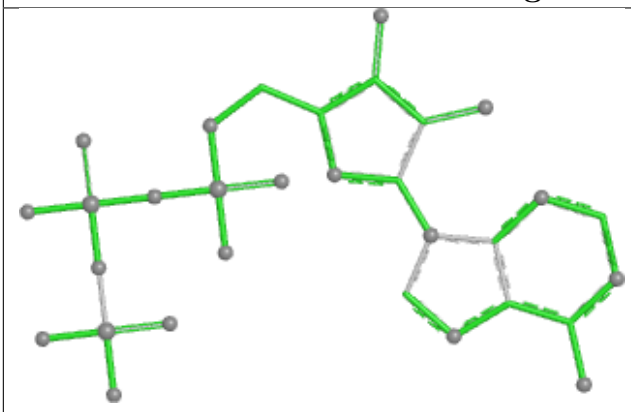


Torsions

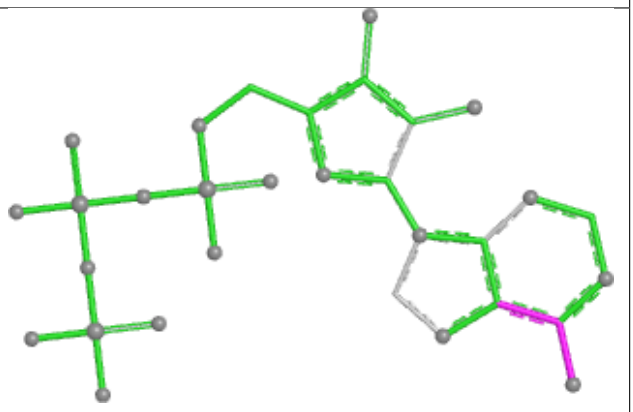


Rings

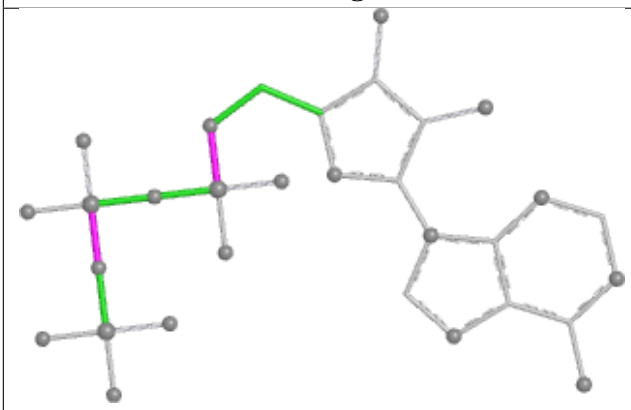
Ligand ATP D 501



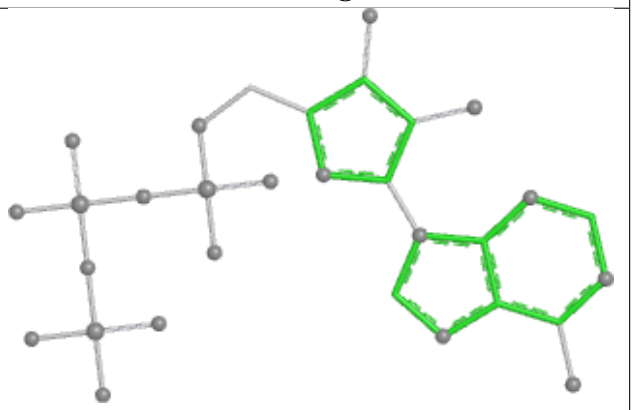
Bond lengths



Bond angles

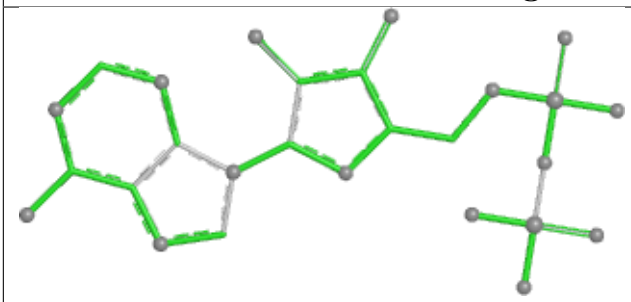


Torsions

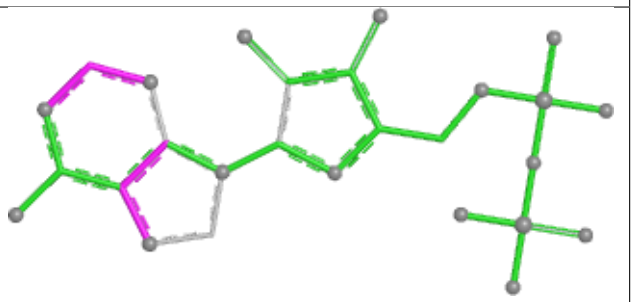


Rings

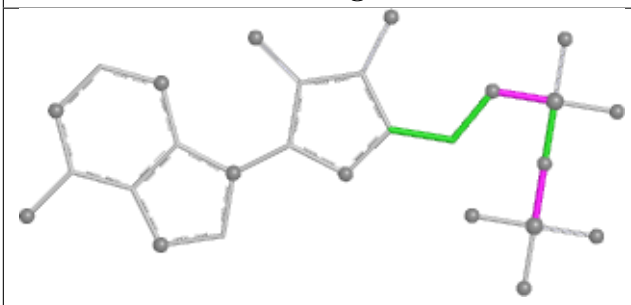
Ligand ADP B 501



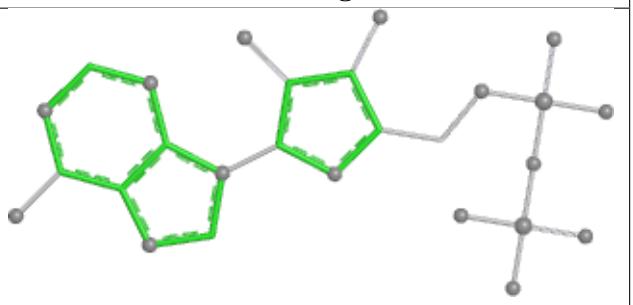
Bond lengths



Bond angles

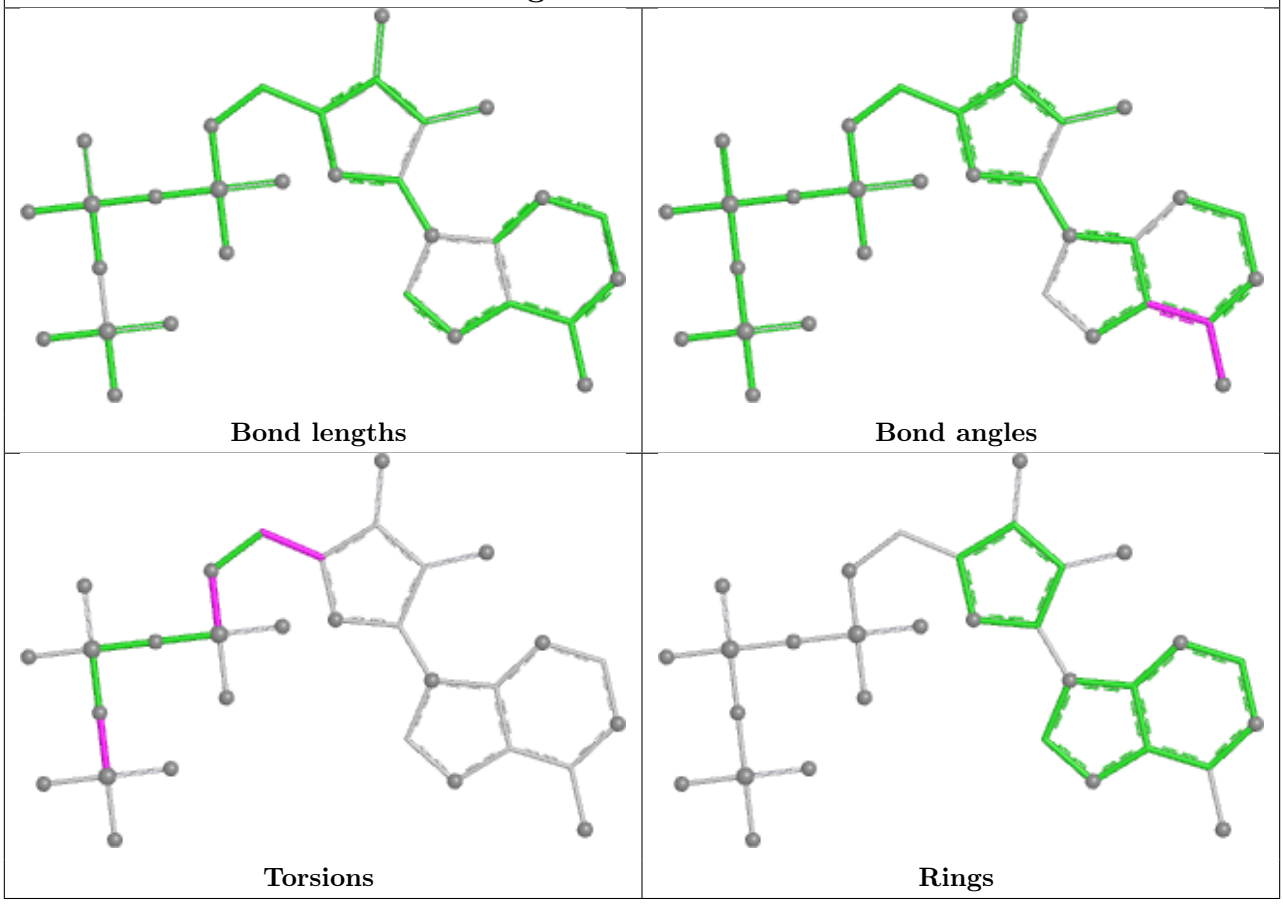


Torsions



Rings

Ligand ATP F 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

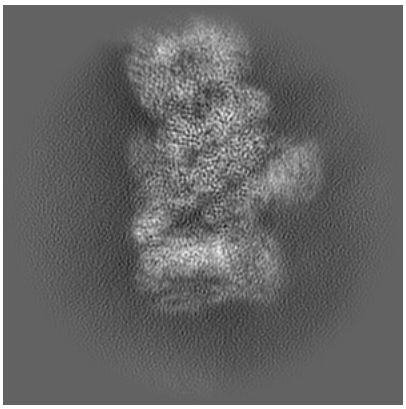
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44930. These allow visual inspection of the internal detail of the map and identification of artifacts.

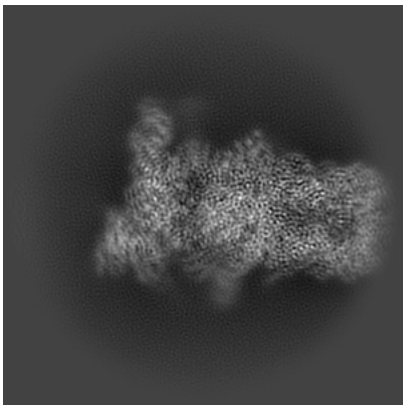
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

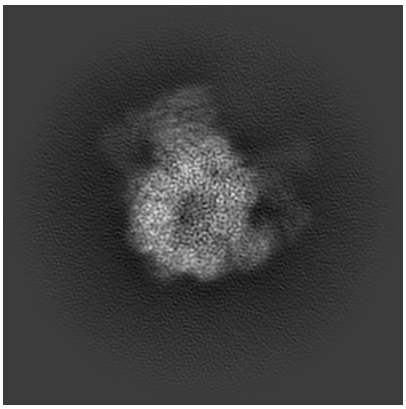
6.1.1 Primary map



X

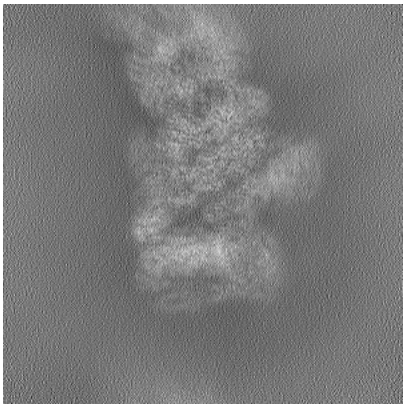


Y

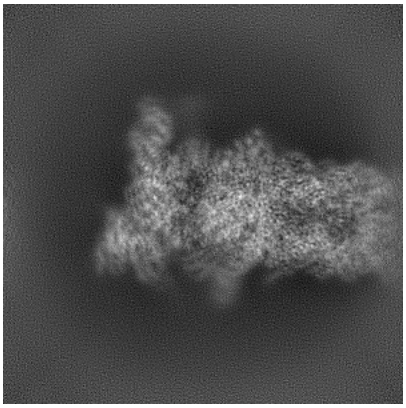


Z

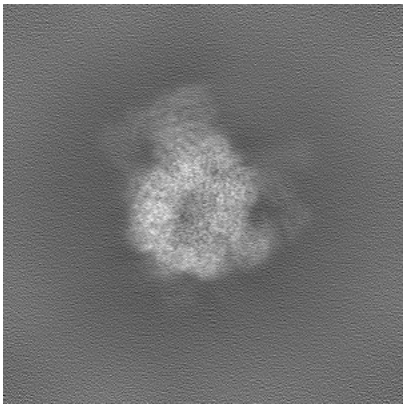
6.1.2 Raw map



X



Y

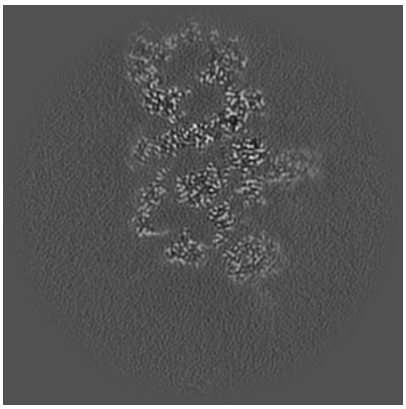


Z

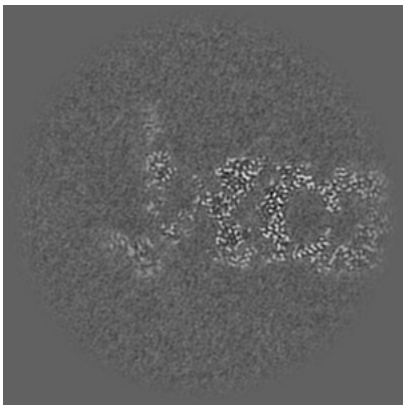
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



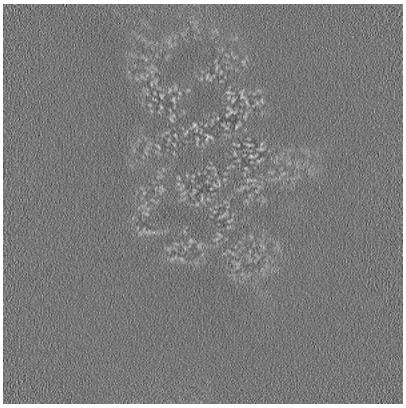
X Index: 220



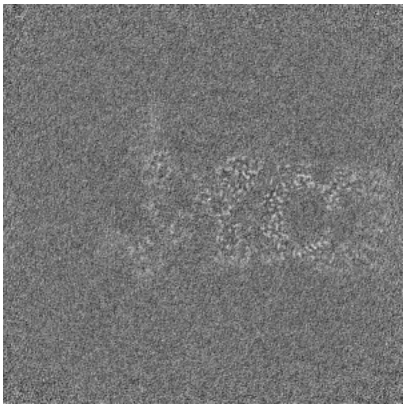
Y Index: 220

Z Index: 220

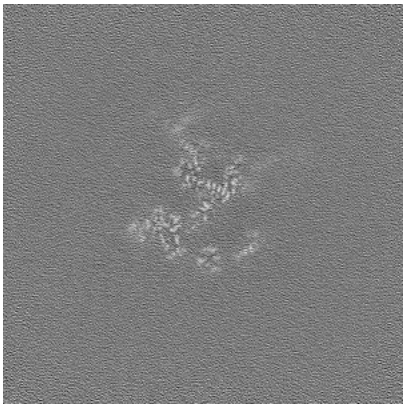
6.2.2 Raw map



X Index: 220



Y Index: 220

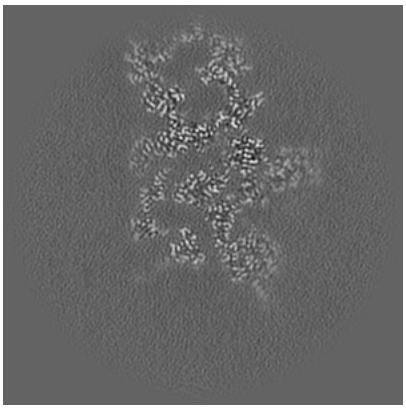


Z Index: 220

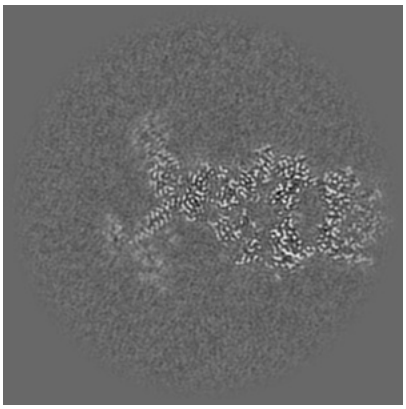
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

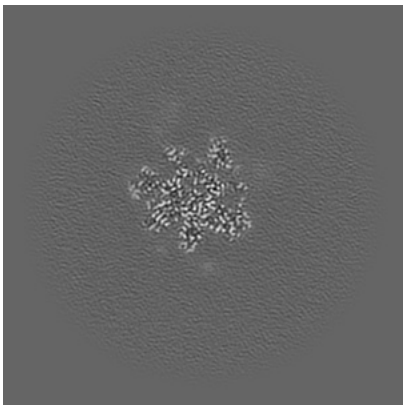
6.3.1 Primary map



X Index: 217

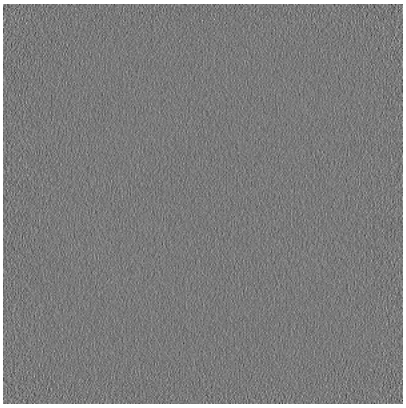


Y Index: 237

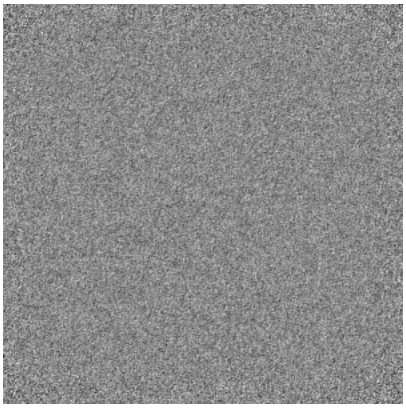


Z Index: 303

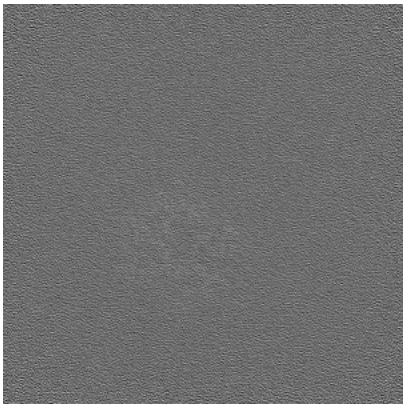
6.3.2 Raw map



X Index: 0



Y Index: 0

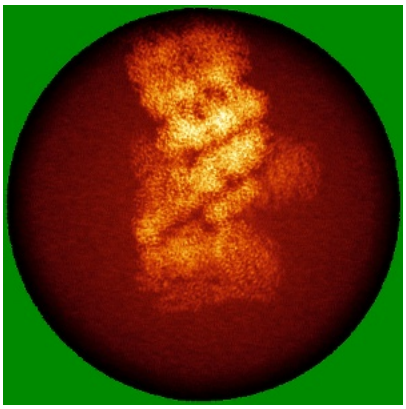


Z Index: 0

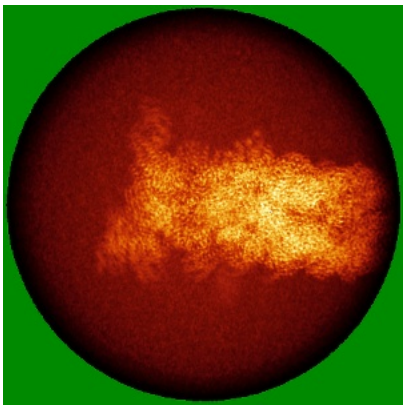
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

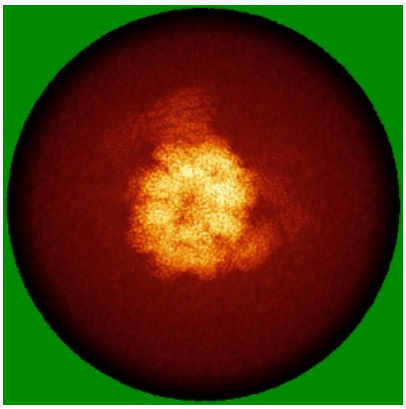
6.4.1 Primary map



X

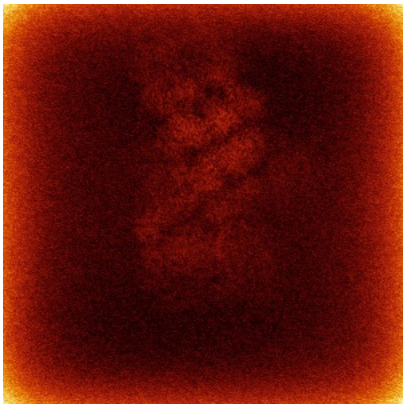


Y

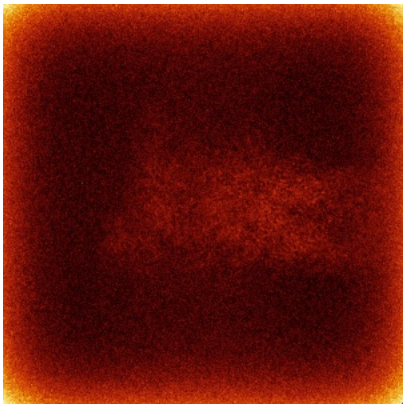


Z

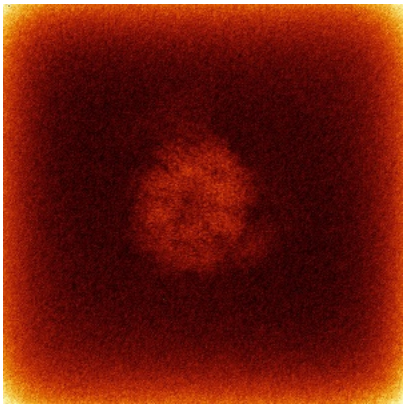
6.4.2 Raw map



X



Y

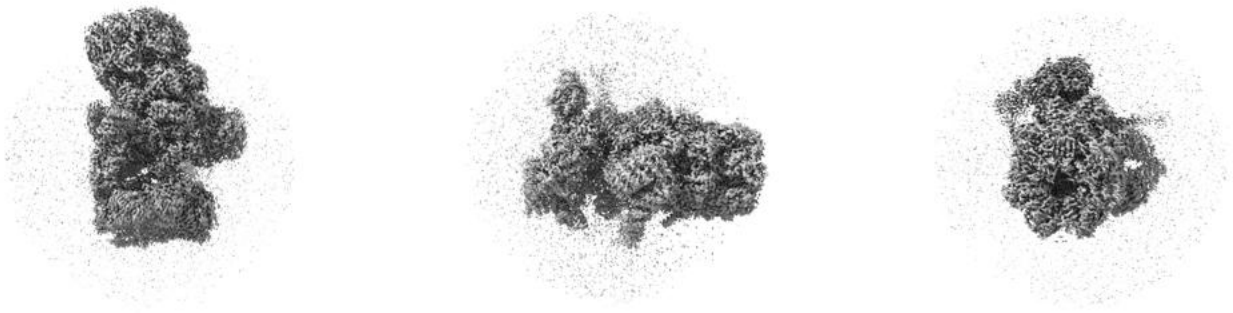


Z

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

6.5 Orthogonal surface views (i)

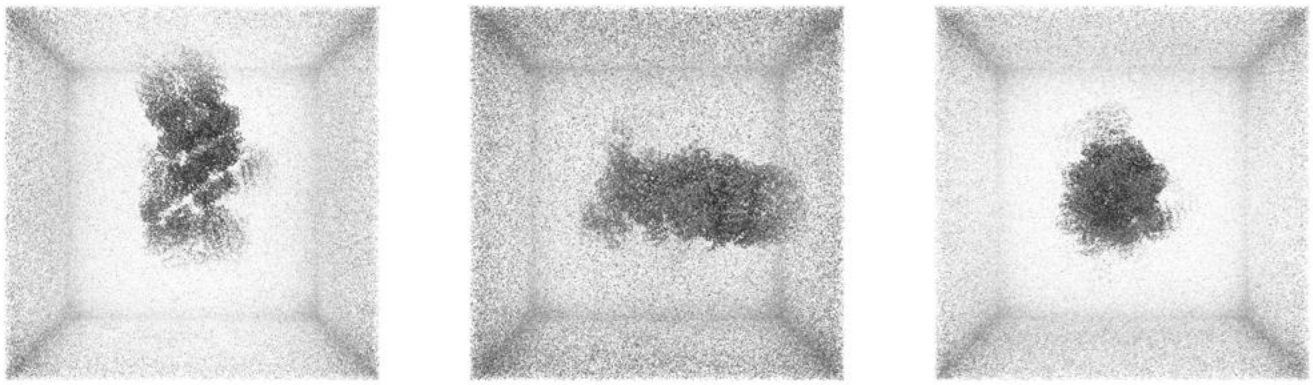
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

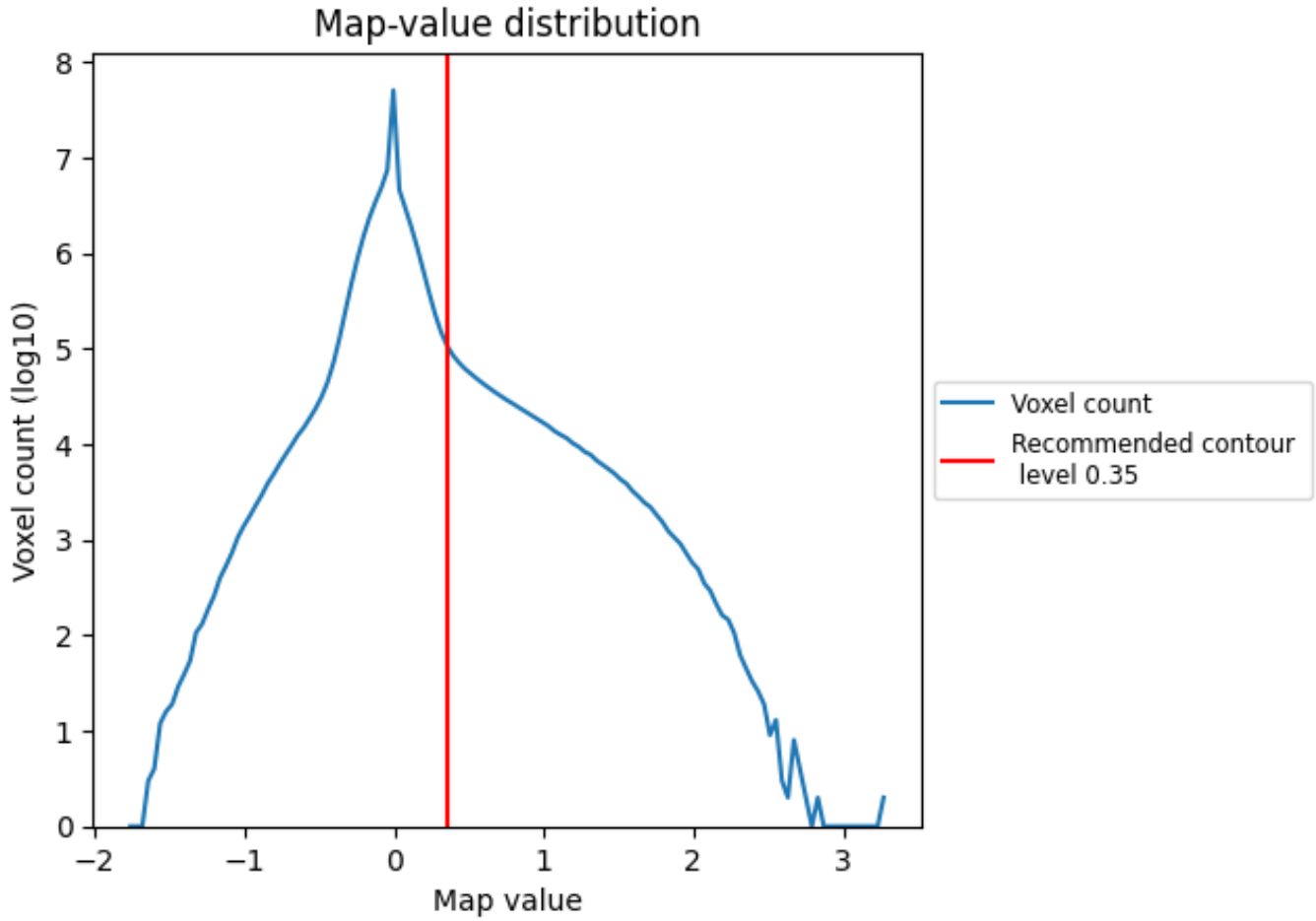
6.6 Mask visualisation (i)

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

7 Map analysis

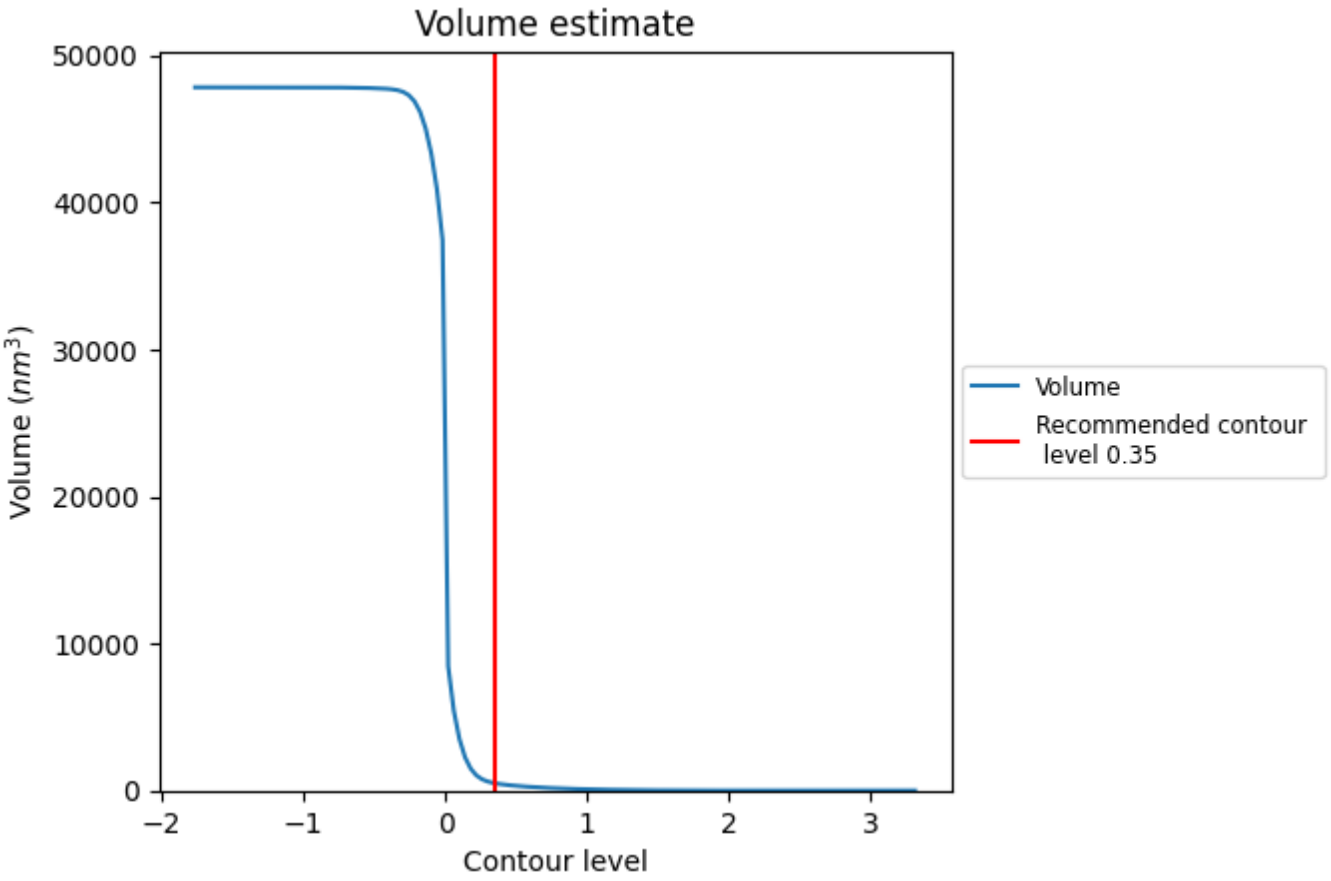
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

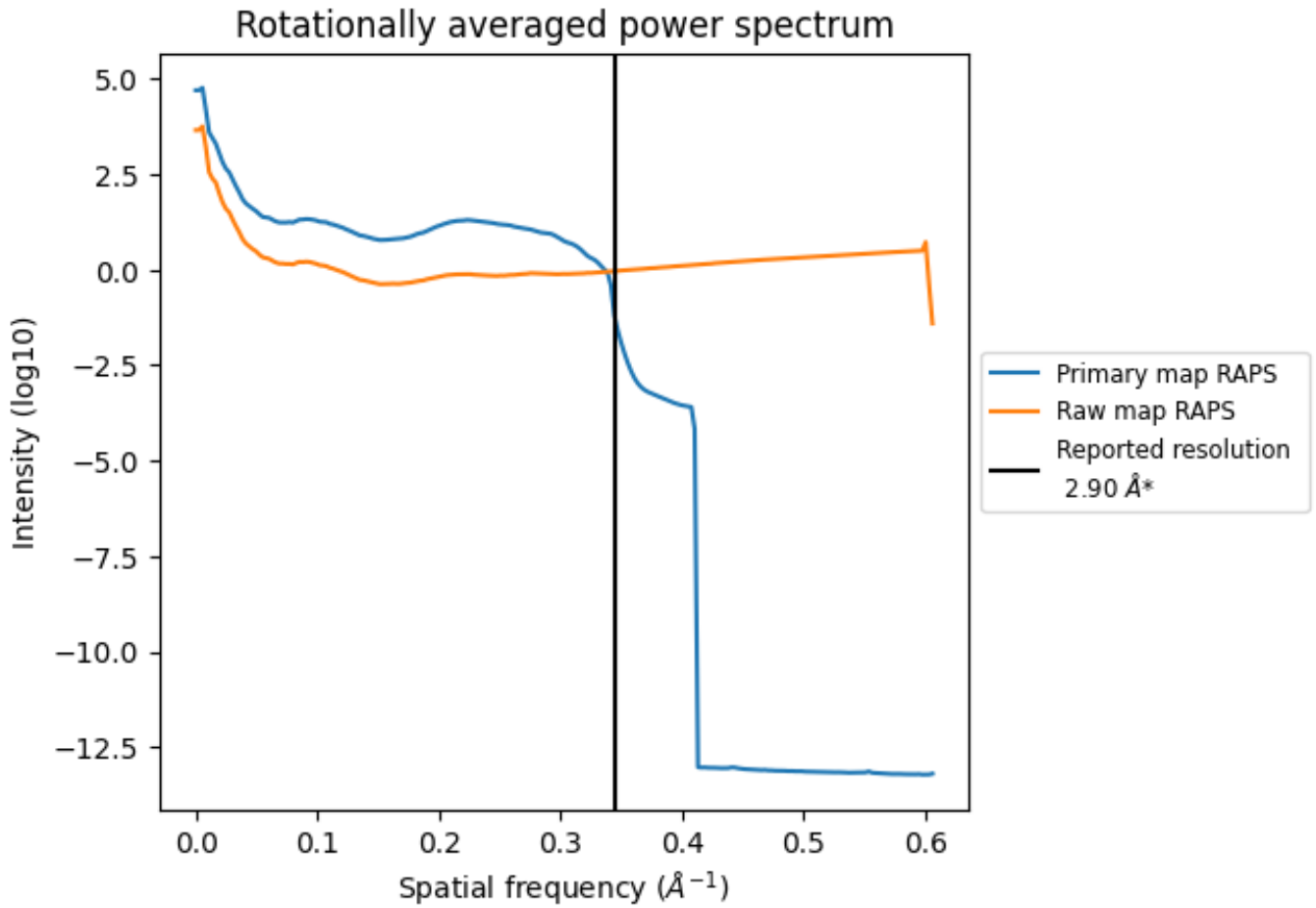
7.2 Volume estimate



The volume at the recommended contour level is 501 nm^3; this corresponds to an approximate mass of 452 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 (i)

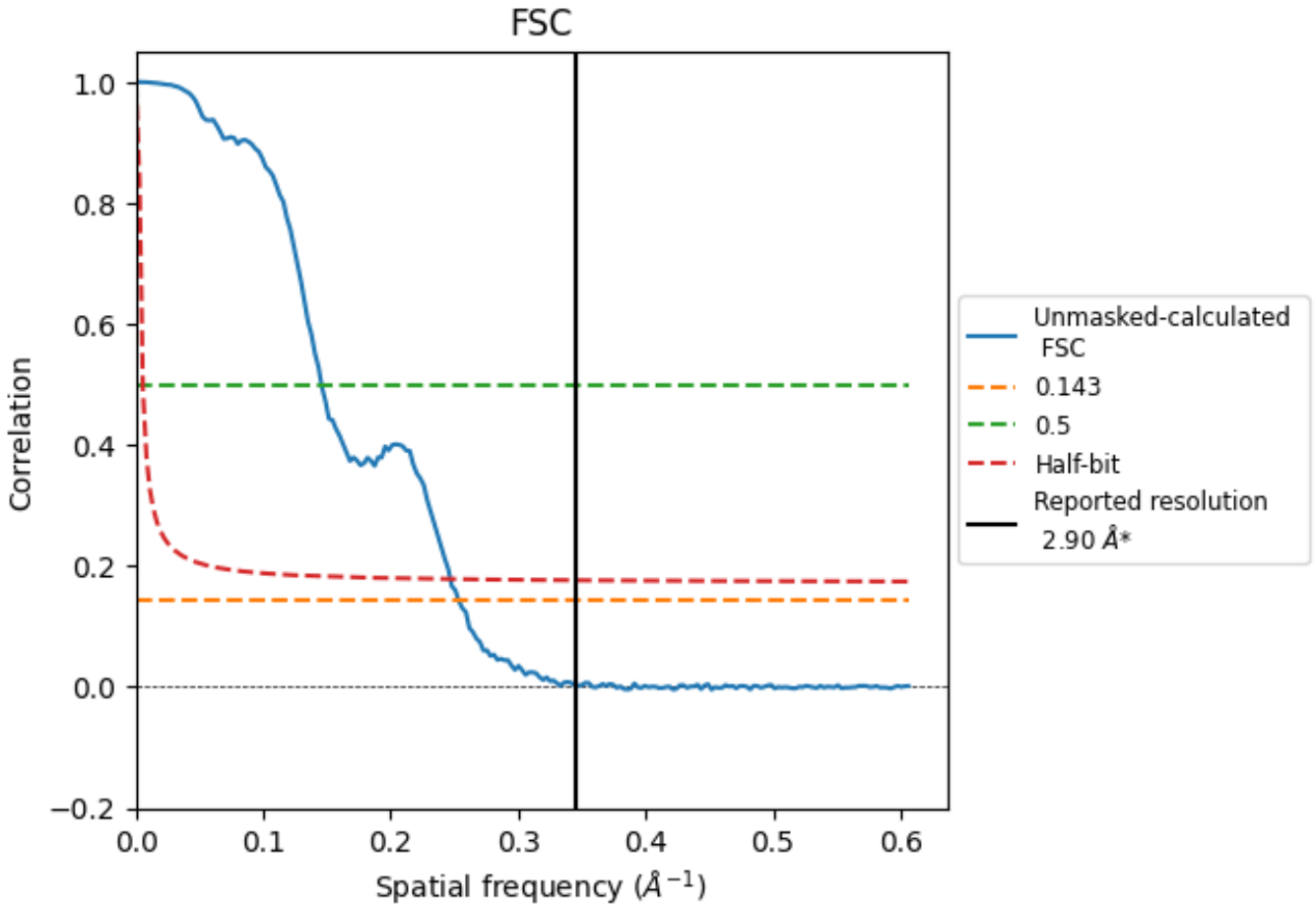


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

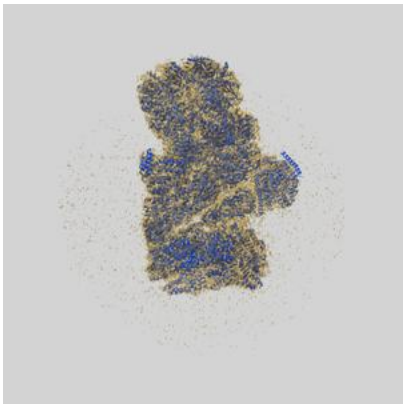
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	6.87	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.9 by more than 10 %

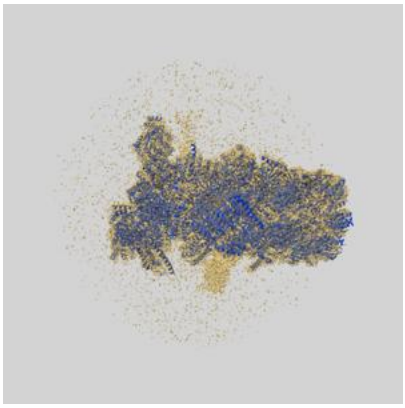
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44930 and PDB model 9BV3. Per-residue inclusion information can be found in section 3 on page 15.

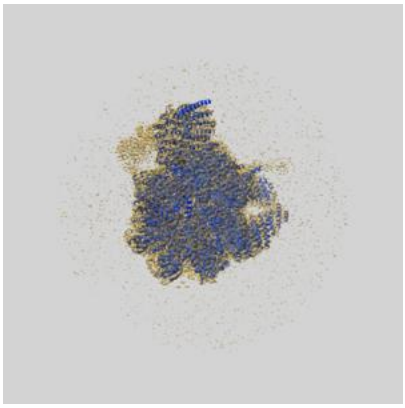
9.1 Map-model overlay



X



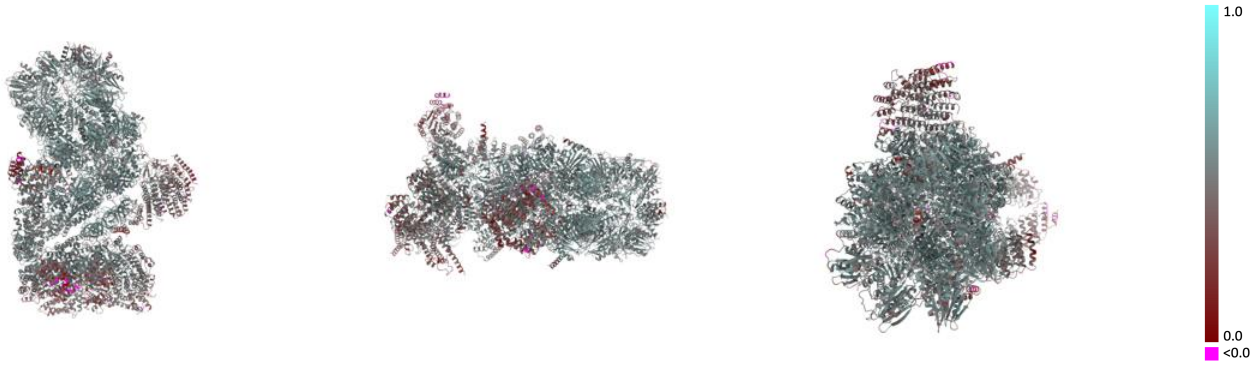
Y



Z

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

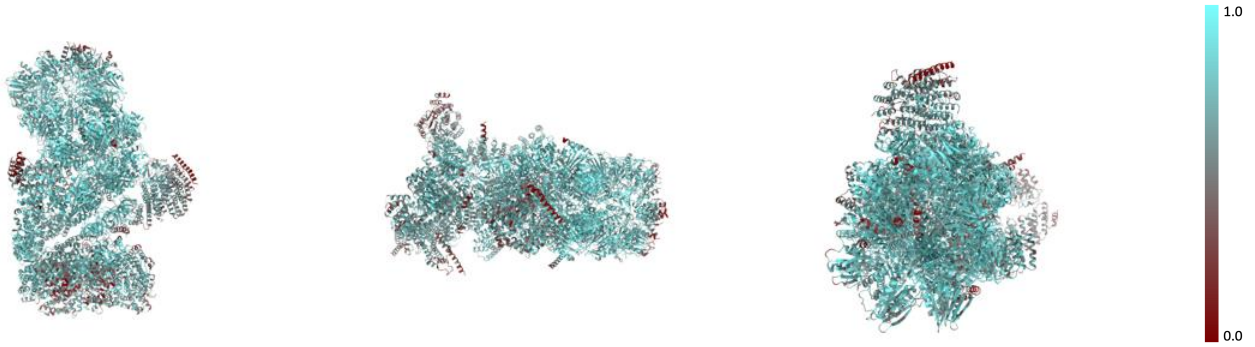
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

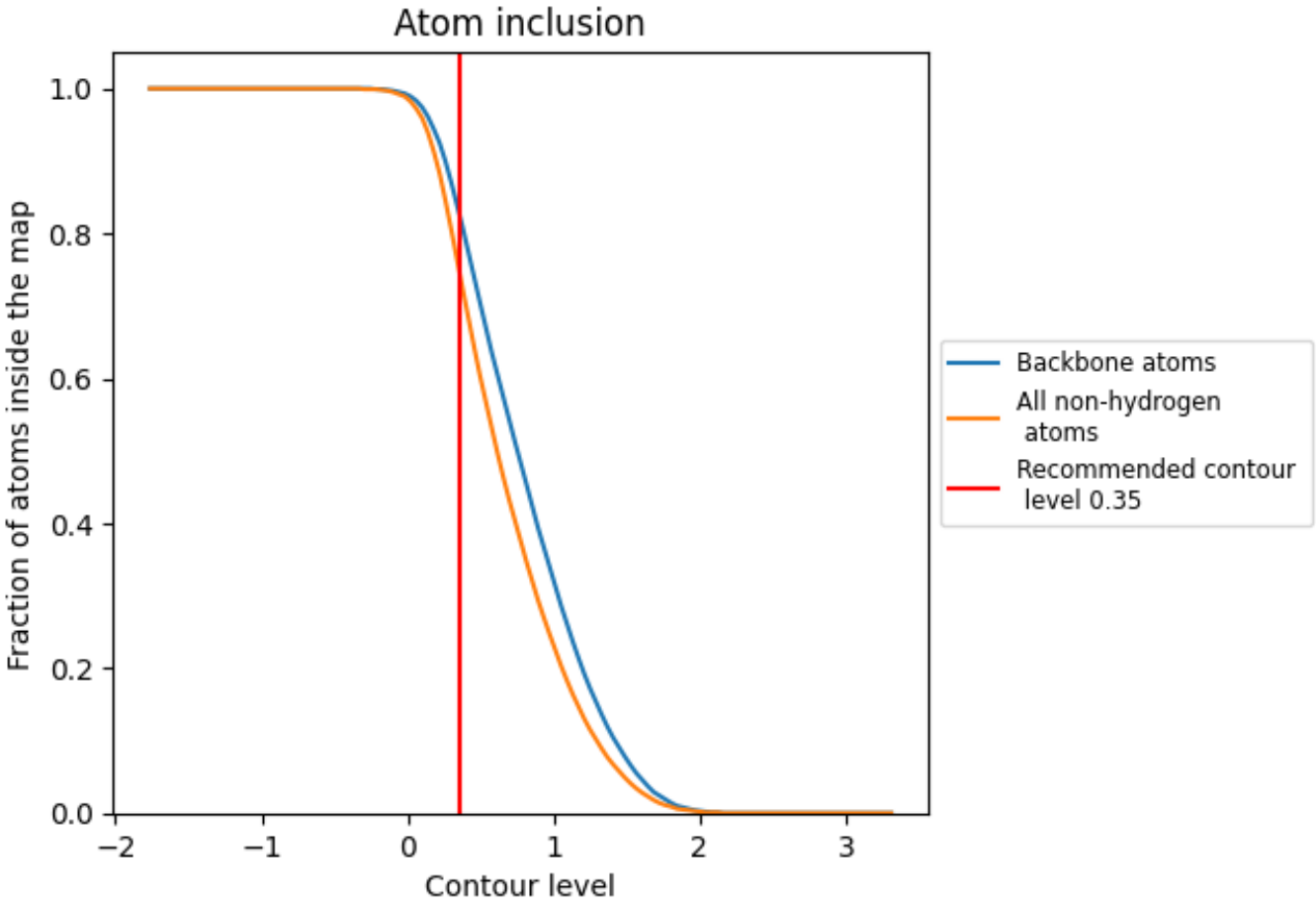
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4970
A	0.8130	0.5260
B	0.7640	0.5050
C	0.8230	0.5450
D	0.8080	0.5330
E	0.8290	0.5460
F	0.8230	0.5360
G	0.8560	0.5510
H	0.8750	0.5660
I	0.8210	0.5410
J	0.8250	0.5360
K	0.8710	0.5590
L	0.8830	0.5660
M	0.8350	0.5480
N	0.8680	0.5580
O	0.8330	0.5390
P	0.8600	0.5490
Q	0.8640	0.5550
R	0.8530	0.5510
S	0.8380	0.5440
T	0.8440	0.5430
U	0.6860	0.4430
V	0.6420	0.4250
W	0.7400	0.4810
X	0.6610	0.4590
Y	0.8190	0.5260
Z	0.7480	0.5130
a	0.6290	0.4040
b	0.4580	0.3570
c	0.7720	0.5200
d	0.6150	0.4020
e	0.6710	0.4790
f	0.5930	0.3810
n	0.7530	0.5130
o	0.6710	0.4850

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Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.5890	0.4800
q	0.6330	0.5060
r	0.7390	0.4920
s	0.7580	0.5050
t	0.7650	0.5180
y	0.0470	0.2240