



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:29 AM UTC

PDB ID : 5M32 / pdb_00005m32
EMDB ID : EMD-4146
Title : Human 26S proteasome in complex with Oprozomib
Authors : Haselbach, D.; Schrader, J.; Lambrecht, F.; Henneberg, F.; Chari, A.; Stark, H.
Deposited on : 2016-10-14
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

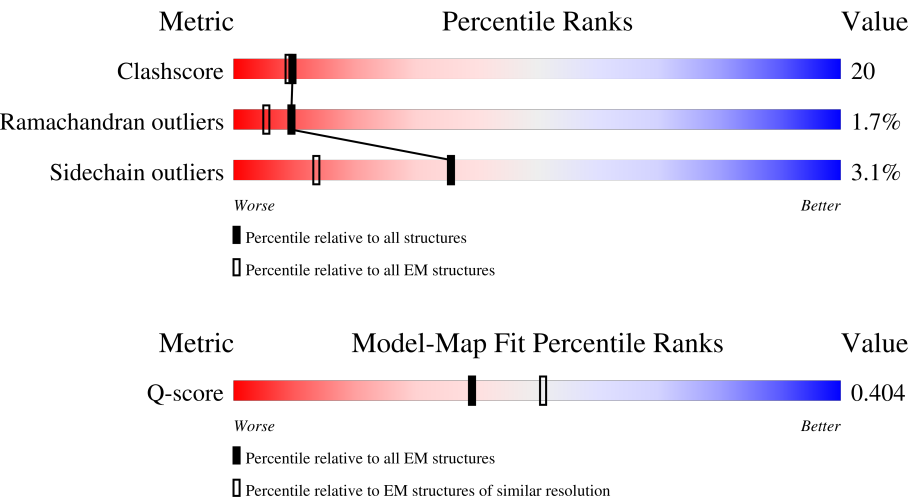
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



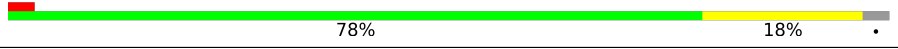
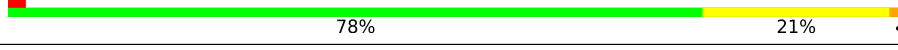
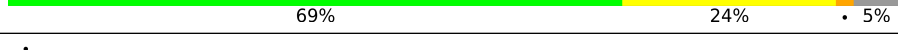
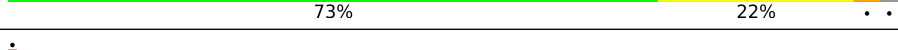
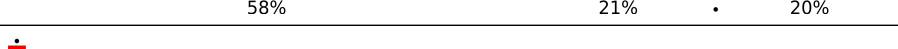
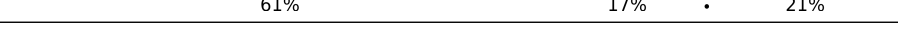
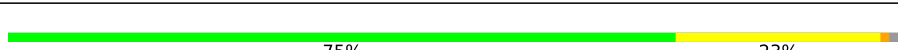
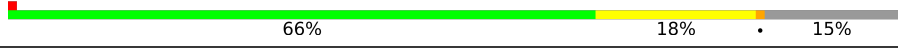
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	234	74%24%..
1	O	234	76%22%.
2	B	261	69%18%.10%
2	P	261	5% 71%19%..7%

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Mol	Chain	Length	Quality of chain
3	C	234	
4	D	241	
4	R	241	
5	E	234	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	196	
10	X	196	
11	K	204	
11	Y	204	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	Q	235	
16	S	238	
17	c	433	

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Mol	Chain	Length	Quality of chain
18	d	428	
19	e	418	
20	f	379	
21	g	439	
22	h	355	
23	i	953	
24	j	534	
25	k	456	
26	l	422	
27	m	389	
28	n	324	
29	o	376	
30	p	377	
31	q	310	
32	r	350	
33	s	70	
34	t	4	
34	u	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	6V9	t	1	-	X	-	-
34	6V9	u	1	-	X	-	-
35	ADP	d	501	-	-	X	-
35	ADP	e	501	-	-	X	-
35	ADP	g	501	-	-	X	-
35	ADP	h	401	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 76085 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1763	1132	297	328	6		
1	O	230	Total	C	N	O	S	0	0
			1764	1126	301	331	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1836	1164	315	348	9		
2	P	244	Total	C	N	O	S	0	0
			1875	1187	323	355	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	234	Total	C	N	O	S	0	0
			1771	1107	315	344	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	LYS	conflict	UNP O14818
C	179	ASP	GLU	conflict	UNP O14818
C	200	GLU	GLN	conflict	UNP O14818

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total	C	N	O	S	0	0
			1757	1103	290	353	11		
4	R	233	Total	C	N	O	S	0	0
			1768	1112	294	351	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	234	Total	C	N	O	S	0	0
			1805	1133	321	340	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	185	ASP	ASN	conflict	UNP P25786
E	234	ASP	GLU	conflict	UNP P25786

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	232	Total	C	N	O	S	0	0
			1818	1153	310	344	11		
6	T	240	Total	C	N	O	S	0	0
			1877	1190	320	356	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1806	1147	301	345	13		
7	U	241	Total	C	N	O	S	0	0
			1841	1168	308	352	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	221	Total	C	N	O	S	0	0
			1663	1047	283	321	12		
8	V	220	Total	C	N	O	S	1	0
			1627	1025	273	318	11		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1590	1013	265	293	19		
9	W	204	Total	C	N	O	S	0	0
			1586	1010	263	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1560	1001	266	284	9		
10	X	196	Total	C	N	O	S	0	0
			1563	1002	267	285	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	182	VAL	ILE	conflict	UNP P49721
J	186	ASP	ASN	conflict	UNP P49721
J	190	ASN	ASP	conflict	UNP P49721
J	192	GLU	ASP	conflict	UNP P49721
J	195	ALA	SER	conflict	UNP P49721
X	182	VAL	ILE	conflict	UNP P49721
X	186	ASP	ASN	conflict	UNP P49721
X	190	ASN	ASP	conflict	UNP P49721
X	192	GLU	ASP	conflict	UNP P49721
X	195	ALA	SER	conflict	UNP P49721

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	200	Total	C	N	O	S	0	0
			1545	974	269	293	9		
11	Y	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	1	0
			1637	1038	277	312	10		
12	Z	213	Total	C	N	O	S	0	0
			1642	1040	281	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	216	Total	C	N	O	S	0	0
			1679	1059	290	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1513	948	258	295	12		
14	b	203	Total	C	N	O	S	0	0
			1519	952	259	296	12		

- Molecule 15 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	235	Total	C	N	O	S	0	0
			1785	1118	318	344	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	ASP	GLU	conflict	UNP O14818

- Molecule 16 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	238	Total	C	N	O	S	0	0
			1834	1147	329	347	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	PHE	conflict	UNP P25786
S	3	ALA	ARG	conflict	UNP P25786
S	185	ASP	ASN	conflict	UNP P25786
S	234	ASP	GLU	conflict	UNP P25786

- Molecule 17 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	347	Total	C	N	O	S	0	0
			2728	1722	485	503	18		

- Molecule 18 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	333	Total	C	N	O	S	0	0
			2560	1614	433	501	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	361	Total	C	N	O	S	0	0
			2776	1752	488	525	11		

- Molecule 20 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	348	Total	C	N	O	S	0	0
			2692	1692	483	501	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	g	363	Total	C	N	O	S	0	0
			2777	1753	480	529	15		

- Molecule 22 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	332	Total	C	N	O	S	0	0
			2518	1589	447	466	16		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	i	230	Total	C	N	O	0	0
			1145	685	230	230		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	j	155	Total	C	N	O	0	0
			779	470	155	154		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	k	364	Total	C	N	O	0	0
			1819	1092	364	363		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	l	415	Total	C	N	O	S	0	0
			2572	1598	474	494	6		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	375	Total	C	N	O	S	0	0
			2421	1513	434	468	6		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	n	206	Total	C	N	O	0	0
			1030	618	206	206		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	75	Total	C	N	O	0	0
			377	227	75	75		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	101	Total	C	N	O	0	0
			504	303	101	100		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	q	259	Total	C	N	O	0	0
			1311	789	261	261		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	8	Total	C	N	O	0	0
			40	25	8	7		

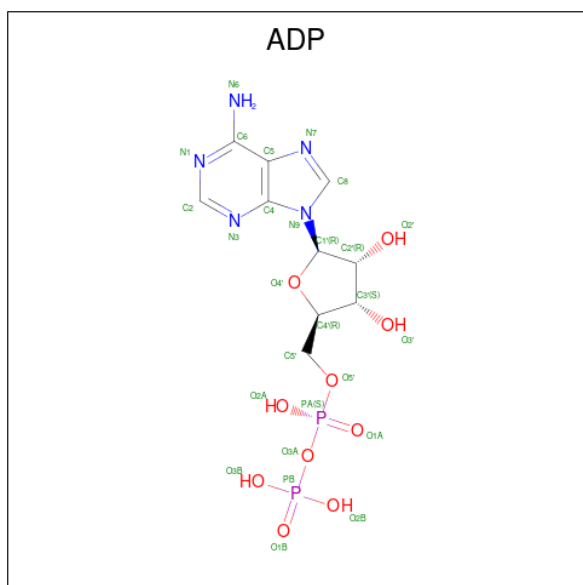
- Molecule 33 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	s	26	Total	C	N	O	0	0
			130	79	26	25		

- Molecule 34 is a protein called bound Oprozomib.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	t	4	Total	C	N	O	S	0	0
			37	25	4	7	1		
34	u	4	Total	C	N	O	S	0	0
			37	25	4	7	1		

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

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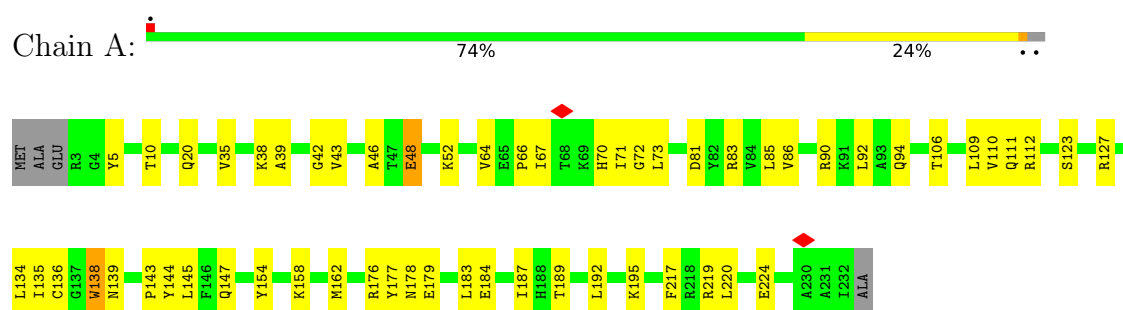
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Mol	Chain	Residues	Atoms					AltConf
35	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	g	1	Total	C	N	O	P	0
			27	10	5	10	2	
35	h	1	Total	C	N	O	P	0
			27	10	5	10	2	

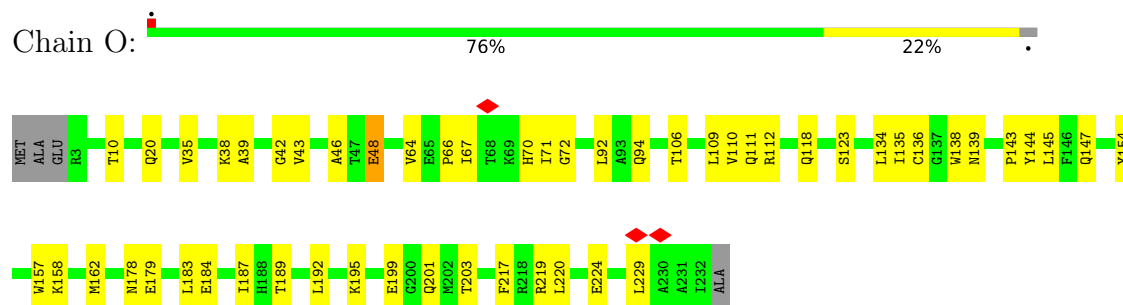
3 Residue-property plots

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

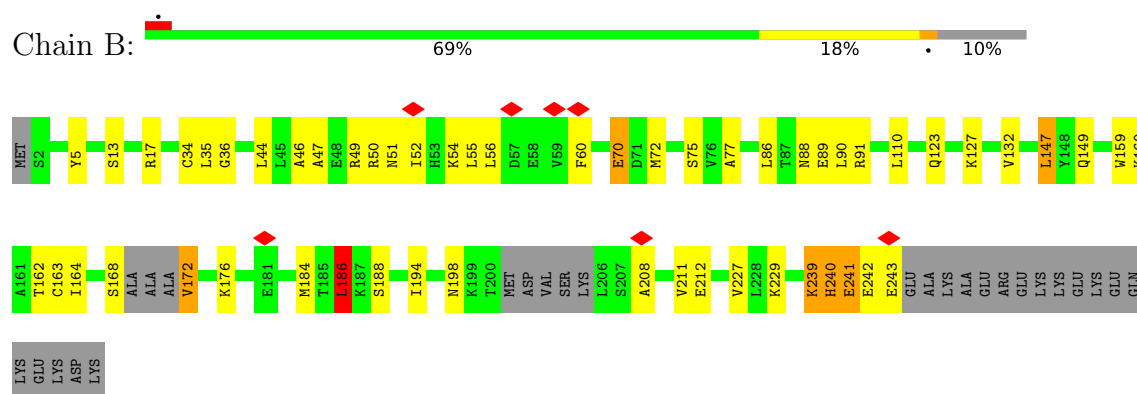
- Molecule 1: Proteasome subunit alpha type-2



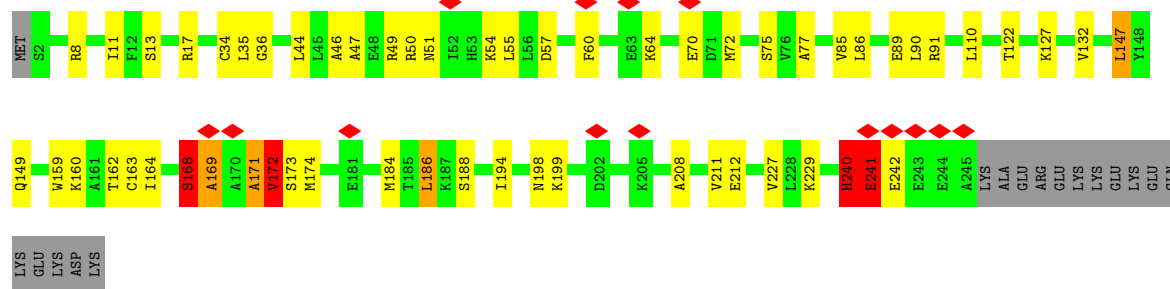
- Molecule 1: Proteasome subunit alpha type-2



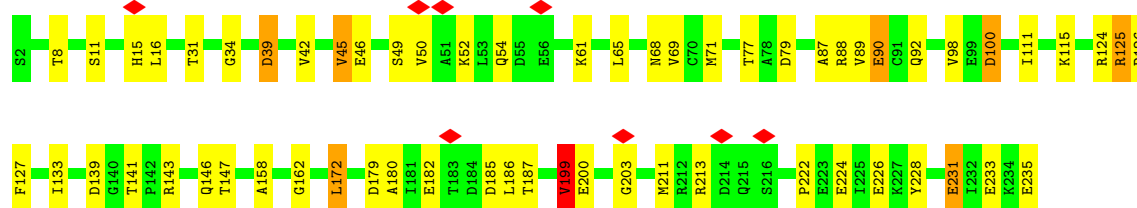
- Molecule 2: Proteasome subunit alpha type-4



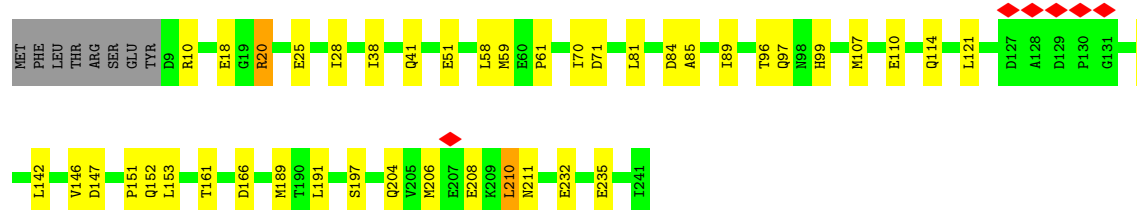
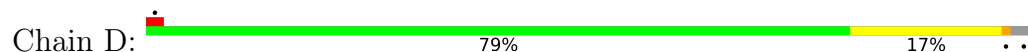
- Molecule 2: Proteasome subunit alpha type-4



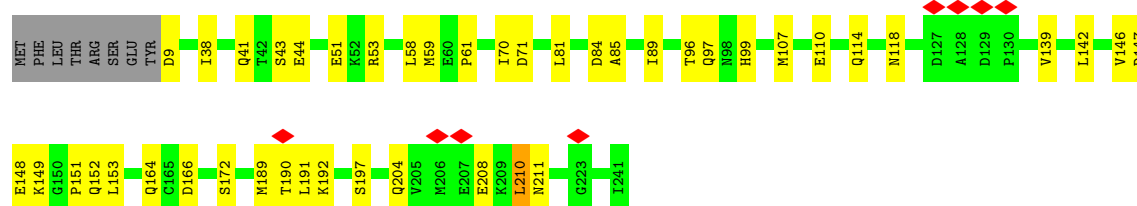
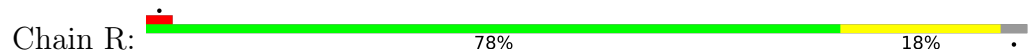
• Molecule 3: Proteasome subunit alpha type-7



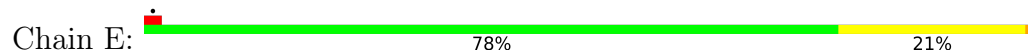
• Molecule 4: Proteasome subunit alpha type-5

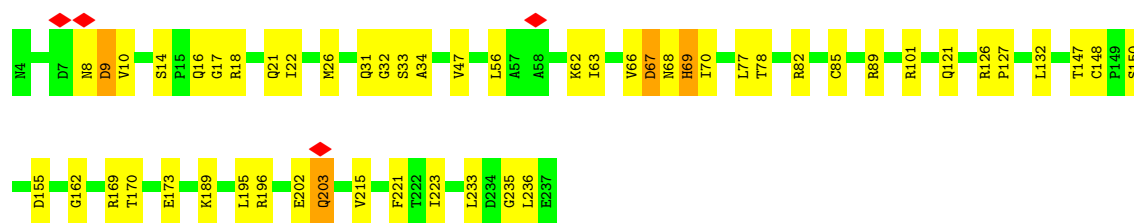


• Molecule 4: Proteasome subunit alpha type-5



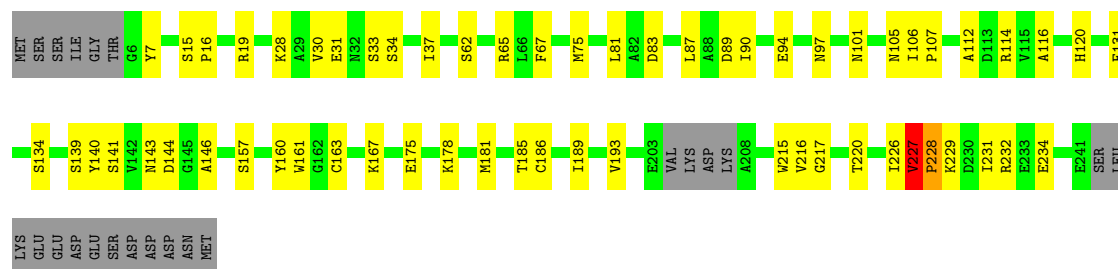
• Molecule 5: Proteasome subunit alpha type-1





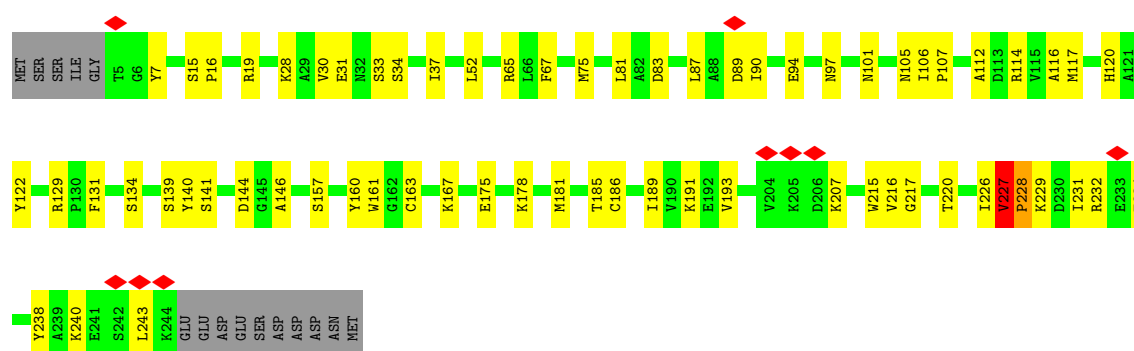
• Molecule 6: Proteasome subunit alpha type-3

Chain F: 67% 23% 9%



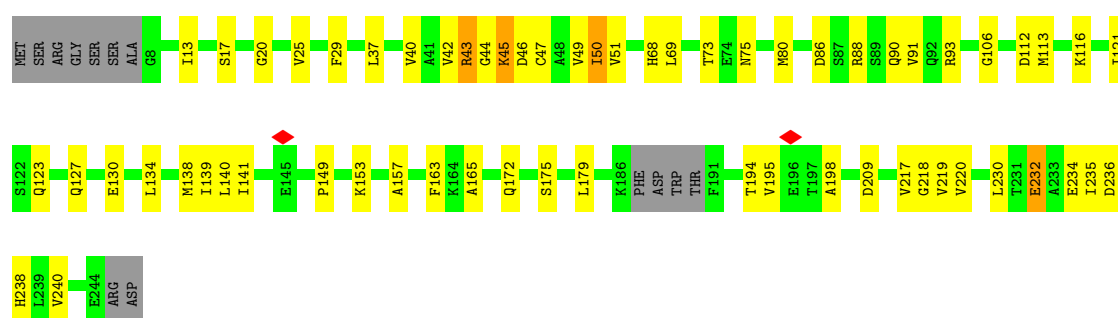
• Molecule 6: Proteasome subunit alpha type-3

Chain T: 68% 25% 6%



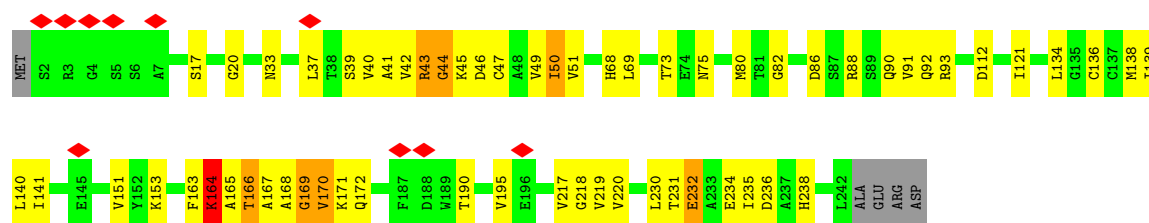
• Molecule 7: Proteasome subunit alpha type-6

Chain G: 69% 24% 5%



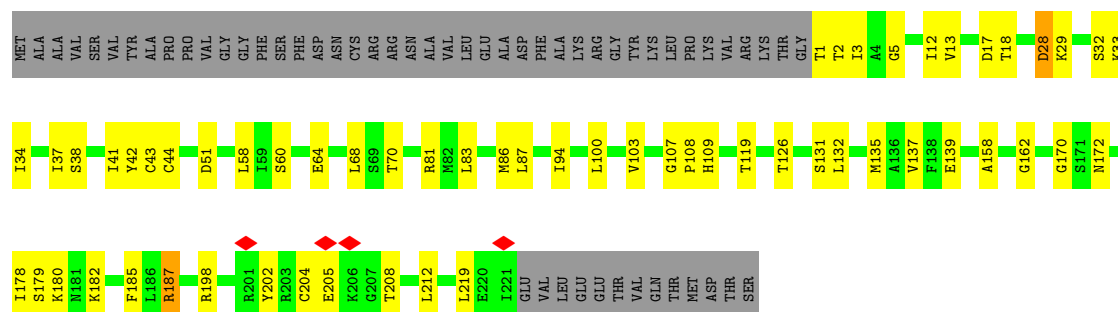
• Molecule 7: Proteasome subunit alpha type-6

Chain U: 



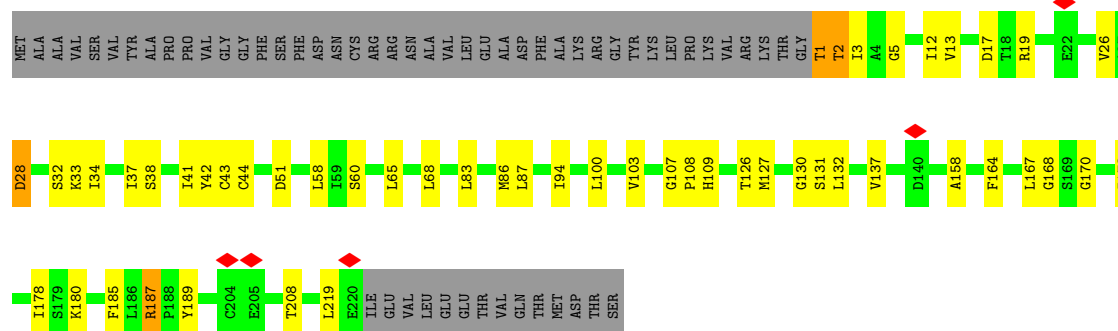
• Molecule 8: Proteasome subunit beta type-7

Chain H: 



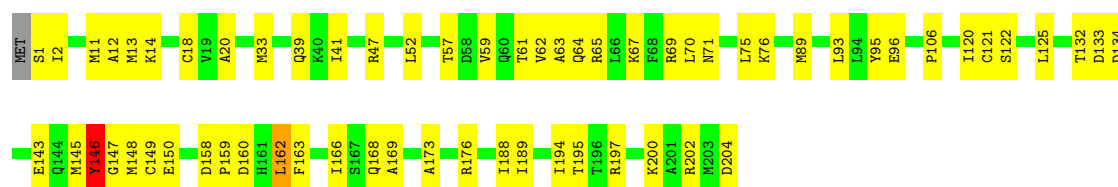
• Molecule 8: Proteasome subunit beta type-7

Chain V: 



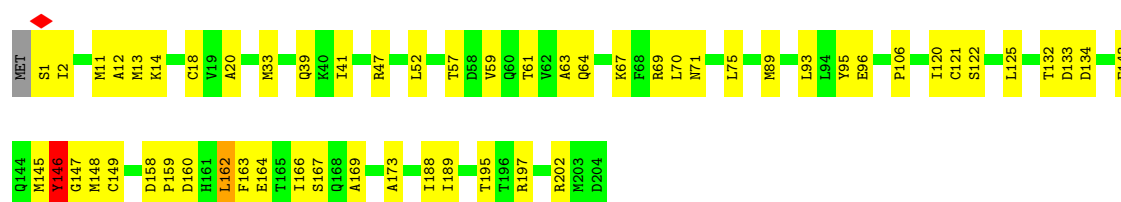
• Molecule 9: Proteasome subunit beta type-3

Chain I: 



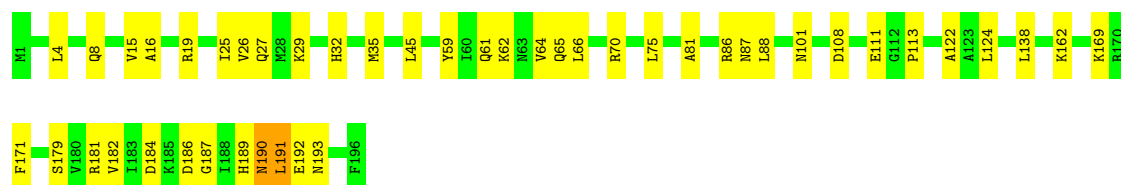
• Molecule 9: Proteasome subunit beta type-3

Chain W:  72% 26%



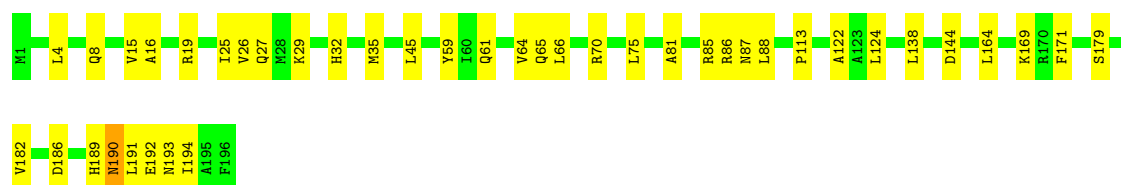
- Molecule 10: Proteasome subunit beta type-2

Chain J:  77% 22%



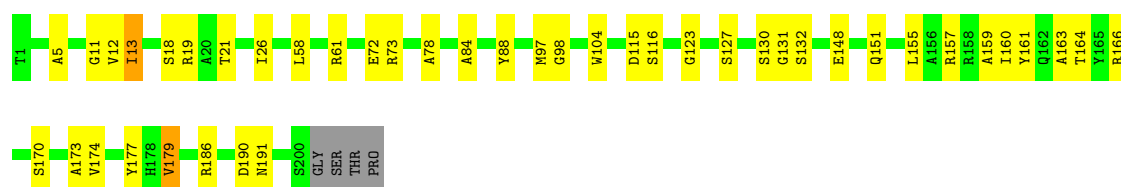
- Molecule 10: Proteasome subunit beta type-2

Chain X:  79% 20%



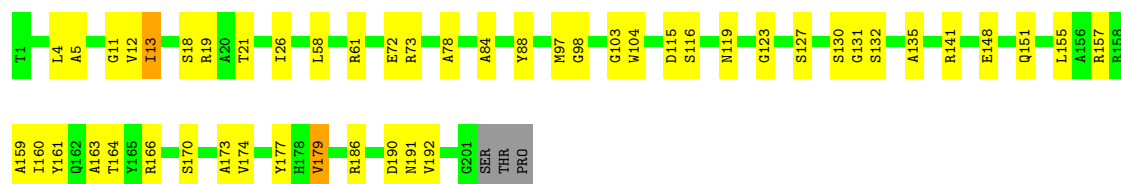
- Molecule 11: Proteasome subunit beta type-5

Chain K:  77% 20%



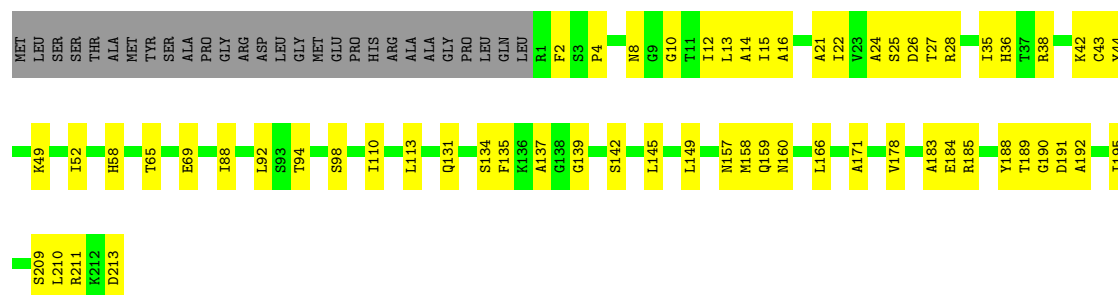
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  75% 23%



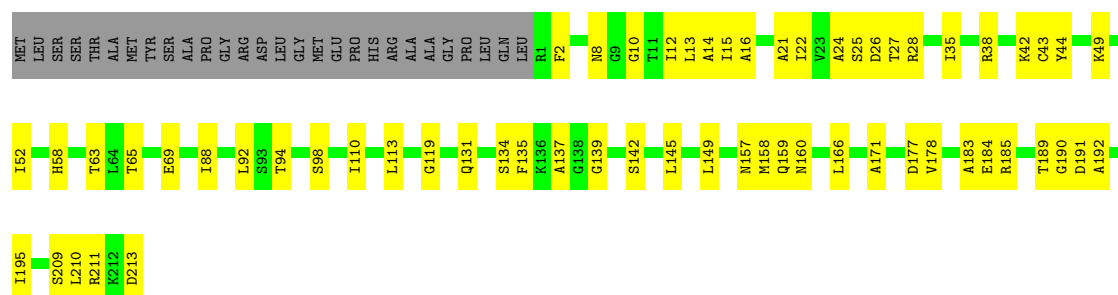
- Molecule 12: Proteasome subunit beta type-1

Chain L: 



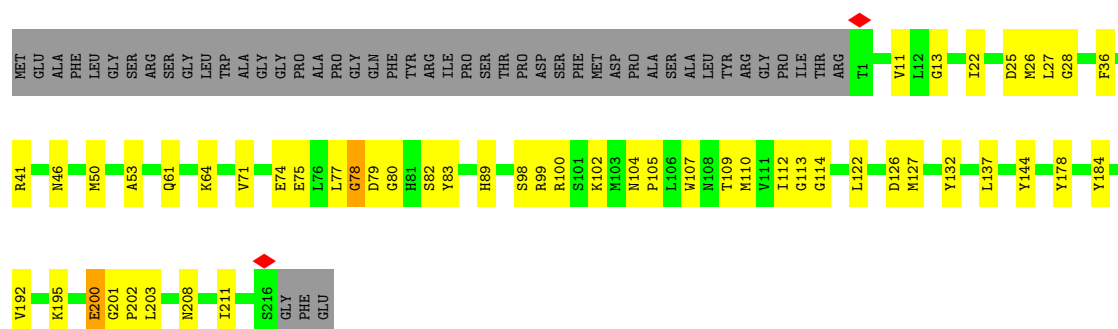
- Molecule 12: Proteasome subunit beta type-1

Chain Z: 



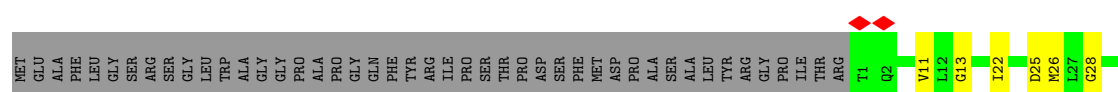
- Molecule 13: Proteasome subunit beta type-4

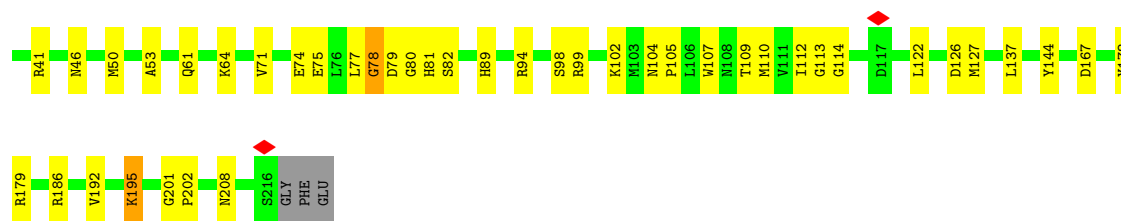
Chain M: 



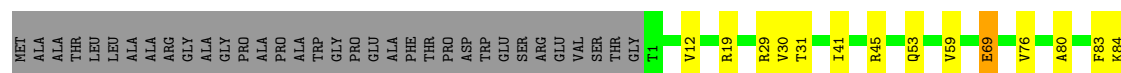
- Molecule 13: Proteasome subunit beta type-4

Chain a: 

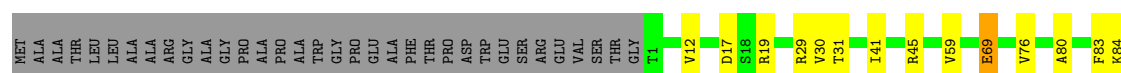




• Molecule 14: Proteasome subunit beta type-6



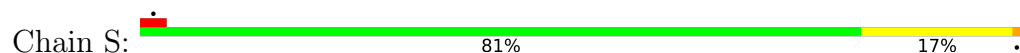
• Molecule 14: Proteasome subunit beta type-6

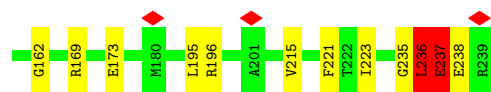


• Molecule 15: Proteasome subunit alpha type-7

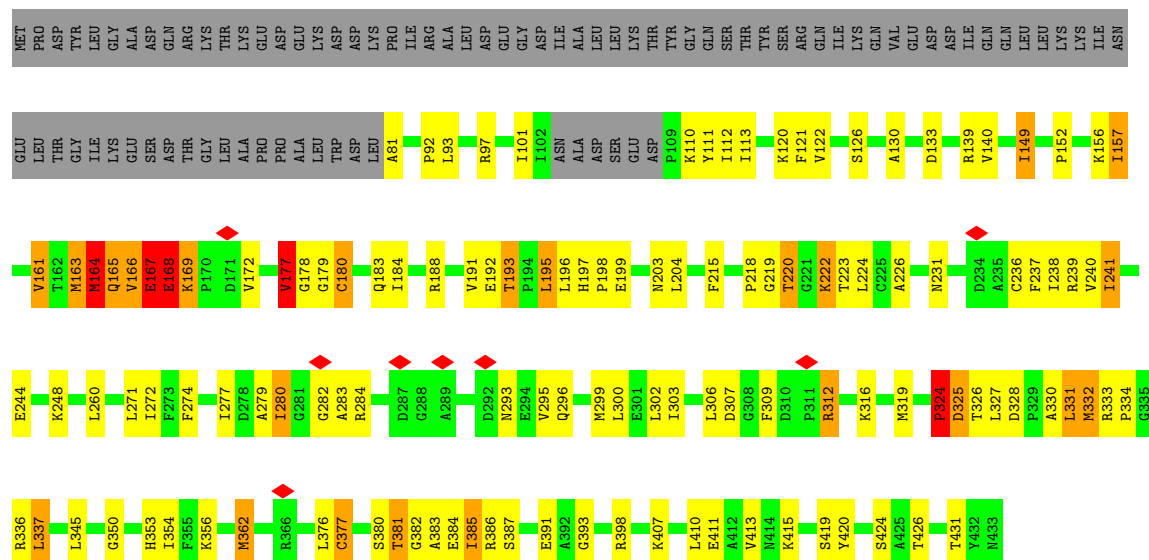


• Molecule 16: Proteasome subunit alpha type-1

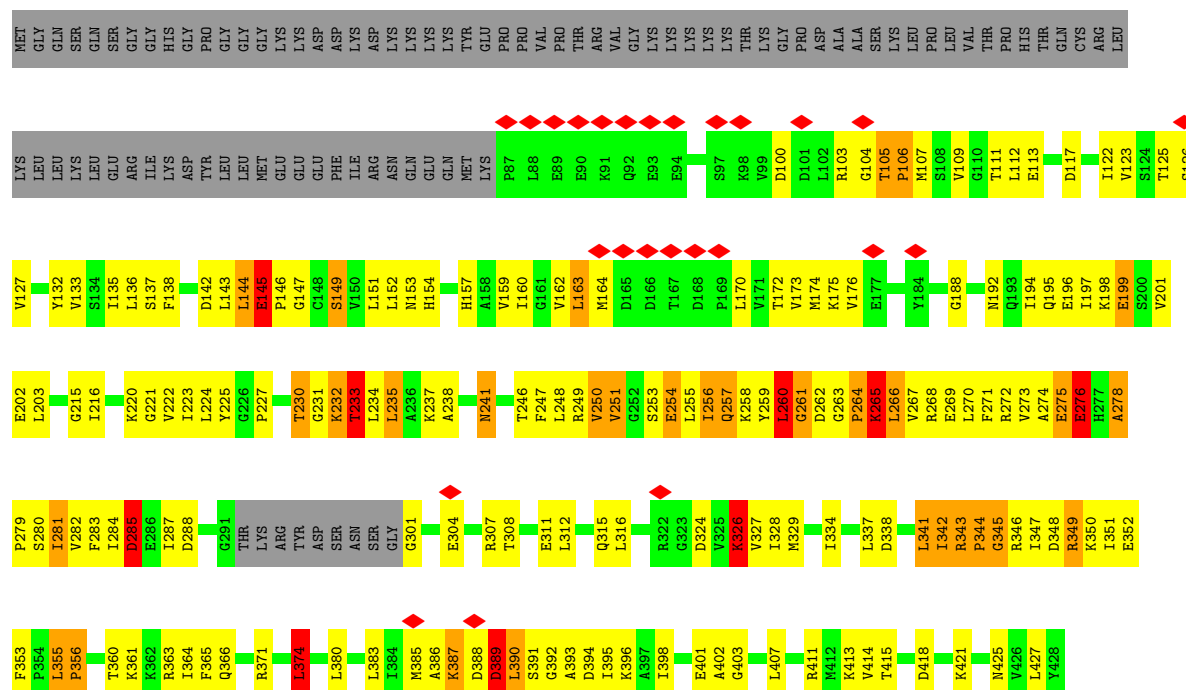




• Molecule 17: 26S protease regulatory subunit 7

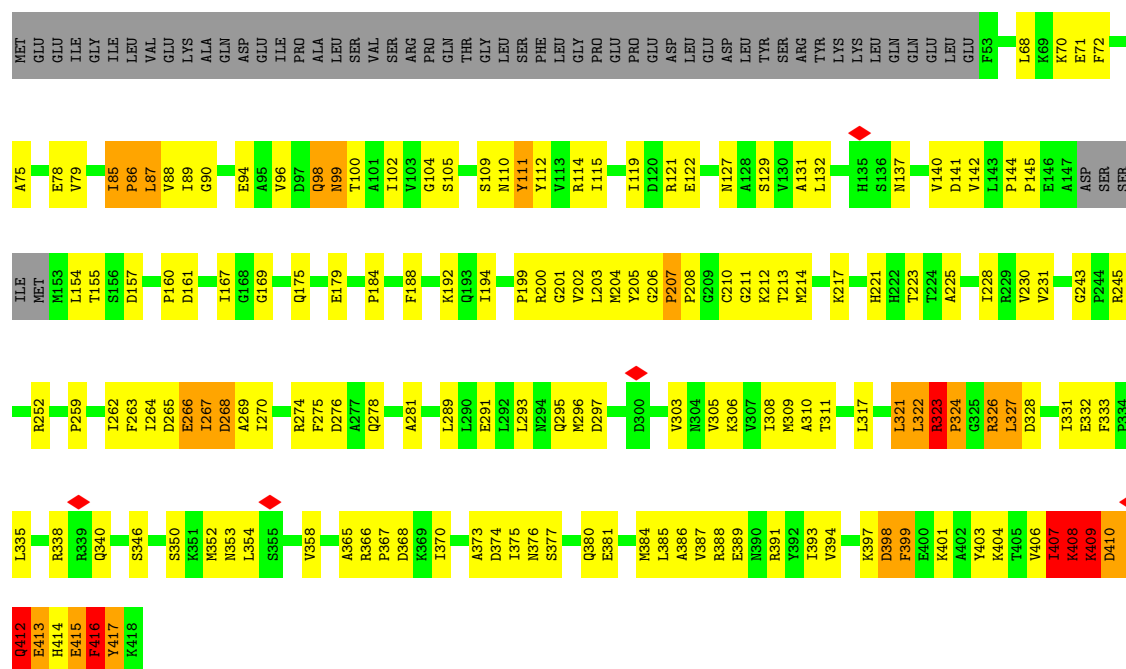


• Molecule 18: 26S protease regulatory subunit 4



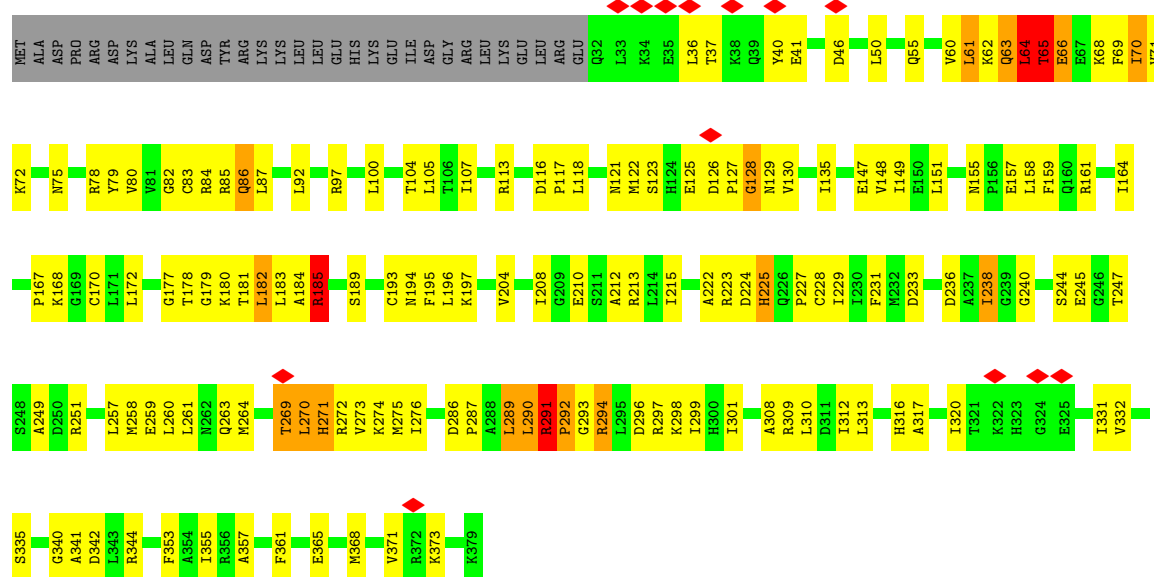
• Molecule 19: 26S protease regulatory subunit 6B

Chain e: 

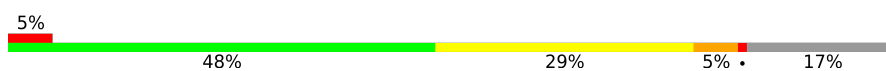


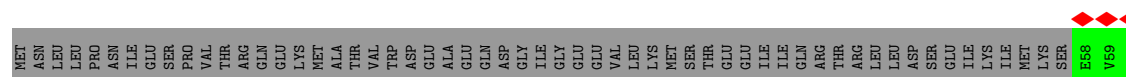
• Molecule 20: 26S protease regulatory subunit 10B

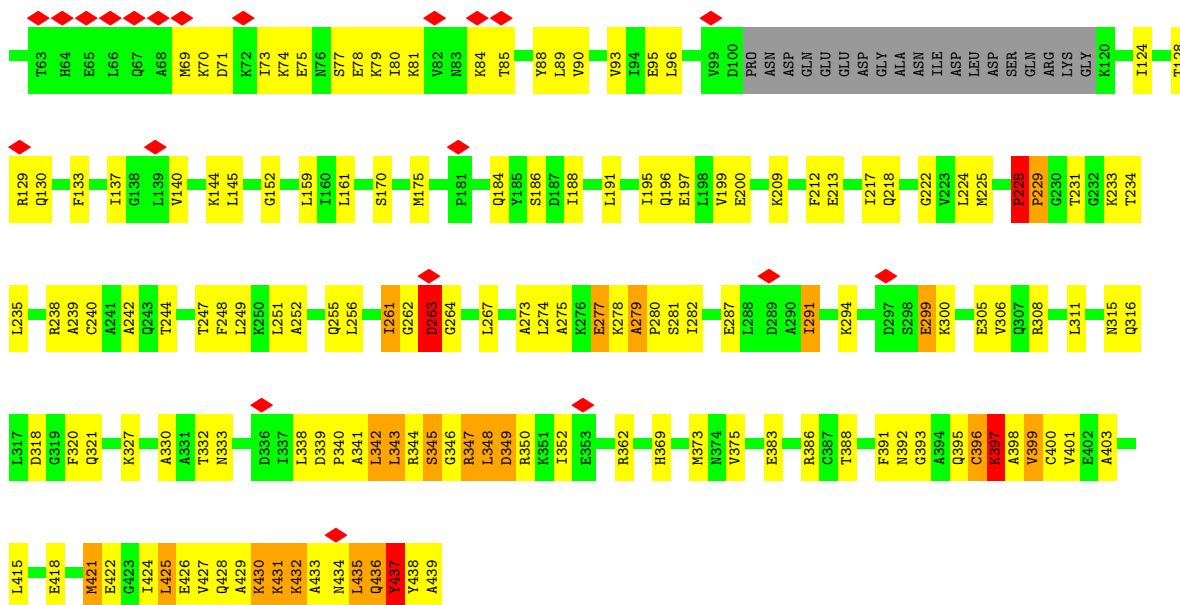
Chain f: 



• Molecule 21: 26S protease regulatory subunit 6A

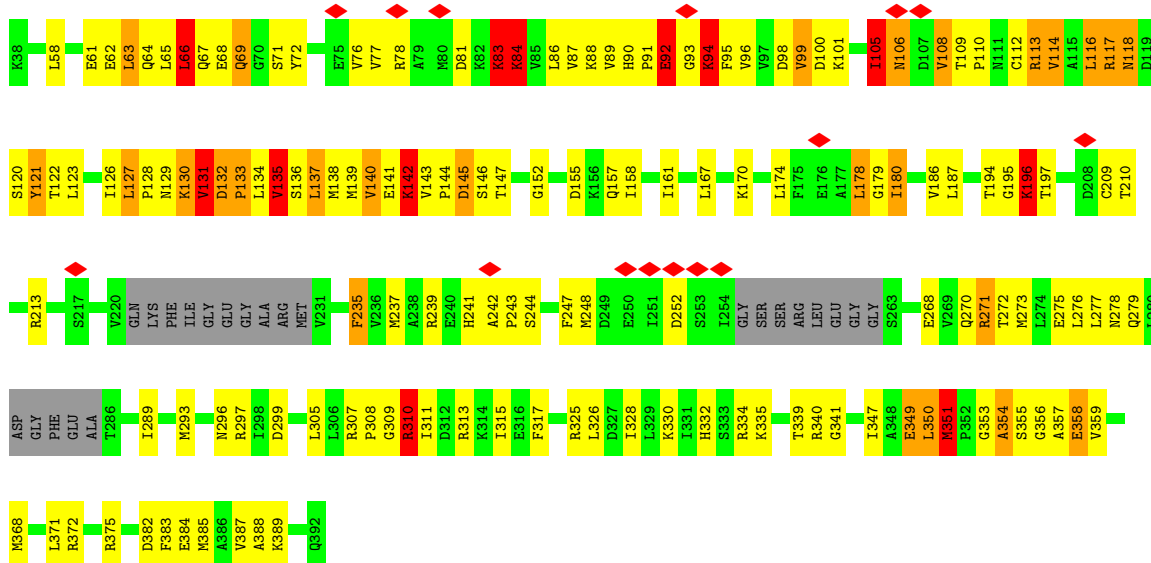
Chain g: 





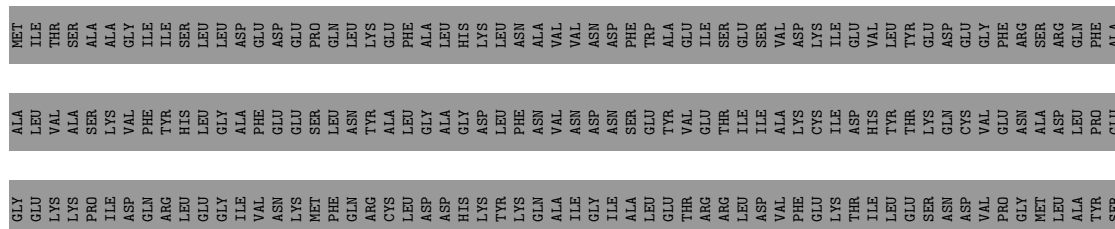
• Molecule 22: 26S protease regulatory subunit 8

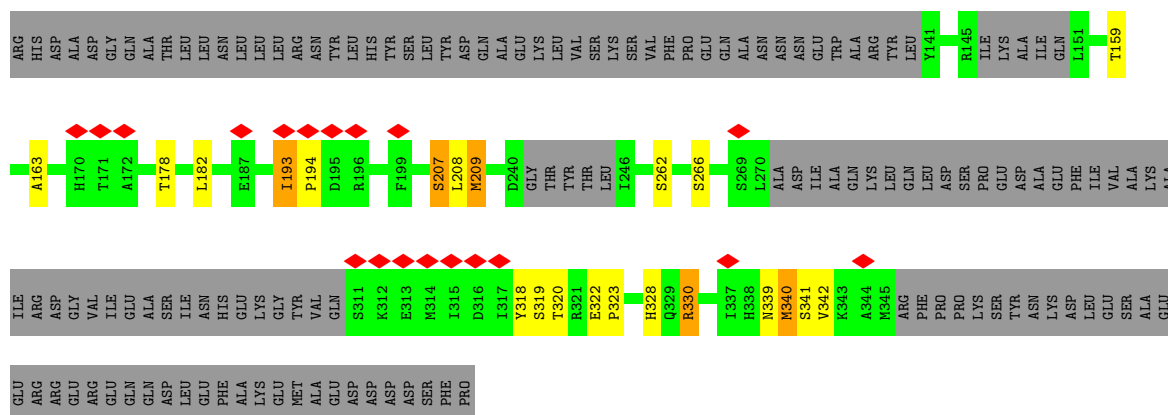
Chain h: 50% 33% 7% 6%



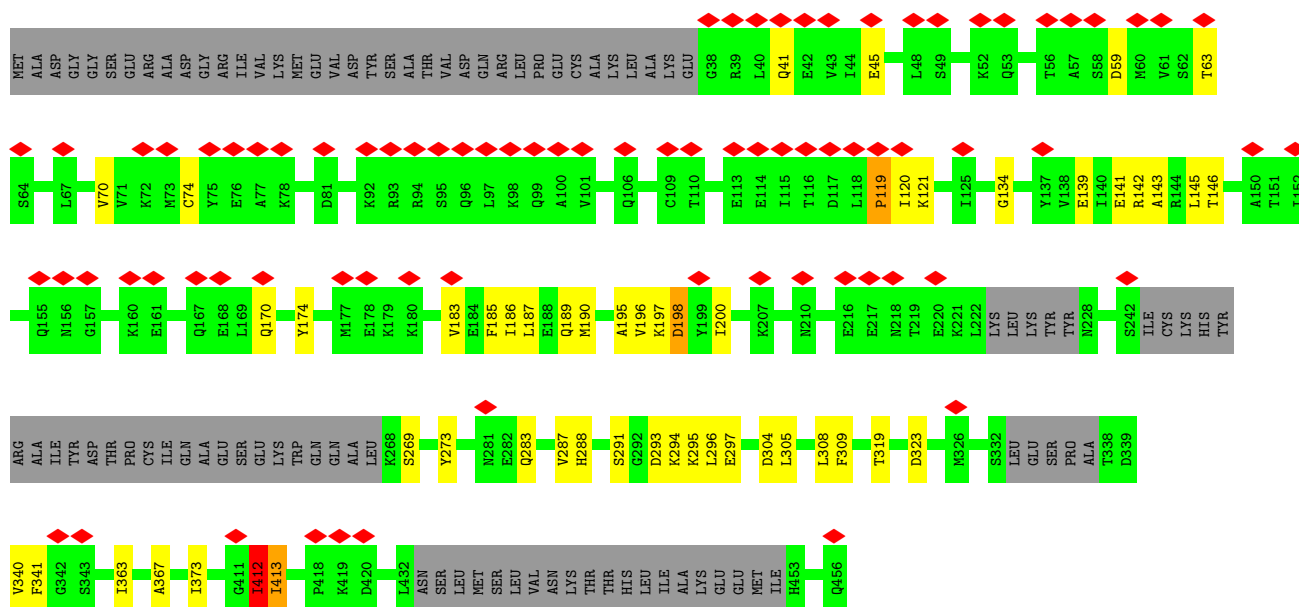
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 1

Chain i: 16% 7% 76%

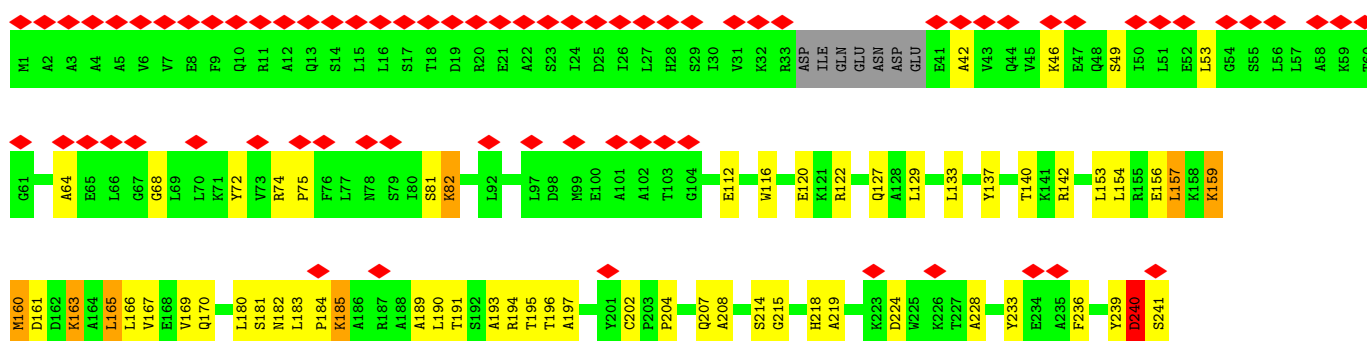


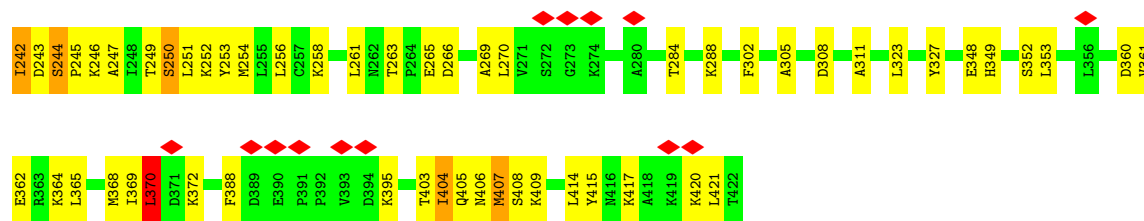


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 12



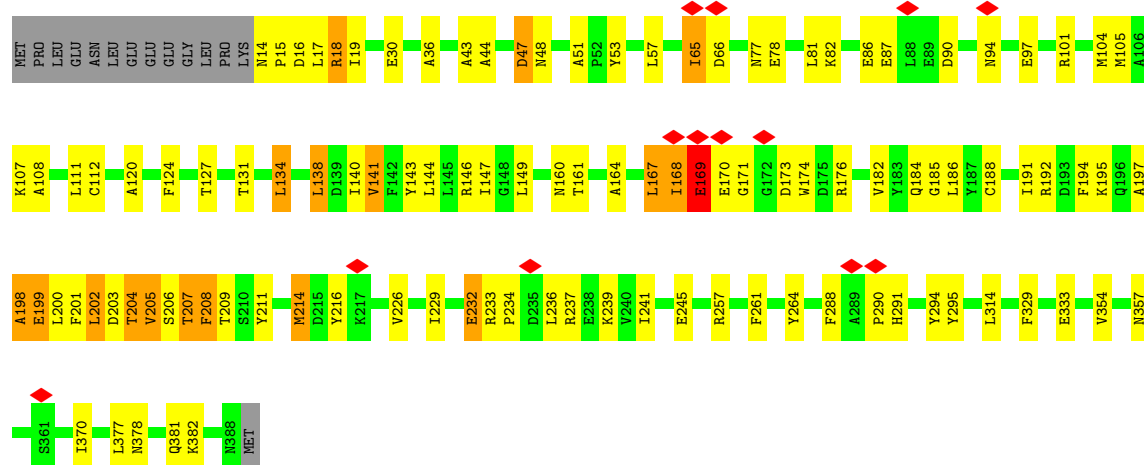
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 11





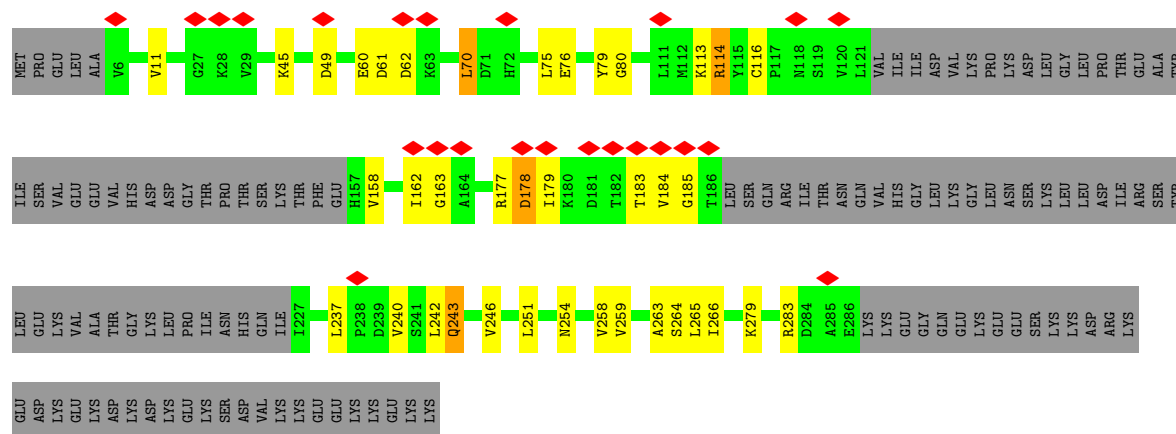
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 6

Chain m: 68% 24%



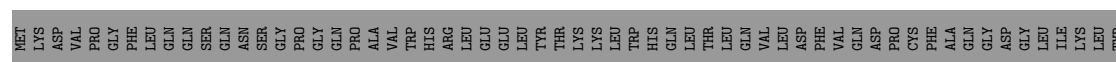
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 7

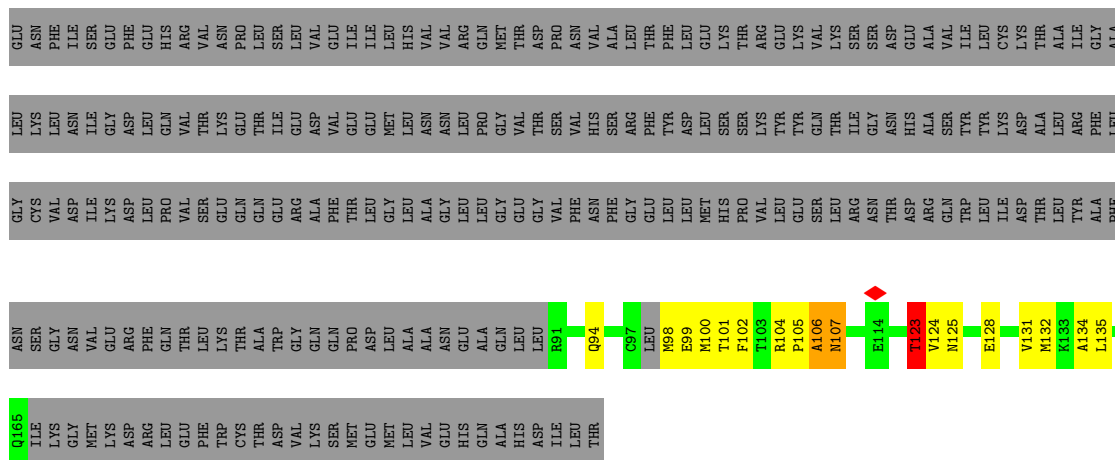
Chain n: 7% 52% 10% 36%



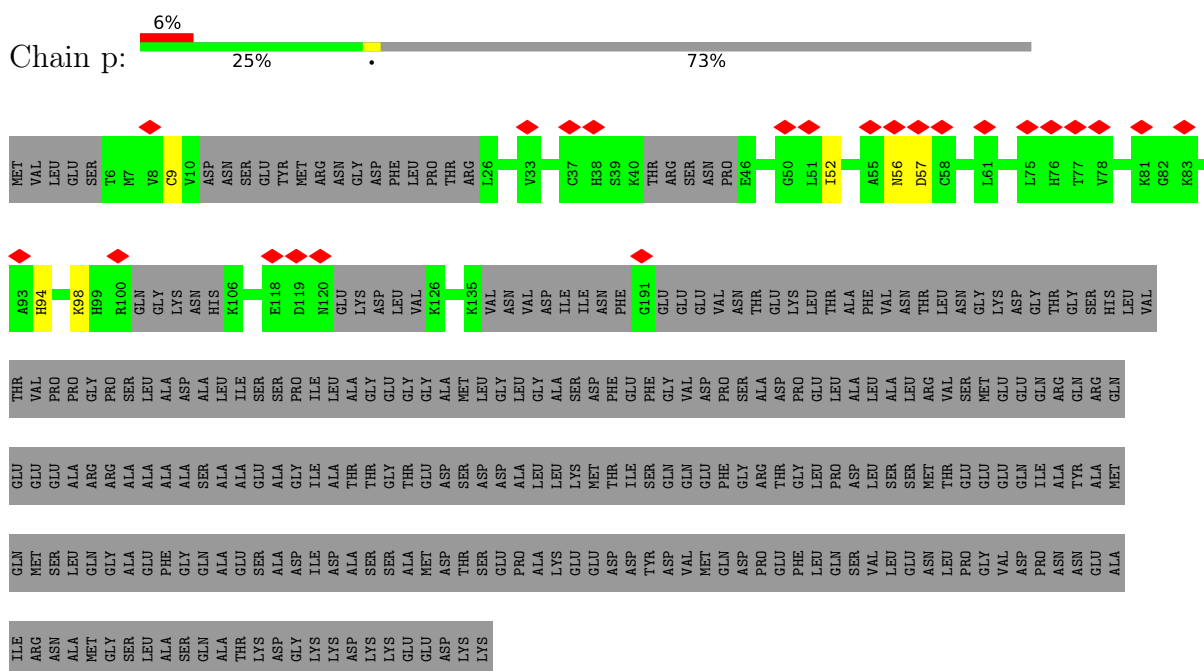
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 13

Chain o: 15% 80%

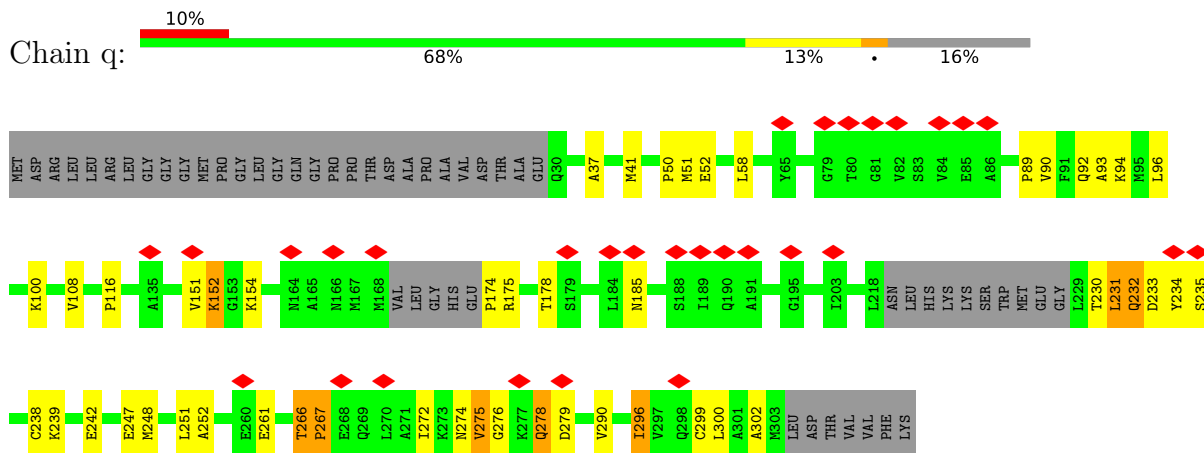




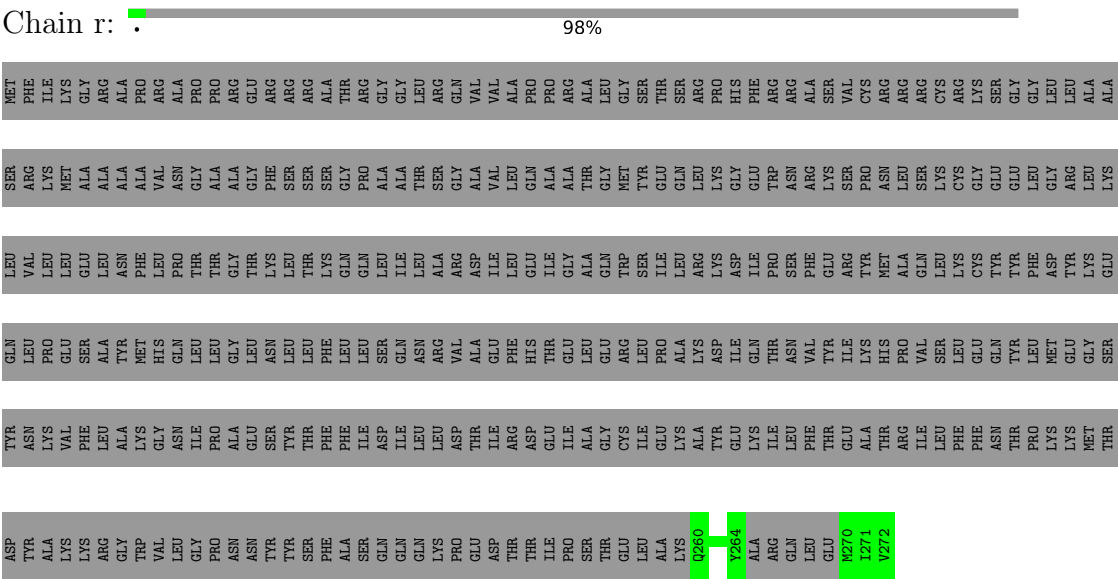
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 4



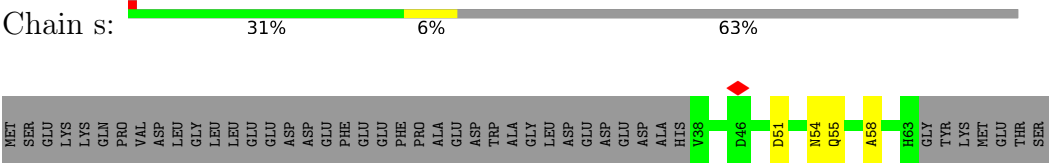
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 14



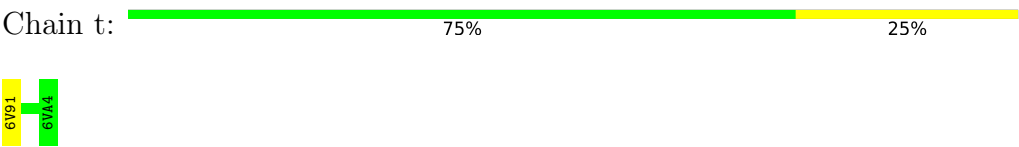
● Molecule 32: 26S proteasome non-ATPase regulatory subunit 8



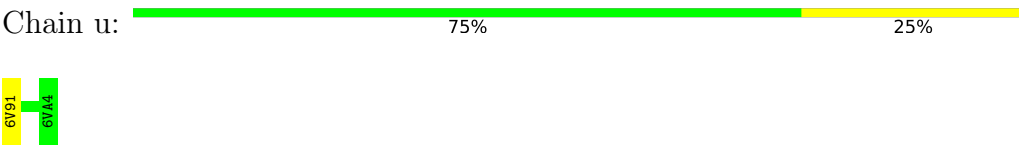
● Molecule 33: 26S proteasome complex subunit SEM1



● Molecule 34: bound Oprozomib



● Molecule 34: bound Oprozomib



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	233000	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	8400	Depositor
Magnification	110236	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.275	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.72, 426.72, 426.72	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6VA, 7C9, ADP, 6V9

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/1802	0.80	3/2446 (0.1%)
1	O	0.33	0/1802	0.81	4/2446 (0.2%)
2	B	0.34	0/1864	0.86	4/2513 (0.2%)
2	P	0.38	1/1904 (0.1%)	0.94	9/2573 (0.3%)
3	C	0.35	0/1796	0.81	5/2438 (0.2%)
4	D	0.31	0/1784	0.66	1/2416 (0.0%)
4	R	0.31	0/1795	0.67	1/2424 (0.0%)
5	E	0.39	0/1839	0.94	6/2492 (0.2%)
6	F	0.37	0/1852	0.78	5/2494 (0.2%)
6	T	0.37	1/1912 (0.1%)	0.79	5/2576 (0.2%)
7	G	0.35	0/1836	0.76	3/2481 (0.1%)
7	U	0.40	0/1875	0.79	8/2542 (0.3%)
8	H	0.37	0/1690	0.70	1/2289 (0.0%)
8	V	0.36	0/1657	0.69	1/2252 (0.0%)
9	I	0.34	0/1619	0.71	4/2184 (0.2%)
9	W	0.34	0/1614	0.71	4/2176 (0.2%)
10	J	0.34	0/1592	0.61	0/2153
10	X	0.34	0/1595	0.60	0/2157
11	K	0.37	0/1576	0.66	0/2131
11	Y	0.37	0/1590	0.67	0/2147
12	L	0.36	0/1670	0.70	0/2254
12	Z	0.35	0/1672	0.70	0/2253
13	M	0.36	0/1720	0.76	3/2328 (0.1%)
13	a	0.36	0/1712	0.75	2/2319 (0.1%)
14	N	0.36	0/1539	0.63	1/2082 (0.0%)
14	b	0.37	0/1546	0.67	3/2094 (0.1%)
15	Q	1.29	2/1810 (0.1%)	1.01	9/2456 (0.4%)
16	S	0.42	1/1868 (0.1%)	0.93	7/2531 (0.3%)
17	c	0.38	0/2774	0.89	4/3739 (0.1%)
18	d	0.47	1/2597 (0.0%)	1.12	19/3514 (0.5%)
19	e	0.38	0/2818	0.93	3/3812 (0.1%)
20	f	0.36	0/2734	0.91	14/3690 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	g	0.37	0/2815	0.92	11/3804 (0.3%)
22	h	0.36	0/2550	0.99	15/3442 (0.4%)
23	i	0.46	0/1150	1.17	6/1599 (0.4%)
24	j	0.41	0/780	1.11	2/1086 (0.2%)
25	k	0.33	0/1819	1.05	7/2536 (0.3%)
26	l	0.33	1/2601 (0.0%)	0.94	9/3569 (0.3%)
27	m	0.37	1/2450 (0.0%)	1.04	15/3356 (0.4%)
28	n	0.44	1/1032 (0.1%)	1.19	7/1438 (0.5%)
29	o	0.39	0/378	0.91	0/528
30	p	0.23	0/501	0.64	0/691
31	q	0.38	0/1318	1.11	7/1836 (0.4%)
32	r	0.35	0/38	0.85	0/50
33	s	0.45	0/129	0.97	0/179
All	All	0.41	9/77015 (0.0%)	0.86	208/104516 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	O	0	1
2	B	0	4
2	P	0	10
3	C	0	1
4	D	0	1
4	R	0	1
5	E	0	4
6	F	0	3
6	T	0	3
7	G	0	3
7	U	0	2
8	H	0	1
8	V	0	1
9	I	0	2
9	W	0	2
10	J	0	1
10	X	0	1
13	a	0	1
14	b	0	2
15	Q	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	5
17	c	0	7
18	d	0	12
19	e	0	4
20	f	0	3
21	g	0	3
22	h	0	4
23	i	0	4
24	j	0	4
25	k	0	8
26	l	0	7
27	m	0	8
28	n	0	9
29	o	0	1
30	p	0	1
31	q	0	6
All	All	0	136

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	45	VAL	C-N	-50.01	0.63	1.33
15	Q	63	CYS	C-N	16.35	1.55	1.33
16	S	237	GLU	CA-C	-6.31	1.44	1.52
2	P	241	GLU	CA-C	-6.00	1.44	1.52
26	l	183	LEU	C-N	5.35	1.40	1.33
28	n	237	LEU	C-N	5.29	1.39	1.33
18	d	326	LYS	N-CA	-5.16	1.39	1.46
27	m	51	ALA	C-N	5.09	1.39	1.34
6	T	227	VAL	CA-C	5.00	1.58	1.52

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	63	CYS	O-C-N	-19.30	98.84	123.16
19	e	323	ARG	C-N-CD	-15.20	62.68	125.00
18	d	145	GLU	C-N-CD	-14.96	63.65	125.00
21	g	228	PRO	C-N-CD	-13.09	71.32	125.00
15	Q	62	ILE	O-C-N	11.40	136.85	122.94
21	g	437	TYR	CA-C-N	-10.64	103.05	122.31
21	g	437	TYR	C-N-CA	-10.64	103.05	122.31
18	d	278	ALA	C-N-CD	-10.38	97.77	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	m	370	ILE	N-CA-C	-10.21	100.83	110.42
2	P	171	ALA	CA-C-N	-10.17	103.66	121.97
2	P	171	ALA	C-N-CA	-10.17	103.66	121.97
5	E	9	ASP	N-CA-C	10.11	128.09	113.02
16	S	9	ASP	N-CA-C	10.11	128.08	113.02
15	Q	49	SER	N-CA-C	-9.84	89.85	110.80
18	d	265	LYS	N-CA-C	-9.10	101.97	113.43
31	q	266	THR	C-N-CD	-9.06	87.84	125.00
22	h	132	ASP	CA-C-N	9.05	131.16	119.84
22	h	132	ASP	C-N-CA	9.05	131.16	119.84
27	m	197	ALA	N-CA-C	8.74	120.58	111.14
31	q	261	GLU	N-CA-C	8.40	120.21	111.14
13	M	201	GLY	C-N-CD	-8.38	102.17	120.60
20	f	85	ARG	CA-C-N	8.33	137.45	121.54
20	f	85	ARG	C-N-CA	8.33	137.45	121.54
18	d	261	GLY	N-CA-C	-8.21	93.73	113.18
15	Q	45	VAL	CA-C-N	-8.16	105.95	121.54
15	Q	45	VAL	C-N-CA	-8.16	105.95	121.54
23	i	665	ASN	N-CA-C	8.09	128.03	110.80
18	d	232	LYS	N-CA-C	8.08	122.58	112.24
2	P	168	SER	O-C-N	-7.79	109.89	122.42
28	n	240	VAL	N-CA-C	-7.78	105.73	113.20
21	g	338	LEU	CA-C-N	7.66	132.32	120.68
21	g	338	LEU	C-N-CA	7.66	132.32	120.68
31	q	235	SER	N-CA-C	-7.60	103.08	114.64
31	q	290	VAL	N-CA-C	7.51	118.28	110.62
18	d	233	THR	N-CA-CB	7.51	123.18	110.49
18	d	343	ARG	N-CA-C	-7.44	93.36	109.81
20	f	238	ILE	N-CA-C	-7.28	105.50	113.43
1	O	48	GLU	CA-CB-CG	7.20	128.50	114.10
1	A	48	GLU	CA-CB-CG	7.20	128.49	114.10
5	E	203	GLN	N-CA-C	7.19	126.11	110.80
6	T	227	VAL	CA-C-N	-7.17	110.88	119.84
6	T	227	VAL	C-N-CA	-7.17	110.88	119.84
2	B	172	VAL	N-CA-C	7.16	124.23	109.34
2	P	172	VAL	N-CA-C	7.15	124.21	109.34
6	F	227	VAL	CA-C-N	-7.14	110.91	119.84
6	F	227	VAL	C-N-CA	-7.14	110.91	119.84
20	f	185	ARG	N-CA-C	-7.13	102.70	111.40
26	l	239	TYR	N-CA-C	-7.07	97.03	108.41
23	i	629	THR	C-N-CD	-7.05	96.10	125.00
28	n	62	ASP	N-CA-C	-7.03	106.61	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	68	ASN	CA-C-N	6.99	134.89	121.54
5	E	68	ASN	C-N-CA	6.99	134.89	121.54
18	d	250	VAL	N-CA-C	6.98	123.86	109.34
3	C	90	GLU	CA-CB-CG	6.97	128.05	114.10
15	Q	90	GLU	CA-CB-CG	6.97	128.04	114.10
21	g	262	GLY	N-CA-C	6.97	121.69	112.77
16	S	68	ASN	CA-C-N	6.96	134.83	121.54
16	S	68	ASN	C-N-CA	6.96	134.83	121.54
21	g	263	ASP	N-CA-C	6.88	118.78	111.28
22	h	310	ARG	N-CA-C	-6.85	105.05	113.41
25	k	197	LYS	CA-C-N	6.84	134.60	121.54
25	k	197	LYS	C-N-CA	6.84	134.60	121.54
9	I	95	TYR	CA-C-N	6.83	134.59	121.54
9	I	95	TYR	C-N-CA	6.83	134.59	121.54
22	h	94	LYS	N-CA-C	6.82	120.09	109.52
27	m	232	GLU	CA-C-N	6.82	129.58	120.58
27	m	232	GLU	C-N-CA	6.82	129.58	120.58
9	W	95	TYR	CA-C-N	6.81	134.55	121.54
9	W	95	TYR	C-N-CA	6.81	134.55	121.54
7	U	164	LYS	N-CA-C	-6.79	103.81	111.14
21	g	316	GLN	N-CA-C	-6.78	104.58	112.92
25	k	373	ILE	CA-C-N	6.76	134.46	121.54
25	k	373	ILE	C-N-CA	6.76	134.46	121.54
14	b	202	LEU	C-N-CD	-6.74	97.35	125.00
7	G	209	ASP	CA-CB-CG	6.74	119.34	112.60
15	Q	45	VAL	O-C-N	6.74	130.68	123.00
18	d	253	SER	CA-C-O	-6.72	113.77	120.82
27	m	65	ILE	CA-C-N	6.64	133.65	121.70
27	m	65	ILE	C-N-CA	6.64	133.65	121.70
18	d	326	LYS	CB-CA-C	6.60	123.55	110.42
15	Q	39	ASP	N-CA-C	-6.58	107.12	114.62
20	f	236	ASP	N-CA-C	-6.55	104.89	114.39
3	C	39	ASP	N-CA-C	-6.54	107.17	114.62
23	i	597	LYS	N-CA-C	-6.50	104.11	111.14
22	h	113	ARG	N-CA-C	6.46	119.98	110.30
26	l	249	THR	CA-C-N	-6.37	112.56	122.37
26	l	249	THR	C-N-CA	-6.37	112.56	122.37
27	m	47	ASP	CA-C-N	6.36	133.68	121.54
27	m	47	ASP	C-N-CA	6.36	133.68	121.54
18	d	231	GLY	N-CA-C	6.26	123.96	115.32
22	h	209	CYS	CA-C-N	6.26	133.51	121.54
22	h	209	CYS	C-N-CA	6.26	133.51	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	n	70	LEU	CB-CA-C	6.22	120.88	110.43
18	d	388	ASP	CA-C-N	6.21	133.40	121.54
18	d	388	ASP	C-N-CA	6.21	133.40	121.54
17	c	312	ARG	N-CA-CB	-6.18	107.12	114.17
15	Q	90	GLU	CB-CG-CD	6.17	123.09	112.60
7	U	169	GLY	N-CA-C	-6.15	98.60	113.18
3	C	90	GLU	CB-CG-CD	6.14	123.04	112.60
21	g	397	LYS	N-CA-C	-6.14	104.50	111.07
18	d	285	ASP	N-CA-C	6.05	123.68	110.80
2	P	227	VAL	N-CA-C	-5.93	106.53	112.17
2	B	227	VAL	N-CA-C	-5.92	106.54	112.17
4	R	210	LEU	CA-CB-CG	5.91	136.99	116.30
4	D	210	LEU	CA-CB-CG	5.90	136.97	116.30
22	h	83	LYS	CA-C-N	5.89	132.79	121.54
22	h	83	LYS	C-N-CA	5.89	132.79	121.54
2	P	186	LEU	CA-CB-CG	5.82	136.68	116.30
2	B	186	LEU	CA-CB-CG	5.81	136.65	116.30
28	n	116	CYS	N-CA-C	5.81	122.66	109.81
18	d	326	LYS	N-CA-C	-5.79	98.46	110.80
22	h	131	VAL	N-CA-C	5.76	121.33	109.34
25	k	413	ILE	N-CA-C	5.76	121.31	109.34
18	d	254	GLU	N-CA-CB	5.75	119.19	110.28
23	i	647	HIS	N-CA-C	-5.70	105.59	113.18
22	h	196	LYS	N-CA-C	5.67	118.87	110.48
7	U	44	GLY	CA-C-N	-5.66	110.74	121.54
7	U	44	GLY	C-N-CA	-5.66	110.74	121.54
18	d	256	ILE	N-CA-C	5.64	116.20	110.05
22	h	135	VAL	N-CA-CB	5.61	120.48	111.23
22	h	109	THR	CA-C-N	5.61	125.61	119.89
22	h	109	THR	C-N-CA	5.61	125.61	119.89
5	E	67	ASP	N-CA-C	5.60	115.96	108.23
17	c	362	MET	N-CA-CB	-5.57	107.82	114.17
16	S	67	ASP	N-CA-C	5.57	115.91	108.23
20	f	361	PHE	CA-C-N	5.55	131.96	121.97
20	f	361	PHE	C-N-CA	5.55	131.96	121.97
27	m	66	ASP	N-CA-C	5.55	126.54	111.00
27	m	357	ASN	CA-C-N	-5.54	116.09	122.52
27	m	357	ASN	C-N-CA	-5.54	116.09	122.52
19	e	111	TYR	CA-CB-CG	5.54	123.87	113.90
20	f	291	ARG	C-N-CD	-5.50	102.45	125.00
7	U	170	VAL	CA-C-N	-5.49	114.29	122.36
7	U	170	VAL	C-N-CA	-5.49	114.29	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	m	198	ALA	N-CA-C	5.48	117.06	111.14
14	b	202	LEU	N-CA-C	-5.47	97.72	109.81
20	f	86	GLN	CA-CB-CG	5.45	125.00	114.10
3	C	200	GLU	CA-C-N	5.44	128.96	120.75
3	C	200	GLU	C-N-CA	5.44	128.96	120.75
27	m	169	GLU	N-CA-C	5.44	117.21	111.28
26	l	414	LEU	N-CA-C	-5.42	105.37	111.28
26	l	388	PHE	N-CA-C	5.41	119.04	111.74
22	h	84	LYS	N-CA-C	-5.40	99.30	110.80
23	i	756	HIS	CA-C-N	5.39	127.70	120.58
23	i	756	HIS	C-N-CA	5.39	127.70	120.58
6	T	227	VAL	N-CA-CB	-5.38	103.68	111.21
1	O	199	GLU	CA-CB-CG	5.38	124.86	114.10
6	F	227	VAL	N-CA-CB	-5.37	103.69	111.21
8	H	28	ASP	CA-CB-CG	5.34	117.94	112.60
2	P	240	HIS	CA-C-N	5.34	131.74	121.54
2	P	240	HIS	C-N-CA	5.34	131.74	121.54
26	l	240	ASP	CA-C-N	5.33	131.73	121.54
26	l	240	ASP	C-N-CA	5.33	131.73	121.54
8	V	28	ASP	CA-CB-CG	5.33	117.93	112.60
24	j	266	SER	N-CA-C	5.31	116.09	107.32
31	q	185	ASN	N-CA-C	-5.28	106.84	113.28
20	f	294	ARG	N-CA-C	-5.28	105.20	111.69
28	n	158	VAL	N-CA-C	-5.28	108.36	113.53
31	q	235	SER	CA-C-N	5.28	128.13	120.79
31	q	235	SER	C-N-CA	5.28	128.13	120.79
20	f	269	THR	CA-C-N	5.27	131.60	121.54
20	f	269	THR	C-N-CA	5.27	131.60	121.54
28	n	113	LYS	CA-C-N	5.27	131.60	121.54
28	n	113	LYS	C-N-CA	5.27	131.60	121.54
2	B	147	LEU	CA-CB-CG	5.26	134.73	116.30
2	P	147	LEU	CA-CB-CG	5.26	134.73	116.30
18	d	276	GLU	N-CA-C	5.24	116.99	111.28
19	e	243	GLY	N-CA-C	5.21	122.97	112.34
21	g	436	GLN	CA-C-N	-5.18	114.45	122.49
21	g	436	GLN	C-N-CA	-5.18	114.45	122.49
20	f	270	LEU	CA-C-N	5.18	131.43	121.54
20	f	270	LEU	C-N-CA	5.18	131.43	121.54
24	j	330	ARG	N-CA-C	-5.17	104.57	111.24
7	G	50	ILE	CA-C-N	-5.14	114.51	122.69
7	G	50	ILE	C-N-CA	-5.14	114.51	122.69
25	k	412	ILE	CA-C-N	5.14	131.22	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	412	ILE	C-N-CA	5.14	131.22	121.97
6	F	185	THR	CA-C-N	5.14	131.35	121.54
6	F	185	THR	C-N-CA	5.14	131.35	121.54
27	m	214	MET	CA-C-N	5.13	131.35	121.54
27	m	214	MET	C-N-CA	5.13	131.35	121.54
7	U	50	ILE	CA-C-N	-5.13	114.53	122.69
7	U	50	ILE	C-N-CA	-5.13	114.53	122.69
14	b	69	GLU	CB-CG-CD	5.13	121.32	112.60
26	l	81	SER	CA-C-N	5.12	131.32	121.54
26	l	81	SER	C-N-CA	5.12	131.32	121.54
6	T	185	THR	CA-C-N	5.11	131.30	121.54
6	T	185	THR	C-N-CA	5.11	131.30	121.54
14	N	69	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	183	LEU	CA-C-N	5.09	131.27	121.54
1	A	183	LEU	C-N-CA	5.09	131.27	121.54
13	a	78	GLY	CA-C-N	5.08	131.25	121.54
13	a	78	GLY	C-N-CA	5.08	131.25	121.54
13	M	78	GLY	CA-C-N	5.08	131.24	121.54
13	M	78	GLY	C-N-CA	5.08	131.24	121.54
1	O	183	LEU	CA-C-N	5.07	131.21	121.54
1	O	183	LEU	C-N-CA	5.07	131.21	121.54
17	c	377	CYS	CA-C-N	5.06	126.16	119.84
17	c	377	CYS	C-N-CA	5.06	126.16	119.84
9	I	162	LEU	CA-C-N	5.05	129.22	121.19
9	I	162	LEU	C-N-CA	5.05	129.22	121.19
16	S	236	LEU	CA-C-N	5.05	131.18	121.54
16	S	236	LEU	C-N-CA	5.05	131.18	121.54
5	E	69	HIS	N-CA-C	5.04	121.54	110.80
9	W	162	LEU	CA-C-N	5.02	129.17	121.19
9	W	162	LEU	C-N-CA	5.02	129.17	121.19
16	S	69	HIS	N-CA-C	5.02	121.49	110.80
18	d	374	LEU	CA-CB-CG	5.01	133.85	116.30

There are no chirality outliers.

All (136) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TRP	Peptide
1	A	139	ASN	Peptide
2	B	229	LYS	Peptide
2	B	240	HIS	Peptide
2	B	54	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	B	60	PHE	Peptide
3	C	199	VAL	Mainchain
4	D	58	LEU	Peptide
5	E	202	GLU	Peptide
5	E	203	GLN	Peptide
5	E	66	VAL	Peptide
5	E	8	ASN	Peptide
6	F	226	ILE	Peptide
6	F	227	VAL	Peptide
6	F	228	PRO	Peptide
7	G	163	PHE	Peptide
7	G	37	LEU	Peptide
7	G	68	HIS	Peptide
8	H	187	ARG	Peptide
9	I	146	TYR	Mainchain
9	I	96	GLU	Peptide
10	J	32	HIS	Peptide
1	O	139	ASN	Peptide
2	P	168	SER	Peptide,Mainchain
2	P	169	ALA	Peptide
2	P	171	ALA	Peptide
2	P	229	LYS	Peptide
2	P	240	HIS	Peptide,Mainchain
2	P	241	GLU	Peptide
2	P	54	LYS	Peptide
2	P	60	PHE	Peptide
15	Q	199	VAL	Mainchain
15	Q	45	VAL	Mainchain
15	Q	49	SER	Peptide
15	Q	63	CYS	Mainchain
4	R	58	LEU	Peptide
16	S	236	LEU	Peptide,Mainchain
16	S	237	GLU	Peptide
16	S	66	VAL	Peptide
16	S	8	ASN	Peptide
6	T	226	ILE	Peptide
6	T	227	VAL	Peptide
6	T	228	PRO	Peptide
7	U	37	LEU	Peptide
7	U	68	HIS	Peptide
8	V	187	ARG	Peptide
9	W	146	TYR	Mainchain

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Mol	Chain	Res	Type	Group
9	W	96	GLU	Peptide
10	X	32	HIS	Peptide
13	a	201	GLY	Peptide
14	b	201	THR	Mainchain
14	b	202	LEU	Peptide
17	c	193	THR	Peptide
17	c	241	ILE	Peptide
17	c	282	GLY	Peptide
17	c	324	PRO	Peptide
17	c	325	ASP	Peptide
17	c	377	CYS	Peptide
17	c	426	THR	Peptide
18	d	117	ASP	Peptide
18	d	164	MET	Peptide
18	d	172	THR	Peptide
18	d	222	VAL	Peptide
18	d	241	ASN	Peptide
18	d	278	ALA	Peptide
18	d	288	ASP	Peptide
18	d	324	ASP	Peptide
18	d	326	LYS	Peptide,Mainchain
18	d	355	LEU	Peptide
18	d	356	PRO	Peptide
19	e	278	GLN	Peptide
19	e	333	PHE	Peptide
19	e	365	ALA	Peptide
19	e	407	ILE	Peptide
20	f	116	ASP	Peptide
20	f	117	PRO	Peptide
20	f	245	GLU	Peptide
21	g	279	ALA	Peptide
21	g	299	GLU	Peptide
21	g	349	ASP	Peptide
22	h	242	ALA	Peptide
22	h	351	MET	Peptide
22	h	83	LYS	Peptide
22	h	92	GLU	Peptide
23	i	538	GLU	Peptide
23	i	661	ALA	Peptide
23	i	770	TRP	Peptide
23	i	773	PHE	Peptide
24	j	193	ILE	Peptide

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Mol	Chain	Res	Type	Group
24	j	194	PRO	Peptide
24	j	207	SER	Peptide
24	j	209	MET	Peptide
25	k	121	LYS	Peptide
25	k	170	GLN	Peptide
25	k	195	ALA	Peptide
25	k	196	VAL	Peptide
25	k	198	ASP	Peptide
25	k	340	VAL	Peptide
25	k	341	PHE	Peptide
25	k	412	ILE	Peptide
26	l	180	LEU	Peptide
26	l	185	LYS	Peptide
26	l	250	SER	Peptide
26	l	370	LEU	Peptide
26	l	372	LYS	Peptide
26	l	74	ARG	Peptide
26	l	75	PRO	Peptide
27	m	134	LEU	Peptide
27	m	169	GLU	Peptide
27	m	174	TRP	Peptide
27	m	216	TYR	Peptide
27	m	288	PHE	Peptide
27	m	30	GLU	Peptide
27	m	36	ALA	Peptide
27	m	65	ILE	Peptide
28	n	114	ARG	Peptide
28	n	162	ILE	Peptide
28	n	178	ASP	Peptide
28	n	183	THR	Peptide
28	n	45	LYS	Peptide
28	n	49	ASP	Peptide
28	n	60	GLU	Peptide
28	n	61	ASP	Peptide
28	n	70	LEU	Peptide
29	o	123	THR	Peptide
30	p	57	ASP	Peptide
31	q	151	VAL	Peptide
31	q	152	LYS	Peptide
31	q	174	PRO	Peptide
31	q	239	LYS	Peptide
31	q	278	GLN	Peptide

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Mol	Chain	Res	Type	Group
31	q	296	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1741	45	0
1	O	1764	0	1732	32	0
2	B	1836	0	1838	40	0
2	P	1875	0	1865	37	0
3	C	1771	0	1712	59	0
4	D	1757	0	1713	45	0
4	R	1768	0	1756	28	0
5	E	1805	0	1765	41	0
6	F	1818	0	1792	38	0
6	T	1877	0	1857	39	0
7	G	1806	0	1816	64	0
7	U	1841	0	1809	69	0
8	H	1663	0	1681	58	0
8	V	1627	0	1608	48	0
9	I	1590	0	1612	43	0
9	W	1586	0	1607	34	0
10	J	1560	0	1561	40	0
10	X	1563	0	1565	33	0
11	K	1545	0	1495	29	0
11	Y	1559	0	1520	35	0
12	L	1637	0	1620	40	0
12	Z	1642	0	1630	42	0
13	M	1687	0	1666	38	0
13	a	1679	0	1651	37	0
14	N	1513	0	1483	27	0
14	b	1519	0	1487	27	0
15	Q	1785	0	1734	140	0
16	S	1834	0	1788	32	0
17	c	2728	0	2775	174	0
18	d	2560	0	2556	341	0
19	e	2776	0	2740	298	0
20	f	2692	0	2696	248	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	g	2777	0	2782	220	0
22	h	2518	0	2530	300	0
23	i	1145	0	592	88	0
24	j	779	0	366	15	0
25	k	1819	0	809	27	0
26	l	2572	0	1980	111	0
27	m	2421	0	1885	111	0
28	n	1030	0	474	20	0
29	o	377	0	173	14	0
30	p	504	0	238	2	0
31	q	1311	0	656	47	0
32	r	40	0	17	0	0
33	s	130	0	56	2	0
34	t	37	0	0	0	0
34	u	37	0	0	0	0
35	c	27	0	11	7	0
35	d	27	0	11	11	0
35	e	27	0	12	19	0
35	g	54	0	24	22	0
35	h	27	0	12	22	0
All	All	76085	0	70499	2895	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 20.

All (2895) 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)
22:h:114:VAL:HG12	22:h:127:LEU:CG	1.16	1.63
15:Q:192:ILE:CD1	15:Q:228:TYR:HB3	1.27	1.61
7:U:163:PHE:CD2	7:U:166:THR:HG21	1.37	1.57
15:Q:188:ILE:CG2	15:Q:228:TYR:CZ	1.79	1.56
3:C:50:VAL:HA	3:C:54:GLN:CG	1.29	1.56
22:h:114:VAL:CG1	22:h:127:LEU:HG	1.09	1.55
15:Q:192:ILE:HD13	15:Q:228:TYR:CB	1.17	1.54
15:Q:220:LEU:CD2	15:Q:224:GLU:HG3	1.37	1.54
3:C:50:VAL:CA	3:C:54:GLN:CG	1.84	1.53
3:C:50:VAL:CB	3:C:54:GLN:HG3	1.07	1.52
15:Q:32:ALA:HA	15:Q:45:VAL:CG1	1.42	1.49
15:Q:206:ILE:HG23	15:Q:225:ILE:CG2	1.45	1.44
7:U:40:VAL:HA	7:U:167:ALA:CB	1.45	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:188:ILE:HG21	15:Q:228:TYR:CZ	0.91	1.43
15:Q:220:LEU:HB3	15:Q:224:GLU:CB	1.46	1.43
22:h:196:LYS:CB	35:h:401:ADP:O1B	1.65	1.43
15:Q:220:LEU:HD22	15:Q:224:GLU:CG	1.47	1.42
3:C:50:VAL:CB	3:C:54:GLN:CG	1.96	1.40
19:e:323:ARG:NE	22:h:143:VAL:HG22	1.38	1.39
22:h:88:LYS:CA	22:h:93:GLY:O	1.71	1.38
7:U:163:PHE:CD2	7:U:166:THR:CG2	2.05	1.37
2:P:168:SER:C	2:P:172:VAL:H	1.32	1.37
18:d:224:LEU:HD12	18:d:233:THR:CG2	1.52	1.37
8:V:3:ILE:CD1	8:V:44:CYS:HB3	1.51	1.37
19:e:323:ARG:CG	22:h:143:VAL:HG22	1.54	1.37
19:e:397:LYS:O	19:e:401:LYS:HB2	1.23	1.36
22:h:271:ARG:HH22	22:h:275:GLU:CA	1.35	1.36
17:c:165:GLN:HA	17:c:237:PHE:O	1.20	1.35
18:d:283:PHE:HE2	18:d:285:ASP:CB	1.36	1.35
22:h:88:LYS:CB	22:h:93:GLY:O	1.74	1.34
18:d:283:PHE:CE2	18:d:285:ASP:CA	2.09	1.34
17:c:168:GLU:OE1	17:c:169:LYS:C	1.69	1.34
3:C:50:VAL:CA	3:C:54:GLN:HG3	1.49	1.34
5:E:31:GLN:NE2	21:g:435:LEU:HD21	1.42	1.34
22:h:271:ARG:NH2	22:h:275:GLU:CA	1.83	1.34
18:d:283:PHE:CE2	18:d:285:ASP:CB	2.10	1.33
18:d:257:GLN:OE1	18:d:266:LEU:CD1	1.76	1.33
5:E:31:GLN:NE2	21:g:435:LEU:CD2	1.92	1.32
23:i:630:PRO:O	23:i:632:GLN:N	1.62	1.32
19:e:122:GLU:OE2	31:q:278:GLN:C	1.71	1.32
22:h:141:GLU:O	22:h:143:VAL:N	1.58	1.32
19:e:323:ARG:CD	22:h:143:VAL:CB	2.06	1.32
15:Q:188:ILE:CG2	15:Q:228:TYR:CE1	2.11	1.32
18:d:283:PHE:CE2	18:d:285:ASP:HB3	1.64	1.31
22:h:114:VAL:HG11	22:h:127:LEU:N	1.42	1.31
17:c:168:GLU:OE1	17:c:169:LYS:N	1.61	1.31
8:V:3:ILE:HD11	8:V:44:CYS:CB	1.61	1.31
15:Q:32:ALA:CA	15:Q:45:VAL:CG1	2.08	1.30
22:h:78:ARG:CB	22:h:110:PRO:HG3	1.60	1.30
20:f:342:ASP:OD1	21:g:345:SER:HB3	1.27	1.30
15:Q:206:ILE:CG2	15:Q:225:ILE:HG22	1.59	1.30
17:c:168:GLU:OE1	17:c:169:LYS:CA	1.80	1.29
20:f:64:LEU:O	20:f:66:GLU:N	1.61	1.29
27:m:208:PHE:CD2	27:m:211:TYR:HA	1.65	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:384:GLU:O	17:c:386:ARG:N	1.61	1.29
7:U:39:SER:O	7:U:167:ALA:HB1	1.27	1.28
22:h:83:LYS:HD2	22:h:98:ASP:OD1	1.21	1.28
22:h:136:SER:O	22:h:140:VAL:HG12	1.12	1.28
19:e:323:ARG:HD3	22:h:143:VAL:CB	1.61	1.28
22:h:88:LYS:HA	22:h:93:GLY:O	1.20	1.28
15:Q:188:ILE:HD13	15:Q:228:TYR:OH	1.13	1.27
15:Q:188:ILE:HG21	15:Q:228:TYR:CE1	1.69	1.27
18:d:232:LYS:O	18:d:234:LEU:N	1.65	1.27
19:e:397:LYS:O	19:e:401:LYS:CB	1.80	1.27
7:U:163:PHE:CE2	7:U:166:THR:HG21	1.70	1.26
22:h:196:LYS:HB2	35:h:401:ADP:O1B	1.19	1.26
18:d:284:ILE:HG22	18:d:287:ILE:CG2	1.65	1.26
22:h:356:GLY:HA3	35:h:401:ADP:C8	1.68	1.26
15:Q:206:ILE:CG2	15:Q:225:ILE:CG2	2.10	1.26
22:h:196:LYS:CG	35:h:401:ADP:O1B	1.82	1.25
3:C:50:VAL:CA	3:C:54:GLN:HG2	1.51	1.25
18:d:105:THR:CG2	18:d:106:PRO:HD3	1.64	1.25
17:c:168:GLU:CD	17:c:169:LYS:H	1.43	1.25
22:h:83:LYS:HD2	22:h:98:ASP:CG	1.60	1.25
19:e:385:LEU:CG	19:e:398:ASP:OD1	1.87	1.23
22:h:139:MET:O	22:h:142:LYS:HG3	1.38	1.23
35:e:501:ADP:O2B	20:f:291:ARG:NH1	1.71	1.22
7:U:43:ARG:CG	7:U:164:LYS:O	1.87	1.22
20:f:185:ARG:NH1	21:g:321:GLN:CG	2.02	1.22
23:i:584:TYR:O	23:i:587:ALA:HB2	1.38	1.22
18:d:390:LEU:HD11	18:d:395:ILE:CG2	1.70	1.22
18:d:232:LYS:CB	35:d:501:ADP:O4'	1.88	1.21
19:e:323:ARG:CG	22:h:143:VAL:CG2	2.15	1.21
19:e:122:GLU:CD	31:q:278:GLN:CB	2.13	1.21
18:d:259:TYR:HE2	19:e:276:ASP:OD1	1.16	1.21
22:h:114:VAL:CG2	22:h:126:ILE:HD12	1.68	1.21
21:g:424:ILE:O	21:g:426:GLU:N	1.73	1.21
19:e:200:ARG:N	19:e:328:ASP:OD2	1.71	1.20
18:d:283:PHE:CE2	18:d:285:ASP:HA	1.75	1.20
22:h:114:VAL:HG21	22:h:126:ILE:CD1	1.69	1.20
23:i:623:GLY:HA2	23:i:655:ALA:O	1.41	1.19
22:h:78:ARG:HB2	22:h:110:PRO:CG	1.71	1.19
15:Q:192:ILE:HD12	15:Q:228:TYR:C	1.66	1.19
18:d:255:LEU:CD1	18:d:267:VAL:HG11	1.71	1.19
17:c:168:GLU:CD	17:c:169:LYS:N	2.00	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:230:THR:O	18:d:353:PHE:CZ	1.94	1.18
15:Q:192:ILE:CD1	15:Q:228:TYR:C	2.16	1.18
23:i:584:TYR:O	23:i:587:ALA:CB	1.92	1.18
17:c:336:ARG:O	17:c:337:LEU:CD1	1.91	1.18
20:f:341:ALA:C	21:g:345:SER:HG	1.52	1.18
17:c:177:VAL:HB	17:c:224:LEU:CD1	1.71	1.18
18:d:105:THR:HG22	18:d:106:PRO:CD	1.72	1.17
18:d:105:THR:HB	18:d:106:PRO:HD2	1.19	1.17
31:q:231:LEU:O	31:q:232:GLN:O	1.61	1.17
20:f:286:ASP:OD1	20:f:287:PRO:HD2	1.40	1.17
15:Q:188:ILE:HG21	15:Q:228:TYR:CE2	1.79	1.16
21:g:273:ALA:O	21:g:277:GLU:HG2	1.44	1.16
2:P:240:HIS:C	2:P:242:GLU:H	1.37	1.16
17:c:220:THR:O	35:c:501:ADP:O2A	1.57	1.16
20:f:341:ALA:C	21:g:345:SER:OG	1.88	1.16
18:d:227:PRO:O	18:d:230:THR:CG2	1.92	1.16
28:n:263:ALA:O	28:n:265:LEU:N	1.79	1.16
20:f:61:LEU:CD2	20:f:78:ARG:HD3	1.76	1.15
8:H:1:THR:HG22	8:H:33:LYS:HZ1	1.12	1.15
20:f:128:GLY:HA3	21:g:321:GLN:NE2	1.62	1.15
21:g:397:LYS:NZ	35:g:502:ADP:O3'	1.80	1.14
23:i:625:ILE:O	23:i:627:PHE:N	1.81	1.14
15:Q:188:ILE:HG21	15:Q:228:TYR:OH	1.46	1.14
18:d:260:LEU:C	18:d:262:ASP:H	1.30	1.14
18:d:407:LEU:HD22	22:h:178:LEU:CD1	1.76	1.14
22:h:271:ARG:CZ	22:h:275:GLU:CB	2.04	1.13
15:Q:188:ILE:CG2	15:Q:228:TYR:CE2	2.31	1.13
16:S:236:LEU:C	16:S:238:GLU:H	1.38	1.13
21:g:393:GLY:HA2	21:g:396:CYS:SG	1.89	1.13
18:d:257:GLN:HE21	18:d:260:LEU:HD23	1.01	1.12
18:d:284:ILE:CG2	18:d:287:ILE:CG2	2.26	1.12
19:e:385:LEU:HG	19:e:398:ASP:OD1	1.47	1.12
26:l:154:LEU:HA	26:l:157:LEU:HD23	1.14	1.12
27:m:205:VAL:HG12	27:m:245:GLU:OE2	1.49	1.12
15:Q:32:ALA:CA	15:Q:45:VAL:HG12	1.70	1.12
20:f:126:ASP:HB3	21:g:320:PHE:HB3	1.32	1.12
20:f:185:ARG:HH11	21:g:321:GLN:HG3	0.95	1.12
19:e:205:TYR:OH	19:e:332:GLU:HB2	1.50	1.11
18:d:390:LEU:CD1	18:d:395:ILE:HG23	1.78	1.11
26:l:243:ASP:O	26:l:245:PRO:N	1.81	1.11
19:e:167:ILE:O	35:e:501:ADP:N1	1.84	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:185:ARG:HH11	21:g:321:GLN:CG	1.63	1.11
18:d:259:TYR:CE2	19:e:276:ASP:OD1	2.03	1.11
18:d:283:PHE:CD2	18:d:285:ASP:HB3	1.83	1.11
22:h:83:LYS:CD	22:h:98:ASP:OD1	1.97	1.11
22:h:116:LEU:O	22:h:118:ASN:N	1.84	1.11
8:H:1:THR:HG22	8:H:33:LYS:NZ	1.63	1.11
7:G:29:PHE:CD2	19:e:414:HIS:CE1	2.39	1.10
20:f:126:ASP:CB	21:g:320:PHE:HB3	1.79	1.10
27:m:208:PHE:CE2	27:m:211:TYR:HA	1.85	1.10
15:Q:206:ILE:HG23	15:Q:225:ILE:HG21	1.24	1.09
20:f:64:LEU:HA	20:f:69:PHE:CD1	1.86	1.09
21:g:342:LEU:C	21:g:343:LEU:HD13	1.77	1.09
2:B:240:HIS:CE1	2:B:243:GLU:OE1	2.04	1.09
18:d:224:LEU:CD1	18:d:233:THR:CG2	2.29	1.09
21:g:369:HIS:CE1	21:g:397:LYS:HB2	1.86	1.09
23:i:619:VAL:O	23:i:655:ALA:HB2	1.52	1.09
18:d:221:GLY:O	18:d:348:ASP:OD1	1.67	1.09
17:c:165:GLN:CA	17:c:237:PHE:O	1.99	1.09
22:h:271:ARG:NH2	22:h:275:GLU:HA	1.10	1.09
28:n:242:LEU:CB	28:n:246:VAL:CB	2.31	1.09
23:i:623:GLY:CA	23:i:655:ALA:O	2.00	1.08
26:l:163:LYS:HG3	26:l:167:VAL:CG1	1.82	1.08
29:o:105:PRO:O	29:o:107:ASN:N	1.85	1.08
18:d:224:LEU:CD1	18:d:233:THR:HG23	1.82	1.08
19:e:323:ARG:HD3	22:h:143:VAL:CA	1.82	1.08
5:E:31:GLN:HE21	21:g:435:LEU:CD2	1.58	1.08
22:h:114:VAL:CG1	22:h:127:LEU:N	2.15	1.08
2:B:176:LYS:HD2	3:C:52:LYS:HG2	1.34	1.07
7:U:40:VAL:CA	7:U:167:ALA:HB2	1.84	1.07
19:e:385:LEU:CB	19:e:398:ASP:OD1	2.01	1.07
19:e:404:LYS:CA	19:e:407:ILE:HG13	1.60	1.07
21:g:342:LEU:O	21:g:343:LEU:CD1	2.01	1.07
27:m:205:VAL:CG1	27:m:245:GLU:OE2	2.02	1.07
2:B:240:HIS:HE1	2:B:243:GLU:OE1	1.35	1.07
7:U:43:ARG:HG3	7:U:164:LYS:O	0.90	1.07
22:h:140:VAL:O	22:h:142:LYS:CD	2.03	1.07
24:j:339:ASN:O	24:j:341:SER:N	1.88	1.07
4:D:18:GLU:CG	21:g:432:LYS:HE3	1.45	1.07
18:d:257:GLN:HE21	18:d:260:LEU:CD2	1.68	1.07
26:l:163:LYS:HG3	26:l:167:VAL:HG13	1.12	1.07
26:l:157:LEU:H	26:l:157:LEU:HD22	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:ARG:HD3	4:D:25:GLU:OE1	1.53	1.06
15:Q:32:ALA:HA	15:Q:45:VAL:HG13	1.08	1.06
15:Q:192:ILE:CD1	15:Q:228:TYR:CA	2.32	1.06
8:H:3:ILE:HD11	8:H:44:CYS:HB3	1.32	1.06
17:c:179:GLY:O	17:c:180:CYS:SG	2.13	1.06
15:Q:188:ILE:CD1	15:Q:228:TYR:OH	2.02	1.06
19:e:323:ARG:NE	22:h:143:VAL:CG2	2.03	1.06
22:h:88:LYS:HB2	22:h:93:GLY:O	1.54	1.06
18:d:260:LEU:C	18:d:262:ASP:N	2.05	1.05
20:f:185:ARG:NH1	21:g:321:GLN:HG3	1.68	1.05
21:g:342:LEU:O	21:g:343:LEU:HD12	1.55	1.05
22:h:94:LYS:O	22:h:95:PHE:CD2	2.08	1.05
31:q:50:PRO:O	31:q:52:GLU:N	1.89	1.05
18:d:143:LEU:HD13	18:d:162:VAL:HG21	1.38	1.05
18:d:255:LEU:CD1	18:d:267:VAL:CG1	2.33	1.05
7:U:40:VAL:CA	7:U:167:ALA:CB	2.34	1.05
22:h:78:ARG:CZ	22:h:108:VAL:O	2.04	1.05
23:i:475:HIS:HA	23:i:511:ALA:HB2	1.33	1.05
15:Q:188:ILE:HG22	15:Q:228:TYR:CE1	1.91	1.05
18:d:224:LEU:HD12	18:d:233:THR:HG23	1.09	1.05
8:H:1:THR:CG2	8:H:33:LYS:NZ	2.20	1.04
8:H:3:ILE:CD1	8:H:44:CYS:HB3	1.86	1.04
20:f:342:ASP:OD1	21:g:345:SER:CB	2.05	1.04
22:h:132:ASP:O	22:h:135:VAL:HG22	1.57	1.04
18:d:407:LEU:HD22	22:h:178:LEU:HD12	1.07	1.04
22:h:271:ARG:CZ	22:h:275:GLU:HB2	1.52	1.04
18:d:342:ILE:HA	18:d:347:ILE:HG22	1.39	1.04
7:G:29:PHE:CE2	19:e:414:HIS:NE2	2.25	1.04
26:l:154:LEU:CA	26:l:157:LEU:HD23	1.82	1.04
2:B:168:SER:C	2:B:172:VAL:N	2.15	1.04
18:d:105:THR:CB	18:d:106:PRO:HD2	1.87	1.04
18:d:257:GLN:NE2	18:d:260:LEU:HD23	1.73	1.04
18:d:259:TYR:CE1	19:e:275:PHE:O	2.10	1.04
19:e:385:LEU:HB3	19:e:398:ASP:OD1	1.58	1.03
20:f:61:LEU:HD21	20:f:78:ARG:CD	1.86	1.03
22:h:78:ARG:NE	22:h:108:VAL:O	1.89	1.03
23:i:544:ILE:CB	23:i:577:ILE:CB	2.35	1.03
2:P:168:SER:C	2:P:172:VAL:N	2.15	1.03
18:d:105:THR:CB	18:d:106:PRO:CD	2.36	1.03
20:f:182:LEU:HD23	20:f:183:LEU:N	1.71	1.03
7:U:40:VAL:HA	7:U:167:ALA:HB2	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:342:ILE:HG13	18:d:344:PRO:HD3	1.38	1.03
17:c:345:LEU:CD2	17:c:381:THR:HG22	1.88	1.02
19:e:214:MET:HE2	35:e:501:ADP:H2'	1.40	1.02
18:d:259:TYR:OH	19:e:276:ASP:CA	2.07	1.02
2:P:240:HIS:C	2:P:242:GLU:N	2.13	1.02
15:Q:32:ALA:HA	15:Q:45:VAL:HG12	1.26	1.02
18:d:232:LYS:HD3	18:d:235:LEU:HD23	1.39	1.02
20:f:125:GLU:OE1	20:f:195:PHE:O	1.78	1.02
21:g:418:GLU:O	21:g:422:GLU:HB3	1.57	1.02
3:C:46:GLU:OE1	3:C:199:VAL:CB	2.09	1.01
15:Q:220:LEU:HB3	15:Q:224:GLU:HB2	1.03	1.01
7:U:163:PHE:CG	7:U:166:THR:CG2	2.42	1.01
20:f:182:LEU:HD23	20:f:183:LEU:H	1.19	1.01
7:G:29:PHE:HD2	19:e:414:HIS:HE1	1.08	1.01
26:l:243:ASP:O	26:l:245:PRO:CD	2.07	1.01
17:c:248:LYS:HB2	18:d:262:ASP:OD2	1.61	1.01
18:d:105:THR:CG2	18:d:106:PRO:CD	2.33	1.01
20:f:185:ARG:NH1	21:g:321:GLN:HG2	1.76	1.01
26:l:163:LYS:CG	26:l:167:VAL:HG13	1.90	1.01
7:G:29:PHE:HD2	19:e:414:HIS:CE1	1.73	1.01
18:d:257:GLN:OE1	18:d:266:LEU:HD13	1.61	1.01
19:e:263:PHE:CE2	19:e:265:ASP:OD1	2.13	1.01
4:D:18:GLU:OE1	4:D:20:ARG:CZ	2.09	1.00
8:V:3:ILE:HD11	8:V:44:CYS:HB3	1.14	1.00
18:d:259:TYR:OH	19:e:276:ASP:HB2	1.61	1.00
20:f:127:PRO:O	20:f:189:SER:HB2	1.58	1.00
22:h:136:SER:O	22:h:140:VAL:CG1	2.08	1.00
4:D:18:GLU:HG2	21:g:432:LYS:CE	1.54	1.00
10:J:181:ARG:HG2	10:J:190:ASN:HB3	1.44	1.00
16:S:236:LEU:C	16:S:238:GLU:N	2.13	1.00
23:i:475:HIS:HA	23:i:511:ALA:CB	1.91	1.00
18:d:230:THR:O	18:d:353:PHE:CE2	2.14	1.00
20:f:185:ARG:HH12	21:g:321:GLN:CA	1.74	1.00
19:e:404:LYS:HA	19:e:407:ILE:HG13	1.44	1.00
15:Q:220:LEU:CB	15:Q:224:GLU:CB	2.40	1.00
26:l:163:LYS:HD3	26:l:166:LEU:HB3	1.42	1.00
23:i:619:VAL:O	23:i:655:ALA:CB	2.09	1.00
22:h:127:LEU:HB3	22:h:128:PRO:HD2	1.43	1.00
23:i:613:ASP:O	23:i:616:ARG:N	1.95	1.00
20:f:63:GLN:O	20:f:65:THR:N	1.94	0.99
23:i:585:THR:C	23:i:587:ALA:H	1.69	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:n:242:LEU:O	28:n:243:GLN:O	1.78	0.99
18:d:255:LEU:HD11	18:d:267:VAL:HG11	1.39	0.99
7:U:41:ALA:O	7:U:165:ALA:HB1	1.61	0.99
18:d:107:MET:CE	18:d:151:LEU:HD13	1.93	0.99
18:d:259:TYR:OH	19:e:275:PHE:O	1.79	0.99
18:d:259:TYR:OH	19:e:276:ASP:CB	2.10	0.99
2:B:176:LYS:HD2	3:C:52:LYS:CG	1.86	0.99
15:Q:32:ALA:N	15:Q:45:VAL:HG12	1.77	0.99
18:d:371:ARG:HG3	22:h:179:GLY:HA2	1.44	0.99
2:P:34:CYS:HA	2:P:46:ALA:O	1.62	0.99
17:c:177:VAL:CB	17:c:224:LEU:HD12	1.93	0.99
19:e:122:GLU:HA	31:q:278:GLN:CB	1.93	0.99
19:e:323:ARG:CD	22:h:143:VAL:HG23	1.49	0.99
20:f:128:GLY:HA3	21:g:321:GLN:HE22	0.83	0.99
22:h:353:GLY:O	22:h:354:ALA:O	1.81	0.99
19:e:122:GLU:OE2	31:q:279:ASP:N	1.94	0.98
27:m:200:LEU:O	27:m:204:THR:OG1	1.80	0.98
17:c:336:ARG:O	17:c:337:LEU:HD13	1.59	0.98
15:Q:220:LEU:CG	15:Q:224:GLU:HG3	1.92	0.98
7:U:42:VAL:HG22	7:U:49:VAL:O	1.63	0.98
17:c:177:VAL:HB	17:c:224:LEU:HD12	0.98	0.98
21:g:264:GLY:O	21:g:267:LEU:HD23	1.61	0.98
22:h:196:LYS:HG3	35:h:401:ADP:O1B	1.61	0.98
17:c:219:GLY:O	17:c:383:ALA:HB3	1.63	0.98
22:h:140:VAL:O	22:h:142:LYS:HD3	1.61	0.98
20:f:182:LEU:O	20:f:185:ARG:N	1.96	0.97
18:d:227:PRO:O	18:d:230:THR:HG22	1.58	0.97
18:d:284:ILE:HG22	18:d:287:ILE:HG23	1.42	0.97
21:g:74:LYS:O	21:g:78:GLU:HB2	1.64	0.97
2:B:34:CYS:HA	2:B:46:ALA:O	1.62	0.97
18:d:233:THR:N	35:d:501:ADP:O1A	1.72	0.97
20:f:125:GLU:OE2	20:f:197:LYS:HB3	1.63	0.97
15:Q:192:ILE:HD13	15:Q:228:TYR:CA	1.92	0.97
17:c:327:LEU:O	17:c:332:MET:HE3	1.65	0.97
19:e:386:ALA:N	19:e:398:ASP:OD2	1.97	0.97
21:g:424:ILE:C	21:g:426:GLU:H	1.72	0.97
14:N:201:THR:C	14:N:202:PRO:N	2.23	0.96
20:f:128:GLY:CA	21:g:321:GLN:HE22	1.77	0.96
22:h:114:VAL:HG11	22:h:127:LEU:H	1.22	0.96
8:H:1:THR:CB	8:H:33:LYS:NZ	2.28	0.96
19:e:323:ARG:HD3	22:h:143:VAL:HA	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:284:ILE:HG22	18:d:287:ILE:HG22	1.47	0.96
28:n:263:ALA:C	28:n:265:LEU:H	1.71	0.96
21:g:231:THR:O	35:g:502:ADP:O2A	1.82	0.96
18:d:341:LEU:O	18:d:346:ARG:HB2	1.64	0.96
22:h:132:ASP:O	22:h:135:VAL:CG2	2.12	0.96
4:D:18:GLU:OE1	4:D:20:ARG:NH1	1.80	0.96
15:Q:220:LEU:CB	15:Q:224:GLU:HB2	1.96	0.96
7:U:42:VAL:CG2	7:U:49:VAL:O	2.13	0.96
23:i:625:ILE:O	23:i:626:LEU:C	2.07	0.96
22:h:114:VAL:HG11	22:h:126:ILE:C	1.90	0.96
7:G:29:PHE:HE2	19:e:414:HIS:NE2	1.62	0.95
15:Q:47:LYS:HA	15:Q:207:GLU:OE1	1.65	0.95
19:e:87:LEU:HD23	19:e:87:LEU:H	1.30	0.95
18:d:257:GLN:OE1	18:d:266:LEU:HD12	1.62	0.95
18:d:255:LEU:HD21	18:d:312:LEU:HD23	1.48	0.95
22:h:137:LEU:HA	22:h:140:VAL:CG1	1.97	0.95
18:d:260:LEU:CD2	18:d:263:GLY:HA2	1.72	0.95
27:m:195:LYS:O	27:m:199:GLU:OE2	1.84	0.95
20:f:290:LEU:CD2	20:f:298:LYS:HD3	1.97	0.95
20:f:342:ASP:N	21:g:345:SER:OG	1.97	0.95
23:i:522:GLY:O	23:i:558:GLY:CA	2.10	0.95
21:g:393:GLY:CA	21:g:396:CYS:SG	2.54	0.95
18:d:342:ILE:HD12	18:d:350:LYS:NZ	1.81	0.94
23:i:522:GLY:O	23:i:558:GLY:HA3	1.53	0.94
27:m:208:PHE:CE2	27:m:211:TYR:CA	2.50	0.94
7:U:163:PHE:CG	7:U:166:THR:HG22	2.02	0.94
17:c:384:GLU:OE1	17:c:385:ILE:N	1.99	0.94
3:C:50:VAL:O	3:C:54:GLN:HB2	1.66	0.94
20:f:177:GLY:H	21:g:344:ARG:HD2	1.31	0.94
18:d:407:LEU:CD2	22:h:178:LEU:HD12	1.97	0.94
20:f:185:ARG:HH12	21:g:321:GLN:HA	1.30	0.94
27:m:195:LYS:O	27:m:199:GLU:CD	2.10	0.94
15:Q:32:ALA:CA	15:Q:45:VAL:HG13	1.87	0.94
15:Q:32:ALA:CB	15:Q:45:VAL:CG1	2.44	0.94
19:e:266:GLU:HG2	20:f:258:MET:SD	2.07	0.94
8:V:3:ILE:CD1	8:V:44:CYS:CB	2.31	0.93
22:h:235:PHE:CE2	22:h:276:LEU:HD22	2.03	0.93
20:f:181:THR:CG2	35:g:501:ADP:O1B	2.15	0.93
27:m:171:GLY:O	27:m:173:ASP:OD1	1.85	0.93
15:Q:206:ILE:CG2	15:Q:225:ILE:HG21	1.88	0.93
18:d:259:TYR:CZ	19:e:275:PHE:O	2.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:356:GLY:HA3	35:h:401:ADP:H8	1.22	0.93
22:h:356:GLY:CA	35:h:401:ADP:C8	2.52	0.93
18:d:284:ILE:CG2	18:d:287:ILE:HG22	1.94	0.93
23:i:475:HIS:CA	23:i:511:ALA:HB2	1.98	0.93
23:i:539:THR:O	23:i:541:HIS:N	2.01	0.93
23:i:612:ASP:CB	23:i:647:HIS:CB	2.47	0.93
18:d:342:ILE:HB	18:d:347:ILE:CG2	1.98	0.92
23:i:497:LEU:O	23:i:501:LEU:N	2.00	0.92
21:g:273:ALA:O	21:g:277:GLU:CG	2.16	0.92
21:g:342:LEU:C	21:g:343:LEU:CD1	2.41	0.92
18:d:232:LYS:HB2	35:d:501:ADP:O4'	0.92	0.92
22:h:126:ILE:C	22:h:127:LEU:HD23	1.94	0.92
18:d:143:LEU:HD13	18:d:162:VAL:CG2	1.98	0.92
22:h:268:GLU:O	22:h:272:THR:OG1	1.84	0.92
18:d:260:LEU:HD21	18:d:263:GLY:HA2	1.47	0.92
20:f:61:LEU:HD11	20:f:72:LYS:CB	1.99	0.92
18:d:143:LEU:CD1	18:d:162:VAL:HG21	1.99	0.92
23:i:475:HIS:HA	23:i:511:ALA:CA	2.00	0.92
20:f:64:LEU:CA	20:f:69:PHE:CE1	2.50	0.91
4:D:18:GLU:HG2	21:g:432:LYS:HE2	1.52	0.91
19:e:213:THR:OG1	35:e:501:ADP:O1B	1.89	0.91
7:U:163:PHE:CD2	7:U:166:THR:HG22	2.01	0.91
7:U:39:SER:O	7:U:167:ALA:CB	2.17	0.91
15:Q:220:LEU:HB3	15:Q:224:GLU:CG	2.00	0.91
26:l:247:ALA:O	26:l:251:LEU:HB2	1.71	0.91
17:c:168:GLU:OE1	17:c:169:LYS:O	1.87	0.91
18:d:106:PRO:HB3	22:h:121:TYR:HB2	1.53	0.91
18:d:259:TYR:HH	19:e:275:PHE:C	1.79	0.91
19:e:323:ARG:NE	22:h:143:VAL:HG13	1.85	0.91
17:c:384:GLU:O	17:c:387:SER:N	2.04	0.91
19:e:385:LEU:C	19:e:398:ASP:OD2	2.13	0.91
17:c:248:LYS:CB	18:d:262:ASP:CG	2.45	0.90
19:e:403:TYR:O	19:e:407:ILE:N	2.04	0.90
18:d:105:THR:O	18:d:107:MET:N	2.05	0.90
28:n:242:LEU:CA	28:n:246:VAL:CB	2.49	0.90
19:e:403:TYR:O	19:e:407:ILE:CA	2.19	0.90
18:d:105:THR:HB	18:d:106:PRO:CD	1.98	0.90
7:U:40:VAL:HA	7:U:167:ALA:HB3	1.54	0.89
20:f:61:LEU:HD21	20:f:78:ARG:NE	1.85	0.89
22:h:136:SER:C	22:h:140:VAL:HG12	1.96	0.89
31:q:232:GLN:O	31:q:234:TYR:N	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:188:ILE:HD13	15:Q:228:TYR:HH	1.14	0.89
17:c:345:LEU:HD22	17:c:381:THR:HG22	1.53	0.89
20:f:122:MET:CE	20:f:194:ASN:HD22	1.84	0.89
15:Q:47:LYS:HG3	15:Q:206:ILE:O	1.68	0.89
26:l:64:ALA:O	26:l:68:GLY:HA3	1.72	0.89
22:h:137:LEU:HA	22:h:140:VAL:HG13	1.54	0.89
23:i:634:PRO:HG3	23:i:666:LYS:O	1.72	0.89
19:e:206:GLY:HA3	19:e:212:LYS:HE2	1.55	0.89
21:g:434:ASN:O	21:g:437:TYR:HE1	1.55	0.89
18:d:342:ILE:CG1	18:d:344:PRO:HD3	2.02	0.89
8:H:1:THR:CG2	8:H:33:LYS:HZ1	1.81	0.89
18:d:265:LYS:HA	18:d:265:LYS:CE	2.00	0.89
19:e:326:ARG:HG3	19:e:326:ARG:HH11	1.36	0.88
17:c:248:LYS:HB2	18:d:262:ASP:CG	1.99	0.88
23:i:497:LEU:O	23:i:501:LEU:CB	2.22	0.88
25:k:293:ASP:O	25:k:296:LEU:N	2.06	0.88
31:q:274:ASN:O	31:q:276:GLY:O	1.90	0.88
22:h:235:PHE:CD2	22:h:276:LEU:HD22	2.09	0.88
20:f:46:ASP:O	20:f:50:LEU:HB2	1.73	0.88
20:f:181:THR:HG23	35:g:501:ADP:O1B	1.71	0.88
22:h:114:VAL:HG12	22:h:127:LEU:CD2	2.04	0.88
14:b:201:THR:C	14:b:203:PRO:N	2.23	0.88
4:D:20:ARG:CD	4:D:25:GLU:OE1	2.22	0.88
19:e:408:LYS:O	19:e:410:ASP:N	2.06	0.88
5:E:31:GLN:HE22	21:g:435:LEU:HD21	1.37	0.87
18:d:227:PRO:C	18:d:230:THR:HG22	1.99	0.87
27:m:208:PHE:HD2	27:m:211:TYR:HA	1.39	0.87
19:e:85:ILE:HG21	20:f:82:GLY:H	1.38	0.87
19:e:323:ARG:NE	22:h:143:VAL:CG1	2.37	0.87
22:h:140:VAL:O	22:h:142:LYS:HD2	1.73	0.87
15:Q:32:ALA:HB2	15:Q:45:VAL:HG11	1.54	0.87
8:V:3:ILE:HD11	8:V:44:CYS:SG	2.14	0.87
20:f:126:ASP:O	20:f:185:ARG:HG2	1.72	0.87
22:h:114:VAL:HG13	22:h:127:LEU:HG	1.53	0.87
23:i:619:VAL:C	23:i:655:ALA:HB2	1.99	0.87
18:d:107:MET:HE2	18:d:151:LEU:HD13	1.55	0.87
20:f:61:LEU:HD21	20:f:78:ARG:HD3	1.48	0.87
20:f:64:LEU:HA	20:f:69:PHE:CE1	2.00	0.87
19:e:323:ARG:HD2	22:h:143:VAL:HG23	1.17	0.87
18:d:342:ILE:CD1	18:d:350:LYS:NZ	2.38	0.87
18:d:394:ASP:OD1	22:h:308:PRO:HG2	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:192:ILE:CD1	15:Q:228:TYR:CB	2.03	0.87
26:l:243:ASP:O	26:l:245:PRO:HD2	1.72	0.86
7:U:39:SER:C	7:U:167:ALA:HB1	2.00	0.86
8:H:1:THR:HB	8:H:33:LYS:HZ3	1.40	0.86
17:c:336:ARG:O	17:c:337:LEU:HD12	1.73	0.86
19:e:415:GLU:OE1	19:e:415:GLU:N	2.08	0.86
22:h:271:ARG:NH1	22:h:271:ARG:O	2.08	0.86
22:h:127:LEU:CB	22:h:128:PRO:HD2	2.04	0.86
1:A:176:ARG:HG2	26:l:160:MET:SD	2.16	0.86
22:h:114:VAL:CG1	22:h:127:LEU:CG	2.00	0.86
15:Q:206:ILE:HG21	15:Q:225:ILE:HG22	1.56	0.85
18:d:220:LYS:C	18:d:348:ASP:OD1	2.18	0.85
18:d:223:ILE:HB	18:d:347:ILE:HD11	1.56	0.85
19:e:323:ARG:HB3	19:e:323:ARG:HH11	1.40	0.85
4:D:18:GLU:CG	21:g:432:LYS:CE	2.14	0.85
4:D:18:GLU:HG3	21:g:432:LYS:HE3	1.58	0.85
15:Q:188:ILE:HG22	15:Q:228:TYR:CD1	2.12	0.85
22:h:83:LYS:CD	22:h:98:ASP:CG	2.45	0.85
17:c:384:GLU:C	17:c:386:ARG:N	2.31	0.85
23:i:566:LEU:O	23:i:568:GLU:N	2.09	0.85
19:e:214:MET:CE	35:e:501:ADP:H2'	2.06	0.85
26:l:165:LEU:HD13	26:l:166:LEU:N	1.90	0.85
7:U:42:VAL:CG2	7:U:49:VAL:C	2.49	0.85
19:e:267:ILE:CD1	19:e:309:MET:SD	2.65	0.85
15:Q:192:ILE:HD13	15:Q:228:TYR:CG	2.12	0.84
26:l:163:LYS:CD	26:l:166:LEU:CA	2.53	0.84
1:O:39:ALA:HB3	1:O:42:GLY:O	1.77	0.84
23:i:475:HIS:CB	23:i:507:VAL:O	2.25	0.84
23:i:613:ASP:O	23:i:615:ARG:N	2.09	0.84
3:C:45:VAL:HG21	3:C:61:LYS:HG3	1.57	0.84
18:d:259:TYR:OH	19:e:276:ASP:HA	1.76	0.84
20:f:193:CYS:SG	20:f:227:PRO:O	2.36	0.84
18:d:259:TYR:CZ	19:e:276:ASP:HA	2.13	0.84
35:e:501:ADP:O2B	20:f:291:ARG:CZ	2.25	0.84
7:G:44:GLY:O	7:G:46:ASP:N	2.10	0.84
20:f:61:LEU:HD11	20:f:72:LYS:HB2	1.56	0.84
22:h:78:ARG:HG2	22:h:110:PRO:HD3	1.59	0.84
8:H:1:THR:CB	8:H:33:LYS:HZ3	1.86	0.84
18:d:224:LEU:CD1	18:d:233:THR:HG22	2.06	0.84
22:h:114:VAL:CG1	22:h:127:LEU:H	1.84	0.84
20:f:179:GLY:N	35:g:501:ADP:C8	2.45	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:107:MET:CE	18:d:151:LEU:CD1	2.56	0.83
15:Q:221:ASN:O	15:Q:223:GLU:N	2.11	0.83
2:B:176:LYS:CD	3:C:52:LYS:HG2	2.06	0.83
19:e:397:LYS:O	19:e:401:LYS:CG	2.25	0.83
2:B:194:ILE:O	2:B:198:ASN:HB2	1.79	0.83
18:d:255:LEU:HD12	18:d:267:VAL:CG1	2.06	0.83
19:e:122:GLU:OE1	31:q:278:GLN:CB	2.27	0.83
22:h:271:ARG:HD3	22:h:271:ARG:C	2.02	0.83
19:e:373:ALA:HB2	35:e:501:ADP:H5'1	1.61	0.83
1:A:39:ALA:HB3	1:A:42:GLY:O	1.77	0.83
17:c:223:THR:O	17:c:226:ALA:N	2.11	0.83
22:h:335:LYS:NZ	27:m:170:GLU:OE2	2.09	0.83
23:i:570:LEU:CB	23:i:578:LEU:O	2.25	0.83
17:c:303:ILE:HG21	17:c:331:LEU:HD12	1.60	0.83
18:d:263:GLY:O	18:d:265:LYS:N	2.12	0.83
18:d:283:PHE:HE2	18:d:285:ASP:CA	1.70	0.83
19:e:201:GLY:HA3	19:e:327:LEU:HD13	1.60	0.83
20:f:291:ARG:O	20:f:292:PRO:C	2.20	0.82
27:m:167:LEU:C	27:m:168:ILE:HD12	2.04	0.82
19:e:87:LEU:HB2	19:e:132:LEU:O	1.77	0.82
20:f:185:ARG:NH1	21:g:321:GLN:CA	2.42	0.82
17:c:327:LEU:HB2	17:c:332:MET:CE	2.09	0.82
17:c:345:LEU:HD21	17:c:381:THR:HG22	1.62	0.82
19:e:323:ARG:CZ	22:h:143:VAL:HG13	2.09	0.82
21:g:222:GLY:O	21:g:348:LEU:HD12	1.79	0.82
5:E:31:GLN:NE2	21:g:435:LEU:HD23	1.93	0.82
8:H:1:THR:CG2	8:H:33:LYS:HZ3	1.89	0.82
18:d:342:ILE:CA	18:d:347:ILE:HG22	2.09	0.82
19:e:397:LYS:O	19:e:401:LYS:N	2.12	0.82
23:i:630:PRO:C	23:i:632:GLN:H	1.87	0.82
19:e:323:ARG:HD2	22:h:143:VAL:CG2	0.52	0.82
26:l:403:THR:O	26:l:406:ASN:N	2.11	0.82
18:d:227:PRO:O	18:d:230:THR:HG23	1.78	0.82
19:e:205:TYR:OH	19:e:332:GLU:CB	2.28	0.81
20:f:147:GLU:O	20:f:151:LEU:HB2	1.80	0.81
18:d:232:LYS:C	18:d:234:LEU:N	2.36	0.81
19:e:322:LEU:H	19:e:322:LEU:HD12	1.45	0.81
2:P:194:ILE:O	2:P:198:ASN:HB2	1.79	0.81
35:d:501:ADP:O3'	22:h:307:ARG:NH1	2.13	0.81
27:m:86:GLU:O	27:m:90:ASP:HB2	1.79	0.81
18:d:259:TYR:HE1	19:e:275:PHE:O	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:283:PHE:CD2	18:d:285:ASP:N	2.48	0.81
27:m:17:LEU:O	27:m:19:ILE:N	2.13	0.81
17:c:218:PRO:O	18:d:343:ARG:HG3	1.80	0.81
17:c:303:ILE:CG2	17:c:331:LEU:HD12	2.09	0.81
17:c:336:ARG:C	17:c:337:LEU:HD12	2.06	0.81
23:i:665:ASN:O	23:i:666:LYS:C	2.21	0.81
22:h:145:ASP:N	22:h:145:ASP:OD1	2.14	0.81
17:c:166:VAL:O	17:c:167:GLU:HB2	1.81	0.81
26:l:163:LYS:HE3	26:l:166:LEU:O	1.40	0.81
22:h:126:ILE:O	22:h:127:LEU:HD23	1.80	0.80
3:C:222:PRO:O	3:C:226:GLU:HG2	1.80	0.80
7:G:29:PHE:CD2	19:e:414:HIS:HE1	1.86	0.80
19:e:323:ARG:CD	22:h:143:VAL:CG2	0.88	0.80
19:e:167:ILE:O	35:e:501:ADP:C2	2.35	0.80
8:H:1:THR:HB	8:H:33:LYS:NZ	1.94	0.80
7:U:164:LYS:HB2	7:U:164:LYS:NZ	1.96	0.80
8:V:3:ILE:HD12	8:V:44:CYS:HB3	1.64	0.80
21:g:247:THR:HG23	21:g:281:SER:HB3	1.64	0.80
21:g:369:HIS:HE1	21:g:397:LYS:HB2	1.44	0.80
21:g:393:GLY:C	21:g:396:CYS:SG	2.65	0.80
22:h:61:GLU:O	22:h:65:LEU:HB2	1.81	0.80
28:n:242:LEU:O	28:n:243:GLN:C	2.24	0.80
14:N:29:ARG:HD2	13:a:179:ARG:HH12	1.47	0.80
18:d:342:ILE:HD12	18:d:350:LYS:HZ1	1.42	0.80
20:f:185:ARG:NH1	21:g:321:GLN:N	2.30	0.80
17:c:199:GLU:O	17:c:203:ASN:HB2	1.82	0.80
23:i:585:THR:O	23:i:587:ALA:N	2.14	0.80
19:e:199:PRO:C	19:e:328:ASP:OD2	2.25	0.80
1:A:176:ARG:HE	26:l:161:ASP:CG	1.88	0.79
5:E:31:GLN:HE21	21:g:435:LEU:HD23	1.44	0.79
20:f:125:GLU:CD	20:f:195:PHE:O	2.25	0.79
27:m:208:PHE:CD2	27:m:211:TYR:CA	2.57	0.79
20:f:204:VAL:HG22	21:g:261:ILE:HG21	1.62	0.79
22:h:133:PRO:O	22:h:136:SER:HB2	1.81	0.79
26:l:243:ASP:O	26:l:244:SER:C	2.20	0.79
3:C:50:VAL:CB	3:C:54:GLN:CB	2.59	0.79
21:g:264:GLY:O	21:g:267:LEU:CD2	2.29	0.79
18:d:371:ARG:CG	22:h:179:GLY:HA2	2.12	0.79
23:i:584:TYR:O	23:i:587:ALA:HB3	1.81	0.79
23:i:566:LEU:O	23:i:567:ILE:C	2.26	0.79
7:G:29:PHE:CE2	19:e:414:HIS:CE1	2.70	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:227:PRO:C	18:d:230:THR:CG2	2.55	0.79
20:f:64:LEU:C	20:f:66:GLU:H	1.88	0.79
18:d:144:LEU:H	18:d:144:LEU:HD22	1.47	0.79
13:M:26:MET:HE1	13:M:202:PRO:CG	2.13	0.79
10:X:182:VAL:CG2	10:X:191:LEU:HD11	2.13	0.79
19:e:199:PRO:CA	19:e:328:ASP:OD2	2.31	0.79
22:h:178:LEU:O	22:h:178:LEU:HD22	1.83	0.79
19:e:94:GLU:OE2	22:h:128:PRO:HG3	1.83	0.78
15:Q:31:THR:C	15:Q:45:VAL:HG12	2.08	0.78
8:V:2:THR:OG1	8:V:130:GLY:C	2.25	0.78
18:d:257:GLN:NE2	18:d:260:LEU:CD2	2.40	0.78
18:d:386:ALA:C	18:d:387:LYS:HD2	2.07	0.78
17:c:248:LYS:CB	18:d:262:ASP:OD2	2.31	0.78
17:c:336:ARG:O	17:c:337:LEU:HB2	1.82	0.78
17:c:383:ALA:HB2	35:c:501:ADP:C8	2.16	0.78
21:g:222:GLY:O	21:g:348:LEU:CD1	2.31	0.78
21:g:263:ASP:O	21:g:267:LEU:HD22	1.83	0.78
26:l:163:LYS:HD3	26:l:166:LEU:CB	2.12	0.78
26:l:406:ASN:O	26:l:408:SER:N	2.16	0.78
18:d:260:LEU:O	18:d:262:ASP:N	2.08	0.78
21:g:222:GLY:C	21:g:348:LEU:CD1	2.57	0.78
18:d:343:ARG:O	18:d:345:GLY:N	2.17	0.78
13:a:71:VAL:O	13:a:75:GLU:HB2	1.84	0.77
19:e:321:LEU:HD12	19:e:321:LEU:O	1.84	0.77
20:f:104:THR:HG21	31:q:50:PRO:HB3	1.66	0.77
4:D:20:ARG:HD3	4:D:25:GLU:CD	2.10	0.77
18:d:105:THR:HG22	18:d:106:PRO:HD3	0.82	0.77
23:i:665:ASN:O	23:i:667:GLU:N	2.17	0.77
5:E:31:GLN:HE22	21:g:432:LYS:HG3	1.48	0.77
17:c:219:GLY:O	17:c:383:ALA:CB	2.32	0.77
19:e:267:ILE:HD11	19:e:309:MET:SD	2.24	0.77
20:f:261:LEU:HG	20:f:294:ARG:HH21	1.49	0.77
21:g:435:LEU:HA	21:g:437:TYR:CE1	2.18	0.77
15:Q:221:ASN:HB2	15:Q:222:PRO:HD2	1.67	0.77
18:d:107:MET:HG3	22:h:96:VAL:HB	1.67	0.77
18:d:250:VAL:N	18:d:283:PHE:O	2.18	0.77
13:M:71:VAL:O	13:M:75:GLU:HB2	1.84	0.77
15:Q:220:LEU:HB3	15:Q:224:GLU:HB3	1.63	0.77
18:d:259:TYR:OH	19:e:275:PHE:C	2.26	0.77
18:d:312:LEU:O	18:d:316:LEU:HB2	1.84	0.77
18:d:232:LYS:HD2	35:d:501:ADP:C3'	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:122:GLU:OE1	31:q:279:ASP:CB	2.32	0.76
27:m:171:GLY:C	27:m:173:ASP:H	1.92	0.76
27:m:195:LYS:O	27:m:199:GLU:OE1	2.03	0.76
7:G:25:VAL:HG21	19:e:416:PHE:CE2	2.19	0.76
27:m:208:PHE:HE2	27:m:211:TYR:C	1.93	0.76
19:e:323:ARG:HD2	22:h:143:VAL:CB	1.94	0.76
17:c:336:ARG:O	17:c:337:LEU:CB	2.32	0.76
18:d:248:LEU:O	18:d:282:VAL:HA	1.85	0.76
18:d:255:LEU:CD2	18:d:312:LEU:HD23	2.15	0.76
21:g:75:GLU:O	21:g:79:LYS:HB2	1.85	0.76
18:d:283:PHE:HE2	18:d:285:ASP:HB2	1.49	0.76
17:c:163:MET:HE1	17:c:244:GLU:HB3	1.67	0.76
10:X:182:VAL:HG21	10:X:191:LEU:HD11	1.68	0.76
26:l:214:SER:O	26:l:218:HIS:HB2	1.85	0.76
19:e:96:VAL:HG23	22:h:128:PRO:HD3	1.66	0.76
17:c:384:GLU:O	17:c:385:ILE:C	2.29	0.75
20:f:64:LEU:C	20:f:66:GLU:N	2.43	0.75
26:l:406:ASN:O	26:l:409:LYS:N	2.18	0.75
15:Q:192:ILE:CD1	15:Q:228:TYR:O	2.33	0.75
18:d:283:PHE:CD2	18:d:285:ASP:CA	2.68	0.75
20:f:125:GLU:OE2	20:f:195:PHE:HD2	1.68	0.75
22:h:71:SER:HB3	22:h:116:LEU:HA	1.68	0.75
18:d:232:LYS:O	18:d:233:THR:C	2.29	0.75
22:h:78:ARG:HB2	22:h:110:PRO:HG3	0.83	0.75
23:i:630:PRO:C	23:i:632:GLN:N	2.44	0.75
26:l:243:ASP:OD2	26:l:246:LYS:HG3	1.87	0.75
10:J:187:GLY:O	10:J:189:HIS:CE1	2.39	0.75
18:d:149:SER:OG	18:d:163:LEU:HG	1.86	0.75
15:Q:220:LEU:CB	15:Q:224:GLU:CG	2.65	0.75
18:d:387:LYS:HD2	18:d:387:LYS:N	2.01	0.75
18:d:283:PHE:CZ	18:d:285:ASP:HA	2.21	0.75
23:i:625:ILE:C	23:i:627:PHE:N	2.45	0.75
15:Q:192:ILE:HD11	15:Q:228:TYR:O	1.87	0.74
15:Q:192:ILE:HG21	15:Q:228:TYR:CB	2.16	0.74
7:U:163:PHE:CB	7:U:166:THR:HG22	2.17	0.74
22:h:114:VAL:CG1	22:h:127:LEU:CB	2.65	0.74
27:m:200:LEU:H	27:m:200:LEU:HD12	1.52	0.74
20:f:224:ASP:OD2	20:f:225:HIS:CE1	2.40	0.74
21:g:369:HIS:ND1	21:g:397:LYS:HB2	2.02	0.74
17:c:157:ILE:HD12	17:c:161:VAL:CG1	2.18	0.74
20:f:61:LEU:HD11	20:f:72:LYS:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:177:GLY:N	21:g:344:ARG:HD2	2.02	0.74
21:g:431:LYS:HZ3	21:g:431:LYS:HB2	1.53	0.74
10:J:191:LEU:N	10:J:191:LEU:HD23	2.02	0.74
19:e:225:ALA:HB1	19:e:259:PRO:O	1.87	0.74
21:g:398:ALA:O	21:g:401:VAL:N	2.21	0.74
15:Q:32:ALA:HB2	15:Q:45:VAL:CG1	2.13	0.74
18:d:387:LYS:HG3	18:d:427:LEU:HD11	1.68	0.74
19:e:94:GLU:OE2	22:h:128:PRO:CG	2.36	0.74
21:g:431:LYS:HB2	21:g:431:LYS:NZ	2.01	0.74
27:m:44:ALA:O	27:m:47:ASP:C	2.30	0.74
35:e:501:ADP:O2B	20:f:291:ARG:NH2	2.19	0.74
20:f:291:ARG:O	20:f:291:ARG:HG2	1.88	0.74
27:m:208:PHE:CE2	27:m:211:TYR:C	2.66	0.74
18:d:144:LEU:HD13	18:d:144:LEU:N	2.04	0.73
22:h:141:GLU:C	22:h:143:VAL:N	2.45	0.73
20:f:122:MET:CE	20:f:194:ASN:ND2	2.51	0.73
23:i:498:LYS:O	23:i:502:TYR:CB	2.36	0.73
18:d:273:VAL:O	18:d:276:GLU:HG3	1.88	0.73
18:d:342:ILE:CD1	18:d:350:LYS:HZ1	1.99	0.73
20:f:125:GLU:OE1	20:f:195:PHE:HB3	1.87	0.73
20:f:193:CYS:SG	20:f:227:PRO:HG2	2.28	0.73
22:h:83:LYS:CB	22:h:98:ASP:OD1	2.36	0.73
15:Q:49:SER:O	15:Q:204:LYS:NZ	2.21	0.73
22:h:134:LEU:HD21	22:h:237:MET:CB	2.18	0.73
23:i:634:PRO:CG	23:i:666:LYS:O	2.35	0.73
30:p:9:CYS:HA	30:p:52:ILE:O	1.88	0.73
15:Q:192:ILE:CG1	15:Q:228:TYR:HB3	2.18	0.73
10:J:187:GLY:O	10:J:189:HIS:ND1	2.22	0.73
22:h:271:ARG:O	22:h:271:ARG:HD3	1.88	0.73
21:g:428:GLN:OE1	21:g:428:GLN:N	2.21	0.73
28:n:242:LEU:O	28:n:246:VAL:CB	2.37	0.73
22:h:69:GLN:OE1	22:h:69:GLN:HA	1.88	0.72
22:h:196:LYS:HG3	35:h:401:ADP:PB	2.28	0.72
26:l:204:PRO:O	26:l:208:ALA:HB3	1.88	0.72
31:q:50:PRO:C	31:q:52:GLU:H	1.96	0.72
4:D:161:THR:HG21	21:g:437:TYR:HB3	1.70	0.72
8:H:17:ASP:O	8:H:33:LYS:HD2	1.89	0.72
19:e:267:ILE:HG22	19:e:270:ILE:HD11	1.70	0.72
19:e:386:ALA:CA	19:e:398:ASP:OD2	2.36	0.72
18:d:232:LYS:HB2	35:d:501:ADP:C1'	2.16	0.72
18:d:249:ARG:HA	18:d:283:PHE:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:573:ASP:CB	23:i:578:LEU:CB	2.68	0.72
17:c:306:LEU:HB3	17:c:336:ARG:HB3	1.71	0.72
31:q:274:ASN:O	31:q:275:VAL:C	2.33	0.72
15:Q:220:LEU:HD13	15:Q:224:GLU:HB3	1.71	0.72
17:c:327:LEU:CB	17:c:332:MET:CE	2.66	0.72
22:h:88:LYS:HB3	22:h:93:GLY:O	1.89	0.72
23:i:570:LEU:CB	23:i:582:GLY:CA	2.68	0.72
25:k:293:ASP:O	25:k:297:GLU:N	2.21	0.72
8:V:1:THR:N	8:V:168:GLY:O	2.23	0.72
17:c:81:ALA:N	18:d:137:SER:HG	1.88	0.72
20:f:182:LEU:CD2	20:f:183:LEU:N	2.51	0.72
10:J:182:VAL:O	10:J:189:HIS:O	2.08	0.72
20:f:125:GLU:OE2	20:f:197:LYS:CB	2.27	0.72
19:e:322:LEU:HD12	19:e:322:LEU:N	2.05	0.72
20:f:204:VAL:CG2	21:g:261:ILE:HG21	2.19	0.71
7:U:164:LYS:HB2	7:U:164:LYS:HZ3	1.53	0.71
18:d:126:SER:OG	22:h:92:GLU:HG3	1.89	0.71
19:e:94:GLU:OE2	22:h:128:PRO:CB	2.38	0.71
19:e:323:ARG:NH1	19:e:324:PRO:HD2	2.04	0.71
8:H:3:ILE:HD11	8:H:44:CYS:CB	2.18	0.71
4:R:110:GLU:O	4:R:114:GLN:HB2	1.90	0.71
19:e:263:PHE:CZ	19:e:265:ASP:OD1	2.43	0.71
20:f:64:LEU:CA	20:f:69:PHE:CD1	2.70	0.71
23:i:569:SER:O	23:i:573:ASP:N	2.22	0.71
27:m:199:GLU:CD	27:m:199:GLU:H	1.97	0.71
3:C:50:VAL:O	3:C:54:GLN:CB	2.37	0.71
12:L:8:ASN:HD22	12:L:58:HIS:H	1.38	0.71
2:P:47:ALA:HB3	2:P:212:GLU:O	1.91	0.71
7:U:163:PHE:HB3	7:U:166:THR:HG22	1.73	0.71
18:d:248:LEU:O	18:d:281:ILE:O	2.08	0.71
18:d:284:ILE:HG21	18:d:287:ILE:CG2	2.17	0.71
22:h:117:ARG:O	22:h:117:ARG:HD2	1.89	0.71
26:l:165:LEU:HD13	26:l:165:LEU:C	2.15	0.71
19:e:85:ILE:HD13	19:e:85:ILE:N	2.05	0.71
12:Z:8:ASN:HD22	12:Z:58:HIS:H	1.38	0.71
19:e:71:GLU:O	19:e:75:ALA:HB2	1.89	0.71
22:h:94:LYS:O	22:h:95:PHE:CG	2.44	0.71
19:e:87:LEU:HD23	19:e:87:LEU:N	2.04	0.71
22:h:142:LYS:HD3	22:h:142:LYS:N	2.04	0.71
26:l:157:LEU:H	26:l:157:LEU:CD2	1.97	0.71
20:f:177:GLY:HA2	21:g:344:ARG:NE	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:393:GLY:C	21:g:396:CYS:HG	1.97	0.71
22:h:349:GLU:H	22:h:349:GLU:CD	1.98	0.70
27:m:168:ILE:HD12	27:m:168:ILE:N	2.05	0.70
28:n:242:LEU:HA	28:n:246:VAL:CB	2.21	0.70
15:Q:192:ILE:HG21	15:Q:228:TYR:HB3	1.71	0.70
20:f:289:LEU:HD23	20:f:289:LEU:C	2.16	0.70
31:q:274:ASN:O	31:q:276:GLY:N	2.24	0.70
2:B:47:ALA:HB3	2:B:212:GLU:O	1.91	0.70
17:c:157:ILE:HD12	17:c:161:VAL:HG13	1.71	0.70
20:f:342:ASP:CA	21:g:345:SER:OG	2.39	0.70
29:o:100:MET:C	29:o:102:PHE:H	1.98	0.70
18:d:232:LYS:O	18:d:234:LEU:CA	2.39	0.70
27:m:208:PHE:O	27:m:209:THR:CG2	2.40	0.70
22:h:134:LEU:CD2	22:h:237:MET:HG2	2.22	0.70
26:l:112:GLU:O	26:l:116:TRP:HB2	1.92	0.70
21:g:369:HIS:ND1	21:g:397:LYS:CB	2.55	0.70
18:d:106:PRO:HB3	22:h:121:TYR:CB	2.21	0.70
18:d:257:GLN:OE1	18:d:266:LEU:HD11	1.88	0.70
19:e:122:GLU:OE2	31:q:278:GLN:O	2.08	0.70
24:j:322:GLU:N	24:j:323:PRO:HD2	2.07	0.70
4:D:110:GLU:O	4:D:114:GLN:HB2	1.90	0.70
18:d:390:LEU:HD11	18:d:395:ILE:HG23	0.82	0.70
25:k:293:ASP:CB	25:k:296:LEU:H	2.04	0.70
19:e:323:ARG:HH11	19:e:323:ARG:CB	2.05	0.70
18:d:107:MET:HE3	18:d:151:LEU:HD13	1.71	0.69
19:e:114:ARG:HE	22:h:66:LEU:HD12	1.57	0.69
21:g:299:GLU:HG3	21:g:300:LYS:HD2	1.74	0.69
9:W:69:ARG:HH12	9:W:93:LEU:HD13	1.56	0.69
17:c:407:LYS:O	17:c:411:GLU:HB2	1.92	0.69
18:d:232:LYS:HD2	35:d:501:ADP:H3'	1.73	0.69
18:d:361:LYS:NZ	18:d:390:LEU:H	1.88	0.69
19:e:397:LYS:O	19:e:401:LYS:CA	2.38	0.69
20:f:122:MET:HE3	20:f:194:ASN:ND2	2.07	0.69
22:h:134:LEU:O	22:h:135:VAL:C	2.34	0.69
23:i:570:LEU:CB	23:i:582:GLY:N	2.55	0.69
23:i:630:PRO:O	23:i:633:CYS:N	2.25	0.69
17:c:164:MET:O	17:c:238:ILE:HA	1.92	0.69
15:Q:50:VAL:HA	15:Q:204:LYS:CD	2.11	0.69
20:f:125:GLU:OE2	20:f:195:PHE:CD2	2.45	0.69
24:j:320:THR:HA	28:n:254:ASN:CB	2.22	0.69
26:l:302:PHE:O	26:l:305:ALA:C	2.36	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:208:THR:HG23	12:Z:158:MET:HG3	1.73	0.69
19:e:408:LYS:C	19:e:410:ASP:H	2.00	0.69
20:f:126:ASP:HB3	21:g:320:PHE:CB	2.16	0.69
7:G:50:ILE:O	7:G:217:VAL:HA	1.91	0.69
15:Q:188:ILE:HG22	15:Q:228:TYR:CZ	2.08	0.69
7:U:50:ILE:O	7:U:217:VAL:HA	1.92	0.69
17:c:165:GLN:HG3	17:c:236:CYS:CB	2.18	0.69
19:e:408:LYS:HA	19:e:408:LYS:HZ3	1.56	0.69
20:f:60:VAL:C	20:f:62:LYS:H	2.00	0.69
20:f:63:GLN:N	20:f:63:GLN:OE1	2.25	0.69
23:i:679:PRO:O	23:i:681:ASN:N	2.26	0.69
9:I:69:ARG:HH12	9:I:93:LEU:HD13	1.56	0.69
18:d:232:LYS:O	18:d:232:LYS:HG2	1.92	0.69
18:d:251:VAL:HA	18:d:285:ASP:O	1.92	0.69
18:d:284:ILE:HG21	18:d:287:ILE:HG21	1.73	0.69
18:d:342:ILE:HD12	18:d:350:LYS:CE	2.23	0.69
22:h:117:ARG:HA	22:h:122:THR:H	1.58	0.69
22:h:210:THR:HG21	22:h:241:HIS:HD2	1.58	0.69
23:i:585:THR:C	23:i:587:ALA:N	2.41	0.69
26:l:243:ASP:C	26:l:245:PRO:CD	2.65	0.69
22:h:197:THR:OG1	35:h:401:ADP:O1A	2.04	0.69
5:E:62:LYS:HZ2	21:g:439:ALA:C	2.00	0.68
15:Q:206:ILE:HG22	15:Q:225:ILE:CG2	2.21	0.68
18:d:230:THR:O	18:d:353:PHE:HZ	1.71	0.68
18:d:341:LEU:HD22	18:d:347:ILE:HG21	1.75	0.68
22:h:340:ARG:HD3	27:m:205:VAL:O	1.93	0.68
26:l:153:LEU:HD13	26:l:157:LEU:HD21	1.74	0.68
18:d:255:LEU:HD12	18:d:267:VAL:HG13	1.74	0.68
19:e:206:GLY:H	19:e:212:LYS:HZ1	1.41	0.68
18:d:266:LEU:O	18:d:270:LEU:HB2	1.94	0.68
24:j:339:ASN:C	24:j:341:SER:N	2.50	0.68
7:G:29:PHE:HE2	19:e:414:HIS:HE2	1.16	0.68
18:d:284:ILE:CG2	18:d:287:ILE:HG21	2.23	0.68
19:e:199:PRO:HA	19:e:328:ASP:OD2	1.92	0.68
23:i:679:PRO:O	23:i:680:VAL:C	2.35	0.68
20:f:70:ILE:N	20:f:70:ILE:HD12	2.08	0.68
22:h:134:LEU:CD2	22:h:237:MET:CG	2.71	0.68
7:U:232:GLU:O	7:U:236:ASP:HB2	1.94	0.68
19:e:385:LEU:CD2	19:e:398:ASP:OD1	2.42	0.68
22:h:328:ILE:HD12	35:h:401:ADP:C6	2.29	0.68
4:D:20:ARG:CZ	4:D:25:GLU:OE1	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:134:LEU:HD21	22:h:237:MET:CG	2.24	0.68
26:l:163:LYS:HD3	26:l:166:LEU:CA	2.22	0.68
27:m:205:VAL:HG13	27:m:245:GLU:OE2	1.93	0.68
22:h:88:LYS:HA	22:h:93:GLY:C	2.12	0.68
22:h:326:LEU:O	22:h:330:LYS:HB2	1.94	0.68
25:k:293:ASP:O	25:k:294:LYS:C	2.37	0.68
12:Z:12:ILE:HG22	12:Z:25:SER:HA	1.76	0.68
20:f:290:LEU:HD23	20:f:298:LYS:HD3	1.76	0.68
12:L:12:ILE:HG22	12:L:25:SER:HA	1.76	0.67
20:f:118:LEU:HD13	20:f:121:ASN:HD22	1.59	0.67
20:f:122:MET:HE3	20:f:194:ASN:HD22	1.56	0.67
22:h:140:VAL:C	22:h:142:LYS:H	2.00	0.67
22:h:271:ARG:NH2	22:h:275:GLU:CB	2.36	0.67
18:d:257:GLN:HB3	18:d:260:LEU:HB2	1.75	0.67
19:e:122:GLU:CA	31:q:278:GLN:CB	2.71	0.67
27:m:14:ASN:C	27:m:146:ARG:HH22	2.02	0.67
7:G:232:GLU:O	7:G:236:ASP:HB2	1.94	0.67
18:d:361:LYS:HZ2	18:d:390:LEU:H	1.42	0.67
18:d:411:ARG:HH21	18:d:413:LYS:HB3	1.60	0.67
22:h:130:LYS:HD3	22:h:130:LYS:C	2.18	0.67
22:h:134:LEU:HD21	22:h:237:MET:HB3	1.75	0.67
26:l:243:ASP:OD2	26:l:246:LYS:CG	2.37	0.67
21:g:435:LEU:C	21:g:437:TYR:H	2.01	0.67
22:h:350:LEU:HD12	22:h:350:LEU:O	1.94	0.67
18:d:196:GLU:OE1	18:d:349:ARG:NH2	2.27	0.67
18:d:348:ASP:O	18:d:349:ARG:O	2.10	0.67
8:H:3:ILE:HD13	8:H:44:CYS:HB3	1.76	0.67
6:T:52:LEU:HD22	6:T:207:LYS:HD2	1.76	0.67
18:d:223:ILE:HB	18:d:347:ILE:CD1	2.25	0.67
18:d:343:ARG:O	18:d:344:PRO:C	2.37	0.67
19:e:85:ILE:HG21	20:f:82:GLY:N	2.08	0.67
23:i:623:GLY:HA3	23:i:655:ALA:O	1.91	0.67
20:f:60:VAL:HG22	20:f:62:LYS:H	1.61	0.66
18:d:360:THR:O	18:d:364:ILE:HB	1.95	0.66
20:f:179:GLY:N	35:g:501:ADP:N7	2.42	0.66
18:d:145:GLU:OE2	18:d:145:GLU:N	2.28	0.66
23:i:520:MET:C	23:i:557:TYR:CB	2.68	0.66
23:i:539:THR:O	23:i:540:GLN:C	2.39	0.66
4:D:28:ILE:HG21	21:g:434:ASN:HD22	1.59	0.66
15:Q:220:LEU:CD2	15:Q:224:GLU:CG	2.31	0.66
19:e:267:ILE:CG2	19:e:270:ILE:HD11	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:185:ARG:HH12	21:g:321:GLN:N	1.89	0.66
22:h:132:ASP:O	22:h:135:VAL:HG23	1.95	0.66
22:h:174:LEU:O	22:h:178:LEU:HB2	1.95	0.66
26:l:154:LEU:CA	26:l:157:LEU:CD2	2.66	0.66
23:i:522:GLY:O	23:i:558:GLY:HA2	1.90	0.66
2:P:90:LEU:HD13	2:P:110:LEU:HD21	1.78	0.66
19:e:213:THR:CG2	35:e:501:ADP:O1B	2.43	0.66
22:h:114:VAL:HG11	22:h:126:ILE:CA	2.26	0.66
27:m:202:LEU:HD23	27:m:202:LEU:N	2.10	0.66
15:Q:220:LEU:HD22	15:Q:224:GLU:CD	2.19	0.66
17:c:299:MET:HE2	17:c:331:LEU:CD1	2.26	0.66
20:f:64:LEU:O	20:f:64:LEU:HD13	1.95	0.66
22:h:83:LYS:HB2	22:h:98:ASP:OD1	1.96	0.66
2:B:90:LEU:HD13	2:B:110:LEU:HD21	1.78	0.66
9:W:159:PRO:O	9:W:163:PHE:HB2	1.96	0.66
21:g:437:TYR:H	21:g:437:TYR:HD1	1.42	0.66
7:U:42:VAL:HG23	7:U:49:VAL:O	1.96	0.66
18:d:283:PHE:CD2	18:d:285:ASP:CB	2.57	0.66
15:Q:192:ILE:HD12	15:Q:229:VAL:N	2.11	0.65
17:c:334:PRO:HG2	21:g:395:GLN:HG3	1.78	0.65
9:I:159:PRO:O	9:I:163:PHE:HB2	1.96	0.65
18:d:232:LYS:O	18:d:235:LEU:N	2.29	0.65
18:d:283:PHE:CE2	18:d:285:ASP:N	2.63	0.65
19:e:323:ARG:CD	22:h:143:VAL:CG1	2.75	0.65
19:e:412:GLN:HE21	19:e:412:GLN:C	2.05	0.65
21:g:428:GLN:HG2	21:g:429:ALA:H	1.61	0.65
27:m:44:ALA:O	27:m:47:ASP:O	2.14	0.65
31:q:230:THR:O	31:q:231:LEU:CB	2.43	0.65
10:J:108:ASP:HB3	10:J:111:GLU:HG2	1.78	0.65
13:M:26:MET:HE1	13:M:202:PRO:HG3	1.78	0.65
10:J:190:ASN:OD1	10:J:190:ASN:N	2.28	0.65
19:e:267:ILE:O	19:e:269:ALA:N	2.30	0.65
9:I:132:THR:HG22	9:I:134:ASP:H	1.60	0.65
21:g:369:HIS:CE1	35:g:502:ADP:O2'	2.50	0.65
26:l:157:LEU:HD22	26:l:157:LEU:N	2.03	0.65
17:c:248:LYS:CA	18:d:262:ASP:OD2	2.41	0.65
35:h:401:ADP:H2'	35:h:401:ADP:N3	2.12	0.65
8:H:219:LEU:HD21	9:I:194:ILE:HG12	1.79	0.65
9:I:33:MET:O	11:Y:166:ARG:NH1	2.30	0.65
18:d:270:LEU:HD11	18:d:282:VAL:HG23	1.77	0.65
19:e:202:VAL:HG13	19:e:331:ILE:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:328:ILE:HD12	35:h:401:ADP:C5	2.31	0.65
18:d:342:ILE:HB	18:d:347:ILE:HG21	1.79	0.65
19:e:206:GLY:N	19:e:212:LYS:NZ	2.45	0.65
19:e:210:CYS:O	35:e:501:ADP:N7	2.29	0.65
21:g:435:LEU:C	21:g:437:TYR:N	2.52	0.65
23:i:566:LEU:C	23:i:568:GLU:N	2.55	0.65
10:X:190:ASN:OD1	10:X:190:ASN:N	2.28	0.65
18:d:342:ILE:CB	18:d:347:ILE:CG2	2.75	0.65
19:e:122:GLU:CD	31:q:278:GLN:C	2.64	0.65
22:h:118:ASN:N	22:h:118:ASN:OD1	2.30	0.65
6:F:157:SER:H	7:G:88:ARG:HH22	1.45	0.64
15:Q:226:GLU:OE1	15:Q:226:GLU:HA	1.95	0.64
20:f:64:LEU:C	20:f:69:PHE:CE1	2.75	0.64
35:g:501:ADP:N3	35:g:501:ADP:H2'	2.12	0.64
26:l:240:ASP:OD1	26:l:240:ASP:N	2.29	0.64
31:q:299:CYS:O	31:q:302:ALA:HB3	1.97	0.64
3:C:31:THR:HA	3:C:162:GLY:HA3	1.80	0.64
8:H:2:THR:HG21	8:H:162:GLY:HA3	1.78	0.64
15:Q:220:LEU:CB	15:Q:224:GLU:HG3	2.26	0.64
15:Q:224:GLU:HA	15:Q:224:GLU:OE1	1.97	0.64
18:d:311:GLU:O	18:d:315:GLN:HB3	1.96	0.64
21:g:434:ASN:O	21:g:437:TYR:CE1	2.44	0.64
3:C:46:GLU:CD	3:C:199:VAL:CB	2.70	0.64
7:G:44:GLY:C	7:G:46:ASP:N	2.53	0.64
18:d:342:ILE:CD1	18:d:350:LYS:HZ3	2.10	0.64
19:e:205:TYR:CE2	19:e:332:GLU:HG2	2.32	0.64
20:f:182:LEU:O	20:f:183:LEU:C	2.39	0.64
18:d:224:LEU:HD11	18:d:233:THR:HG22	1.78	0.64
21:g:175:MET:HB3	21:g:249:LEU:HB2	1.78	0.64
2:B:240:HIS:ND1	2:B:243:GLU:HB3	2.13	0.64
9:W:132:THR:HG22	9:W:134:ASP:H	1.61	0.64
14:b:175:ARG:HG2	14:b:188:VAL:HG12	1.80	0.64
19:e:397:LYS:C	19:e:401:LYS:HB2	2.16	0.64
26:l:243:ASP:C	26:l:245:PRO:HD2	2.21	0.64
27:m:171:GLY:O	27:m:173:ASP:N	2.26	0.64
11:K:164:THR:HG22	11:K:170:SER:HB3	1.80	0.64
7:U:42:VAL:HG22	7:U:49:VAL:C	2.17	0.64
21:g:398:ALA:HA	21:g:401:VAL:HG12	1.79	0.64
3:C:50:VAL:HA	3:C:54:GLN:HG2	0.66	0.64
8:V:51:ASP:HB3	8:V:94:ILE:HG23	1.80	0.64
21:g:209:LYS:O	21:g:212:PHE:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:357:ALA:C	22:h:359:VAL:H	2.06	0.64
8:H:119:THR:H	14:N:53:GLN:HE22	1.45	0.64
23:i:613:ASP:C	23:i:615:ARG:N	2.54	0.64
24:j:339:ASN:O	24:j:340:MET:C	2.41	0.64
20:f:63:GLN:C	20:f:65:THR:H	2.01	0.64
18:d:284:ILE:HB	18:d:329:MET:HG2	1.80	0.64
12:L:14:ALA:HA	12:L:22:ILE:O	1.98	0.63
15:Q:192:ILE:HD12	15:Q:228:TYR:HB3	1.66	0.63
8:V:3:ILE:HG23	8:V:127:MET:H	1.63	0.63
17:c:274:PHE:HB2	17:c:319:MET:HG2	1.78	0.63
7:G:44:GLY:C	7:G:46:ASP:H	2.06	0.63
14:N:175:ARG:HG2	14:N:188:VAL:HG12	1.80	0.63
12:Z:14:ALA:HA	12:Z:22:ILE:O	1.98	0.63
14:b:45:ARG:HA	14:b:98:ILE:HG22	1.79	0.63
21:g:274:LEU:HA	21:g:277:GLU:HG3	1.80	0.63
27:m:171:GLY:C	27:m:173:ASP:N	2.56	0.63
18:d:341:LEU:CD1	18:d:341:LEU:H	2.11	0.63
27:m:104:MET:O	27:m:108:ALA:HB2	1.98	0.63
27:m:208:PHE:HE2	27:m:211:TYR:CA	2.05	0.63
2:B:91:ARG:HD3	9:I:75:LEU:HB3	1.81	0.63
14:N:45:ARG:HA	14:N:98:ILE:HG22	1.79	0.63
15:Q:31:THR:HA	15:Q:162:GLY:HA3	1.80	0.63
17:c:299:MET:HE2	17:c:331:LEU:HD12	1.79	0.63
19:e:391:ARG:HG3	25:k:134:GLY:HA3	1.81	0.63
18:d:265:LYS:HA	18:d:265:LYS:HE2	1.80	0.63
7:G:157:ALA:CB	19:e:416:PHE:CE1	2.81	0.63
8:H:208:THR:O	9:I:168:GLN:NE2	2.32	0.63
22:h:78:ARG:CG	22:h:110:PRO:HD3	2.28	0.63
24:j:339:ASN:C	24:j:341:SER:H	2.06	0.63
7:U:51:VAL:HG12	7:U:217:VAL:HG22	1.81	0.63
8:V:17:ASP:HB2	8:V:170:GLY:HA3	1.81	0.63
17:c:299:MET:CE	17:c:331:LEU:HD13	2.29	0.63
10:J:25:ILE:HG23	10:J:26:VAL:HG13	1.81	0.63
17:c:398:ARG:NH2	18:d:196:GLU:OE1	2.32	0.63
18:d:220:LYS:O	18:d:348:ASP:CG	2.33	0.63
18:d:111:THR:HA	18:d:149:SER:HA	1.81	0.62
18:d:232:LYS:O	18:d:234:LEU:C	2.42	0.62
21:g:275:ALA:O	21:g:279:ALA:HB2	1.98	0.62
22:h:127:LEU:CB	22:h:128:PRO:CD	2.76	0.62
12:L:38:ARG:NH2	8:V:164:PHE:O	2.32	0.62
20:f:195:PHE:HD2	20:f:197:LYS:HE3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:570:LEU:O	23:i:579:ARG:HA	1.99	0.62
23:i:613:ASP:O	23:i:614:VAL:C	2.41	0.62
4:D:20:ARG:CD	4:D:20:ARG:H	2.10	0.62
11:Y:164:THR:HG22	11:Y:170:SER:HB3	1.80	0.62
7:G:29:PHE:HZ	19:e:416:PHE:HE1	1.48	0.62
10:X:25:ILE:HG23	10:X:26:VAL:HG13	1.81	0.62
17:c:307:ASP:HB3	17:c:336:ARG:NH2	2.14	0.62
18:d:270:LEU:HD11	18:d:282:VAL:CG2	2.29	0.62
19:e:391:ARG:HG2	19:e:393:ILE:H	1.64	0.62
12:Z:63:THR:OG1	13:a:94:ARG:NH2	2.32	0.62
22:h:108:VAL:O	22:h:108:VAL:HG23	2.00	0.62
22:h:114:VAL:CG2	22:h:126:ILE:CD1	2.51	0.62
27:m:198:ALA:O	27:m:202:LEU:N	2.22	0.62
17:c:168:GLU:CG	17:c:169:LYS:N	2.62	0.62
22:h:116:LEU:HG	22:h:122:THR:O	1.98	0.62
1:A:5:TYR:CZ	7:G:130:GLU:HB3	2.35	0.62
8:H:51:ASP:HB3	8:H:94:ILE:HG23	1.80	0.62
19:e:203:LEU:HB2	19:e:327:LEU:HG	1.81	0.62
12:L:183:ALA:HB2	12:L:210:LEU:HD23	1.82	0.62
15:Q:100:ASP:OD1	15:Q:100:ASP:N	2.31	0.62
15:Q:192:ILE:HD11	15:Q:228:TYR:C	2.14	0.62
15:Q:220:LEU:HD22	15:Q:224:GLU:HG3	0.68	0.62
27:m:202:LEU:HD23	27:m:202:LEU:H	1.64	0.62
12:Z:183:ALA:HB2	12:Z:210:LEU:HD23	1.82	0.62
17:c:177:VAL:CB	17:c:224:LEU:CD1	2.65	0.62
18:d:123:VAL:HG11	18:d:152:LEU:HD11	1.81	0.62
22:h:213:ARG:HG2	22:h:247:PHE:HB3	1.80	0.62
22:h:235:PHE:CE2	22:h:276:LEU:CD2	2.81	0.62
27:m:182:VAL:HG23	27:m:204:THR:HG21	1.82	0.62
31:q:274:ASN:C	31:q:276:GLY:N	2.57	0.62
18:d:255:LEU:HD13	18:d:267:VAL:HG11	1.74	0.62
27:m:168:ILE:HG22	27:m:168:ILE:O	2.00	0.62
20:f:61:LEU:HD23	20:f:78:ARG:HD3	1.80	0.61
21:g:347:ARG:HG3	21:g:347:ARG:NH2	2.15	0.61
6:T:139:SER:HA	6:T:216:VAL:HG11	1.82	0.61
7:U:44:GLY:O	7:U:45:LYS:C	2.41	0.61
8:V:103:VAL:HG22	8:V:108:PRO:HB3	1.82	0.61
17:c:384:GLU:O	17:c:386:ARG:CA	2.46	0.61
18:d:112:LEU:O	18:d:147:GLY:HA3	2.00	0.61
19:e:267:ILE:HG22	19:e:270:ILE:CD1	2.30	0.61
21:g:71:ASP:O	21:g:75:GLU:CB	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:369:HIS:CE1	21:g:397:LYS:CB	2.72	0.61
22:h:368:MET:HE1	22:h:372:ARG:HH21	1.63	0.61
17:c:336:ARG:C	17:c:337:LEU:CD1	2.68	0.61
18:d:227:PRO:CD	18:d:230:THR:HG21	2.30	0.61
20:f:293:GLY:N	20:f:296:ASP:OD1	2.34	0.61
21:g:228:PRO:CG	21:g:229:PRO:HD2	2.18	0.61
21:g:238:ARG:O	21:g:242:ALA:HB2	2.00	0.61
21:g:347:ARG:HH21	21:g:347:ARG:CG	2.14	0.61
25:k:59:ASP:O	25:k:63:THR:N	2.34	0.61
5:E:170:THR:HG21	21:g:383:GLU:HB3	1.82	0.61
18:d:227:PRO:N	18:d:230:THR:HG21	2.15	0.61
27:m:15:PRO:HD2	27:m:146:ARG:HH22	1.65	0.61
8:H:17:ASP:HB2	8:H:170:GLY:HA3	1.81	0.61
20:f:309:ARG:NH2	20:f:335:SER:O	2.33	0.61
22:h:65:LEU:HG	22:h:68:GLU:OE2	2.01	0.61
22:h:78:ARG:CB	22:h:110:PRO:CG	2.49	0.61
20:f:128:GLY:O	20:f:130:VAL:HG12	2.01	0.61
21:g:393:GLY:O	21:g:396:CYS:SG	2.57	0.61
21:g:437:TYR:C	21:g:439:ALA:H	2.09	0.61
2:B:72:MET:HE1	2:B:110:LEU:HD22	1.82	0.61
7:G:51:VAL:HG12	7:G:217:VAL:HG22	1.81	0.61
1:O:38:LYS:HA	1:O:43:VAL:HG12	1.83	0.61
20:f:193:CYS:HB3	20:f:227:PRO:O	2.00	0.61
15:Q:188:ILE:CB	15:Q:228:TYR:CE1	2.83	0.61
19:e:406:VAL:O	19:e:406:VAL:HG12	2.01	0.61
21:g:228:PRO:HG2	21:g:229:PRO:HD2	1.81	0.61
22:h:137:LEU:O	22:h:137:LEU:HD12	2.01	0.61
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.82	0.61
11:Y:173:ALA:HA	11:Y:191:ASN:HA	1.83	0.61
18:d:390:LEU:O	18:d:390:LEU:HG	2.00	0.61
22:h:114:VAL:HG21	22:h:126:ILE:HD12	0.78	0.61
7:G:44:GLY:N	7:G:47:CYS:O	2.33	0.61
11:K:11:GLY:HA3	11:K:179:VAL:O	2.01	0.61
18:d:126:SER:OG	22:h:92:GLU:CG	2.49	0.61
7:G:42:VAL:HG21	7:G:194:THR:HG21	1.83	0.60
8:H:103:VAL:HG22	8:H:108:PRO:HB3	1.82	0.60
7:U:42:VAL:HG23	7:U:49:VAL:N	2.16	0.60
7:U:88:ARG:HA	7:U:91:VAL:HG12	1.83	0.60
18:d:232:LYS:C	18:d:234:LEU:H	2.04	0.60
19:e:122:GLU:OE2	31:q:278:GLN:CB	2.44	0.60
19:e:297:ASP:OD2	22:h:142:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:ARG:HG2	6:F:81:LEU:HD11	1.83	0.60
7:U:44:GLY:O	7:U:46:ASP:N	2.34	0.60
18:d:421:LYS:O	18:d:425:ASN:HB2	2.00	0.60
27:m:208:PHE:O	27:m:209:THR:HG22	2.01	0.60
5:E:67:ASP:OD1	5:E:67:ASP:N	2.33	0.60
6:F:120:HIS:NE2	7:G:86:ASP:OD1	2.23	0.60
11:K:173:ALA:HA	11:K:191:ASN:HA	1.83	0.60
18:d:283:PHE:HD2	18:d:285:ASP:HB3	1.60	0.60
19:e:267:ILE:HD11	19:e:309:MET:HB2	1.83	0.60
21:g:294:LYS:HG3	21:g:339:ASP:H	1.64	0.60
12:L:135:PHE:HB2	12:L:149:LEU:HD13	1.83	0.60
2:P:72:MET:HE1	2:P:110:LEU:HD22	1.82	0.60
16:S:67:ASP:N	16:S:67:ASP:OD1	2.33	0.60
1:A:81:ASP:OD1	7:G:123:GLN:NE2	2.31	0.60
8:H:219:LEU:HG	9:I:47:ARG:HE	1.66	0.60
12:Z:92:LEU:HD13	12:Z:110:ILE:HD11	1.84	0.60
20:f:177:GLY:O	35:g:501:ADP:O2A	2.20	0.60
13:M:28:GLY:HA3	13:M:36:PHE:HB2	1.83	0.60
15:Q:206:ILE:O	15:Q:225:ILE:HD12	2.00	0.60
6:T:65:ARG:HG2	6:T:81:LEU:HD11	1.83	0.60
14:b:41:ILE:HG12	14:b:76:VAL:HG22	1.82	0.60
17:c:299:MET:HE3	17:c:331:LEU:HD13	1.82	0.60
22:h:78:ARG:HB3	22:h:110:PRO:HG3	1.76	0.60
20:f:147:GLU:HA	20:f:151:LEU:HD13	1.83	0.60
20:f:193:CYS:CB	20:f:227:PRO:O	2.50	0.60
20:f:247:THR:HG23	20:f:251:ARG:HH12	1.65	0.60
21:g:373:MET:HE1	21:g:401:VAL:HA	1.82	0.60
23:i:475:HIS:HA	23:i:511:ALA:HA	1.80	0.60
23:i:570:LEU:CB	23:i:582:GLY:H	2.14	0.60
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.34	0.60
17:c:222:LYS:HB2	35:c:501:ADP:O2B	2.01	0.60
23:i:570:LEU:CB	23:i:582:GLY:HA3	2.31	0.60
1:A:38:LYS:HA	1:A:43:VAL:HG12	1.83	0.60
9:I:121:CYS:SG	9:I:122:SER:N	2.75	0.60
11:Y:11:GLY:HA3	11:Y:179:VAL:O	2.01	0.60
20:f:60:VAL:HG22	20:f:62:LYS:N	2.16	0.60
31:q:50:PRO:HA	31:q:116:PRO:HG3	1.84	0.60
8:H:29:LYS:NZ	9:I:150:GLU:OE2	2.32	0.60
12:Z:135:PHE:HB2	12:Z:149:LEU:HD13	1.83	0.60
20:f:290:LEU:HD21	20:f:298:LYS:HD3	1.81	0.60
21:g:398:ALA:O	21:g:399:VAL:C	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:105:ILE:O	22:h:105:ILE:HG22	2.01	0.60
27:m:15:PRO:CD	27:m:146:ARG:HH22	2.15	0.60
27:m:232:GLU:HG3	27:m:234:PRO:HD2	1.83	0.60
8:H:103:VAL:HG11	8:H:180:LYS:HA	1.84	0.59
18:d:348:ASP:O	18:d:349:ARG:C	2.45	0.59
20:f:84:ARG:HB3	20:f:87:LEU:HB2	1.82	0.59
26:l:153:LEU:HD13	26:l:157:LEU:CD2	2.31	0.59
27:m:86:GLU:O	27:m:90:ASP:CB	2.51	0.59
19:e:210:CYS:O	35:e:501:ADP:C8	2.55	0.59
4:R:164:GLN:HB3	16:S:58:ALA:H	1.66	0.59
10:X:193:ASN:HD22	10:X:193:ASN:N	2.00	0.59
14:b:136:TYR:O	14:b:140:ASP:HB2	2.02	0.59
19:e:397:LYS:O	19:e:401:LYS:HG2	2.03	0.59
26:l:68:GLY:O	26:l:72:TYR:CB	2.50	0.59
7:G:88:ARG:HA	7:G:91:VAL:HG12	1.84	0.59
6:T:240:LYS:HA	6:T:243:LEU:HB2	1.84	0.59
9:W:121:CYS:SG	9:W:122:SER:N	2.75	0.59
17:c:165:GLN:CG	17:c:236:CYS:HB2	2.32	0.59
17:c:284:ARG:HH22	21:g:333:ASN:HB2	1.65	0.59
19:e:394:VAL:HG22	19:e:399:PHE:HD1	1.68	0.59
27:m:202:LEU:H	27:m:202:LEU:CD2	2.14	0.59
5:E:155:ASP:HB3	6:F:62:SER:HA	1.85	0.59
19:e:408:LYS:HA	19:e:408:LYS:NZ	2.17	0.59
20:f:341:ALA:HB1	21:g:345:SER:O	2.02	0.59
22:h:106:ASN:O	22:h:106:ASN:ND2	2.36	0.59
22:h:114:VAL:HG11	22:h:126:ILE:HA	1.83	0.59
22:h:310:ARG:HH11	22:h:310:ARG:CG	2.15	0.59
10:X:182:VAL:HG23	10:X:191:LEU:CD1	2.33	0.59
19:e:206:GLY:CA	19:e:212:LYS:HE2	2.31	0.59
19:e:323:ARG:HD3	22:h:143:VAL:HG22	0.94	0.59
20:f:126:ASP:CB	21:g:320:PHE:CB	2.61	0.59
22:h:58:LEU:O	22:h:62:GLU:CB	2.51	0.59
22:h:145:ASP:O	22:h:147:THR:HG23	2.02	0.59
10:X:19:ARG:NH1	10:X:193:ASN:OD1	2.36	0.59
13:a:28:GLY:HA3	13:a:36:PHE:HB2	1.83	0.59
13:a:41:ARG:NH1	13:a:53:ALA:O	2.36	0.59
26:l:163:LYS:CD	26:l:166:LEU:N	2.66	0.59
8:V:103:VAL:HG11	8:V:180:LYS:HA	1.84	0.59
21:g:432:LYS:O	21:g:432:LYS:HG2	2.01	0.59
4:D:20:ARG:HD2	4:D:20:ARG:C	2.27	0.59
8:H:58:LEU:HD22	8:H:86:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:186:ASP:HB2	10:J:189:HIS:CE1	2.37	0.59
18:d:221:GLY:C	18:d:348:ASP:OD1	2.44	0.59
21:g:282:ILE:HG22	21:g:327:LYS:HB2	1.83	0.59
4:D:20:ARG:NE	4:D:25:GLU:OE1	2.36	0.59
6:F:139:SER:HA	6:F:216:VAL:HG11	1.84	0.59
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.36	0.59
17:c:345:LEU:HD22	17:c:381:THR:CG2	2.30	0.59
19:e:296:MET:SD	19:e:326:ARG:HA	2.43	0.59
20:f:185:ARG:NH1	21:g:321:GLN:CB	2.64	0.59
3:C:65:LEU:HB2	3:C:69:VAL:HG23	1.85	0.58
7:G:44:GLY:O	7:G:45:LYS:C	2.44	0.58
12:L:92:LEU:HD13	12:L:110:ILE:HD11	1.84	0.58
17:c:177:VAL:O	17:c:177:VAL:HG22	2.02	0.58
18:d:342:ILE:HD11	18:d:350:LYS:NZ	2.18	0.58
19:e:100:THR:HA	19:e:114:ARG:HA	1.84	0.58
20:f:185:ARG:HD3	21:g:321:GLN:HG3	1.85	0.58
20:f:342:ASP:HA	21:g:345:SER:CB	2.33	0.58
21:g:428:GLN:HG2	21:g:429:ALA:N	2.18	0.58
22:h:134:LEU:CD2	22:h:237:MET:HB3	2.33	0.58
5:E:189:LYS:HE3	5:E:233:LEU:H	1.67	0.58
7:G:90:GLN:HE21	7:G:134:LEU:HD11	1.68	0.58
14:N:136:TYR:O	14:N:140:ASP:HB2	2.02	0.58
27:m:199:GLU:OE1	27:m:199:GLU:N	2.32	0.58
15:Q:33:VAL:HG12	15:Q:44:GLY:O	2.03	0.58
17:c:274:PHE:HB3	17:c:277:ILE:HD13	1.84	0.58
27:m:167:LEU:O	27:m:167:LEU:HD23	2.02	0.58
5:E:101:ARG:NH1	13:M:74:GLU:OE2	2.37	0.58
1:O:111:GLN:NE2	1:O:154:TYR:OH	2.36	0.58
19:e:201:GLY:HA3	19:e:327:LEU:CD1	2.32	0.58
19:e:323:ARG:HD2	22:h:143:VAL:HG21	0.59	0.58
15:Q:51:ALA:HA	15:Q:54:GLN:CG	2.33	0.58
17:c:110:LYS:HG2	21:g:85:THR:HG23	1.85	0.58
17:c:307:ASP:HB3	17:c:336:ARG:HH21	1.68	0.58
18:d:270:LEU:CD1	18:d:282:VAL:HG21	2.33	0.58
19:e:127:ASN:O	19:e:252:ARG:NH2	2.36	0.58
19:e:323:ARG:HD3	22:h:143:VAL:CG2	1.13	0.58
21:g:362:ARG:NH1	21:g:388:THR:O	2.36	0.58
22:h:89:VAL:HG12	22:h:92:GLU:O	2.02	0.58
22:h:252:ASP:HB3	22:h:296:ASN:HD21	1.68	0.58
23:i:475:HIS:N	23:i:511:ALA:HB2	2.18	0.58
3:C:45:VAL:O	3:C:45:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:ARG:NH1	13:M:53:ALA:O	2.36	0.58
8:V:219:LEU:HG	9:W:47:ARG:HE	1.68	0.58
18:d:136:LEU:HD21	18:d:160:ILE:HD13	1.85	0.58
12:L:157:ASN:HD21	9:W:202:ARG:HG2	1.69	0.58
18:d:201:VAL:HG21	18:d:328:ILE:HD11	1.86	0.58
25:k:41:GLN:O	25:k:45:GLU:CB	2.52	0.58
25:k:293:ASP:C	25:k:295:LYS:N	2.57	0.58
18:d:246:THR:HG23	18:d:280:SER:CB	2.33	0.58
18:d:281:ILE:C	18:d:281:ILE:HD13	2.29	0.58
19:e:208:PRO:CD	19:e:335:LEU:HD12	2.33	0.58
22:h:77:VAL:HB	22:h:86:LEU:HD12	1.84	0.58
22:h:170:LYS:NZ	27:m:97:GLU:OE1	2.36	0.58
22:h:332:HIS:CE1	35:h:401:ADP:O2'	2.56	0.58
25:k:185:PHE:O	25:k:189:GLN:CB	2.51	0.58
6:T:97:ASN:O	6:T:101:ASN:HB2	2.04	0.58
7:U:90:GLN:HE21	7:U:134:LEU:HD11	1.68	0.58
8:V:58:LEU:HD22	8:V:86:MET:HE2	1.85	0.58
10:X:182:VAL:HG23	10:X:191:LEU:HG	1.86	0.58
21:g:90:VAL:HA	21:g:152:GLY:HA2	1.83	0.58
22:h:120:SER:O	22:h:121:TYR:HB2	2.03	0.58
3:C:100:ASP:OD1	3:C:100:ASP:N	2.31	0.58
10:J:27:GLN:NE2	10:X:169:LYS:O	2.37	0.57
22:h:325:ARG:HA	22:h:328:ILE:HG22	1.86	0.57
11:K:155:LEU:O	11:K:159:ALA:HB2	2.04	0.57
15:Q:46:GLU:O	15:Q:47:LYS:C	2.46	0.57
15:Q:65:LEU:HB2	15:Q:69:VAL:HG23	1.85	0.57
17:c:164:MET:C	17:c:238:ILE:HD13	2.29	0.57
18:d:398:ILE:O	18:d:402:ALA:HB2	2.04	0.57
22:h:83:LYS:CG	22:h:98:ASP:OD1	2.52	0.57
3:C:50:VAL:CA	3:C:54:GLN:CB	2.76	0.57
12:L:28:ARG:NH2	12:L:213:ASP:OXT	2.37	0.57
1:O:123:SER:HA	2:P:127:LYS:HE3	1.85	0.57
18:d:198:LYS:O	18:d:202:GLU:HB2	2.04	0.57
18:d:393:ALA:O	18:d:396:LYS:N	2.37	0.57
19:e:354:LEU:HD12	19:e:358:VAL:HG11	1.86	0.57
21:g:247:THR:CG2	21:g:281:SER:HB3	2.34	0.57
31:q:296:ILE:O	31:q:300:LEU:N	2.35	0.57
6:F:97:ASN:O	6:F:101:ASN:HB2	2.04	0.57
20:f:342:ASP:HA	21:g:345:SER:OG	2.03	0.57
22:h:144:PRO:HG3	22:h:213:ARG:HD3	1.85	0.57
8:H:1:THR:HG22	8:H:33:LYS:CE	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:42:GLY:H	1:O:143:PRO:HG3	1.70	0.57
11:Y:155:LEU:O	11:Y:159:ALA:HB2	2.04	0.57
18:d:227:PRO:HD2	18:d:230:THR:HG21	1.86	0.57
18:d:271:PHE:HE1	18:d:282:VAL:HG21	1.69	0.57
19:e:228:ILE:HD11	19:e:262:ILE:HG12	1.84	0.57
5:E:10:VAL:HB	5:E:21:GLN:HE21	1.69	0.57
15:Q:221:ASN:O	15:Q:222:PRO:C	2.46	0.57
17:c:93:LEU:HB3	18:d:132:TYR:HB3	1.85	0.57
17:c:165:GLN:HG3	17:c:236:CYS:HB2	1.84	0.57
19:e:385:LEU:HB3	19:e:398:ASP:CG	2.29	0.57
22:h:81:ASP:HB2	22:h:84:LYS:HG3	1.86	0.57
9:I:188:ILE:HB	9:I:195:THR:HB	1.87	0.57
4:R:118:ASN:OD1	16:S:82:ARG:NH1	2.37	0.57
17:c:165:GLN:CB	17:c:237:PHE:O	2.53	0.57
18:d:238:ALA:O	18:d:241:ASN:HB3	2.05	0.57
21:g:78:GLU:HA	21:g:81:LYS:HB2	1.86	0.57
31:q:50:PRO:CA	31:q:116:PRO:HG3	2.35	0.57
1:A:43:VAL:HG21	1:A:136:CYS:HB2	1.85	0.57
15:Q:221:ASN:C	15:Q:223:GLU:N	2.63	0.57
18:d:126:SER:HB2	22:h:92:GLU:CD	2.30	0.57
21:g:437:TYR:N	21:g:437:TYR:CD1	2.73	0.57
23:i:770:TRP:HA	31:q:178:THR:CB	2.35	0.57
27:m:14:ASN:C	27:m:146:ARG:HH12	2.12	0.57
31:q:92:GLN:O	31:q:96:LEU:CB	2.53	0.57
4:D:97:GLN:HB3	11:K:61:ARG:HG3	1.87	0.57
10:J:8:GLN:NE2	10:J:113:PRO:O	2.38	0.57
9:W:188:ILE:HB	9:W:195:THR:HB	1.87	0.57
11:Y:177:TYR:OH	11:Y:186:ARG:NH2	2.38	0.57
22:h:134:LEU:HD23	22:h:237:MET:HG2	1.87	0.57
8:V:3:ILE:HD13	8:V:44:CYS:HB3	1.73	0.57
18:d:250:VAL:CG2	18:d:270:LEU:HD11	2.35	0.57
19:e:175:GLN:O	19:e:179:GLU:HB2	2.05	0.57
20:f:83:CYS:HA	20:f:107:ILE:HG22	1.87	0.57
22:h:357:ALA:O	22:h:359:VAL:N	2.38	0.57
26:l:406:ASN:C	26:l:408:SER:N	2.60	0.57
4:D:20:ARG:H	4:D:20:ARG:HD2	1.70	0.56
1:O:43:VAL:HG21	1:O:136:CYS:HB2	1.85	0.56
22:h:116:LEU:C	22:h:118:ASN:N	2.61	0.56
21:g:231:THR:C	35:g:502:ADP:O2A	2.48	0.56
22:h:358:GLU:HA	22:h:358:GLU:OE2	2.05	0.56
23:i:516:LEU:O	23:i:520:MET:N	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:H	1:A:143:PRO:HG3	1.70	0.56
8:H:132:LEU:HB3	13:a:144:TYR:HB3	1.86	0.56
10:J:193:ASN:HD22	10:J:193:ASN:N	2.02	0.56
11:K:177:TYR:OH	11:K:186:ARG:NH2	2.38	0.56
15:Q:220:LEU:CG	15:Q:224:GLU:CG	2.75	0.56
10:X:8:GLN:NE2	10:X:113:PRO:O	2.38	0.56
18:d:105:THR:C	18:d:107:MET:N	2.62	0.56
19:e:85:ILE:CG2	20:f:82:GLY:H	2.14	0.56
21:g:188:ILE:HD11	21:g:191:LEU:HD12	1.87	0.56
21:g:347:ARG:HG3	21:g:347:ARG:HH21	1.70	0.56
23:i:625:ILE:O	23:i:627:PHE:CA	2.52	0.56
26:l:112:GLU:O	26:l:116:TRP:CB	2.54	0.56
26:l:153:LEU:HD13	26:l:157:LEU:CG	2.34	0.56
28:n:76:GLU:O	28:n:80:GLY:HA3	2.05	0.56
31:q:231:LEU:C	31:q:232:GLN:O	2.40	0.56
10:J:16:ALA:HA	10:J:179:SER:O	2.05	0.56
19:e:323:ARG:CG	22:h:143:VAL:HG23	2.11	0.56
20:f:122:MET:HB3	20:f:196:LEU:CD2	2.36	0.56
21:g:311:LEU:O	21:g:315:ASN:ND2	2.39	0.56
22:h:132:ASP:HB3	22:h:133:PRO:HD2	1.88	0.56
14:N:164:MET:HB2	14:N:171:GLY:HA2	1.87	0.56
17:c:327:LEU:HB2	17:c:332:MET:HE1	1.88	0.56
18:d:199:GLU:HA	18:d:203:LEU:HD13	1.88	0.56
18:d:347:ILE:O	18:d:347:ILE:HG23	2.06	0.56
19:e:267:ILE:HD12	19:e:309:MET:SD	2.43	0.56
23:i:678:ASP:CB	23:i:679:PRO:HD2	2.35	0.56
35:d:501:ADP:HO3'	22:h:307:ARG:HH12	1.50	0.56
19:e:94:GLU:CD	22:h:128:PRO:HG3	2.29	0.56
22:h:134:LEU:C	22:h:136:SER:N	2.58	0.56
26:l:185:LYS:HG2	26:l:189:ALA:HB3	1.87	0.56
26:l:191:THR:HG22	26:l:194:ARG:HH12	1.69	0.56
26:l:215:GLY:O	26:l:219:ALA:HB2	2.06	0.56
31:q:231:LEU:O	31:q:232:GLN:C	2.47	0.56
11:K:13:ILE:HA	11:K:177:TYR:O	2.06	0.56
16:S:10:VAL:HB	16:S:21:GLN:HE21	1.69	0.56
7:U:44:GLY:C	7:U:46:ASP:N	2.62	0.56
18:d:107:MET:HE3	18:d:151:LEU:CD1	2.30	0.56
18:d:249:ARG:NH1	22:h:275:GLU:OE2	2.38	0.56
18:d:343:ARG:C	18:d:345:GLY:N	2.62	0.56
26:l:403:THR:O	26:l:405:GLN:N	2.39	0.56
3:C:50:VAL:C	3:C:54:GLN:HG2	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:GLU:OE2	3:C:186:LEU:N	2.33	0.56
8:H:139:GLU:OE2	13:a:179:ARG:NH2	2.38	0.56
10:X:16:ALA:HA	10:X:179:SER:O	2.05	0.56
19:e:416:PHE:N	19:e:416:PHE:CD1	2.73	0.56
20:f:61:LEU:CD2	20:f:78:ARG:CD	2.50	0.56
20:f:118:LEU:O	20:f:122:MET:HG2	2.05	0.56
20:f:179:GLY:HA2	20:f:182:LEU:HD22	1.88	0.56
20:f:182:LEU:O	20:f:185:ARG:HB2	2.05	0.56
21:g:75:GLU:O	21:g:79:LYS:CB	2.54	0.56
29:o:94:GLN:O	29:o:98:MET:CB	2.53	0.56
3:C:50:VAL:C	3:C:54:GLN:CG	2.74	0.56
2:P:184:MET:O	2:P:188:SER:OG	2.24	0.56
14:b:164:MET:HB2	14:b:171:GLY:HA2	1.87	0.56
17:c:166:VAL:HG22	17:c:239:ARG:HG2	1.87	0.56
18:d:259:TYR:HH	20:f:247:THR:HG21	1.71	0.56
20:f:240:GLY:HA3	20:f:286:ASP:HB2	1.87	0.56
20:f:289:LEU:HD23	20:f:289:LEU:O	2.06	0.56
1:A:176:ARG:CG	26:l:160:MET:SD	2.92	0.56
7:G:80:MET:SD	7:G:80:MET:N	2.79	0.56
9:I:39:GLN:NE2	9:I:41:ILE:O	2.39	0.56
13:M:144:TYR:HB3	8:V:132:LEU:HB3	1.87	0.56
2:P:34:CYS:HG	2:P:75:SER:HG	1.47	0.56
7:U:41:ALA:HB1	7:U:151:VAL:HG21	1.88	0.56
18:d:364:ILE:HD12	35:d:501:ADP:HN62	1.70	0.56
19:e:326:ARG:HG3	19:e:326:ARG:NH1	2.10	0.56
21:g:197:GLU:OE2	21:g:350:ARG:NH2	2.38	0.56
21:g:233:LYS:HB2	35:g:502:ADP:O3B	2.05	0.56
8:H:12:ILE:HD11	8:H:178:ILE:HD12	1.88	0.55
17:c:362:MET:H	18:d:215:GLY:HA3	1.71	0.55
18:d:106:PRO:HB3	22:h:121:TYR:CG	2.41	0.55
18:d:387:LYS:HA	18:d:387:LYS:CE	2.35	0.55
22:h:385:MET:O	22:h:389:LYS:HB2	2.06	0.55
26:l:360:ASP:O	26:l:364:LYS:N	2.37	0.55
33:s:51:ASP:O	33:s:55:GLN:CB	2.55	0.55
2:B:184:MET:O	2:B:188:SER:OG	2.24	0.55
7:U:232:GLU:HA	7:U:235:ILE:HG22	1.88	0.55
9:W:13:MET:HG3	9:W:162:LEU:HD11	1.87	0.55
19:e:122:GLU:OE2	31:q:278:GLN:CA	2.54	0.55
26:l:302:PHE:O	26:l:305:ALA:O	2.24	0.55
5:E:121:GLN:NE2	6:F:83:ASP:OD1	2.40	0.55
7:G:157:ALA:HB3	19:e:416:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:433:ALA:O	21:g:435:LEU:HD13	2.06	0.55
21:g:435:LEU:HA	21:g:437:TYR:CD1	2.41	0.55
26:l:215:GLY:O	26:l:219:ALA:CB	2.55	0.55
5:E:33:SER:HB3	21:g:439:ALA:C	2.31	0.55
9:W:39:GLN:NE2	9:W:41:ILE:O	2.39	0.55
19:e:323:ARG:HH12	19:e:324:PRO:HD2	1.69	0.55
22:h:273:MET:O	22:h:277:LEU:HB2	2.06	0.55
23:i:623:GLY:HA3	23:i:655:ALA:HA	1.88	0.55
26:l:49:SER:O	26:l:53:LEU:CB	2.54	0.55
4:R:97:GLN:HB3	11:Y:61:ARG:HG3	1.89	0.55
16:S:22:ILE:HG22	16:S:127:PRO:HG3	1.89	0.55
17:c:97:ARG:NH2	21:g:170:SER:OG	2.39	0.55
19:e:205:TYR:CZ	19:e:332:GLU:CB	2.90	0.55
19:e:210:CYS:C	35:e:501:ADP:O1A	2.50	0.55
23:i:645:ASN:O	23:i:647:HIS:N	2.38	0.55
31:q:247:GLU:O	31:q:251:LEU:CB	2.55	0.55
11:Y:13:ILE:HA	11:Y:177:TYR:O	2.06	0.55
18:d:342:ILE:HG13	18:d:344:PRO:CD	2.24	0.55
19:e:269:ALA:HB2	20:f:258:MET:HG3	1.89	0.55
25:k:269:SER:O	25:k:273:TYR:CB	2.54	0.55
26:l:129:LEU:O	26:l:133:LEU:HB2	2.07	0.55
27:m:169:GLU:N	27:m:171:GLY:H	2.05	0.55
19:e:230:VAL:HG13	19:e:264:ILE:HG22	1.87	0.55
27:m:378:ASN:O	27:m:382:LYS:N	2.39	0.55
7:G:25:VAL:CG2	19:e:416:PHE:CE2	2.90	0.55
9:I:13:MET:HG3	9:I:162:LEU:HD11	1.87	0.55
10:X:182:VAL:HG23	10:X:191:LEU:HD11	1.88	0.55
13:a:25:ASP:OD1	13:a:41:ARG:NH2	2.40	0.55
19:e:206:GLY:H	19:e:212:LYS:NZ	2.01	0.55
22:h:68:GLU:CD	22:h:68:GLU:H	2.14	0.55
22:h:140:VAL:C	22:h:142:LYS:N	2.64	0.55
13:M:25:ASP:OD1	13:M:41:ARG:NH2	2.40	0.55
8:V:12:ILE:HD11	8:V:178:ILE:HD12	1.88	0.55
18:d:259:TYR:OH	19:e:276:ASP:N	2.40	0.55
26:l:250:SER:HA	26:l:253:TYR:H	1.71	0.55
27:m:15:PRO:N	27:m:146:ARG:HH22	2.05	0.55
6:F:37:ILE:HD11	6:F:193:VAL:HG13	1.89	0.55
12:L:28:ARG:HH11	12:L:35:ILE:HG21	1.72	0.55
1:O:92:LEU:HD13	1:O:112:ARG:HB3	1.89	0.55
17:c:163:MET:HE3	17:c:240:VAL:HG23	1.88	0.55
17:c:241:ILE:HD11	18:d:268:ARG:HH12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:205:TYR:CZ	19:e:332:GLU:HA	2.41	0.55
19:e:374:ASP:CA	20:f:292:PRO:HG3	2.37	0.55
7:G:232:GLU:HA	7:G:235:ILE:HG22	1.88	0.54
15:Q:206:ILE:HG23	15:Q:225:ILE:HG22	1.26	0.54
6:T:157:SER:H	7:U:88:ARG:HH22	1.55	0.54
7:U:80:MET:N	7:U:80:MET:SD	2.79	0.54
14:b:19:ARG:NH1	14:b:168:GLY:O	2.40	0.54
17:c:306:LEU:HD13	17:c:312:ARG:HH12	1.71	0.54
18:d:125:THR:HG23	18:d:127:VAL:H	1.72	0.54
19:e:111:TYR:HB2	22:h:72:TYR:HA	1.88	0.54
19:e:346:SER:O	19:e:350:SER:HB3	2.07	0.54
23:i:619:VAL:CB	23:i:651:GLY:C	2.80	0.54
27:m:138:LEU:HA	27:m:141:VAL:HG12	1.88	0.54
13:M:89:HIS:HB2	13:M:112:ILE:HD11	1.89	0.54
6:T:37:ILE:HD11	6:T:193:VAL:HG13	1.89	0.54
6:T:215:TRP:HZ3	6:T:227:VAL:HG23	1.73	0.54
21:g:305:GLU:OE1	21:g:308:ARG:NH2	2.39	0.54
26:l:165:LEU:H	26:l:165:LEU:HD12	1.72	0.54
30:p:94:HIS:O	30:p:98:LYS:CB	2.55	0.54
10:J:182:VAL:HG21	10:J:191:LEU:HD11	1.89	0.54
6:T:227:VAL:HG11	6:T:232:ARG:HG2	1.90	0.54
18:d:361:LYS:NZ	18:d:389:ASP:HA	2.22	0.54
22:h:152:GLY:N	35:h:401:ADP:N1	2.52	0.54
31:q:58:LEU:HA	31:q:108:VAL:HA	1.89	0.54
5:E:22:ILE:HG22	5:E:127:PRO:HG3	1.88	0.54
6:F:186:CYS:HA	6:F:189:ILE:HG12	1.90	0.54
14:N:19:ARG:NH1	14:N:168:GLY:O	2.41	0.54
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.07	0.54
17:c:383:ALA:HB2	35:c:501:ADP:H8	1.73	0.54
18:d:255:LEU:CD2	18:d:312:LEU:CD2	2.84	0.54
20:f:70:ILE:HG13	20:f:80:VAL:HG22	1.89	0.54
20:f:275:MET:N	20:f:275:MET:SD	2.77	0.54
21:g:140:VAL:HA	21:g:144:LYS:HE3	1.90	0.54
23:i:630:PRO:O	23:i:632:GLN:CA	2.53	0.54
26:l:204:PRO:O	26:l:208:ALA:CB	2.54	0.54
27:m:236:LEU:HB3	27:m:239:LYS:HE2	1.88	0.54
5:E:215:VAL:HB	5:E:221:PHE:HD1	1.73	0.54
13:M:109:THR:HG23	13:M:126:ASP:HA	1.89	0.54
19:e:119:ILE:HD11	19:e:142:VAL:HG13	1.90	0.54
23:i:619:VAL:CA	23:i:655:ALA:HB2	2.37	0.54
25:k:183:VAL:O	25:k:187:LEU:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:308:ASP:H	26:l:311:ALA:HB2	1.72	0.54
2:B:88:ASN:HD21	9:I:76:LYS:HE2	1.73	0.54
8:H:1:THR:CB	8:H:33:LYS:HZ1	2.09	0.54
2:P:169:ALA:HA	2:P:173:SER:H	1.73	0.54
20:f:177:GLY:HA2	21:g:344:ARG:CD	2.38	0.54
21:g:93:VAL:HA	21:g:124:ILE:HA	1.88	0.54
28:n:11:VAL:H	28:n:163:GLY:HA3	1.71	0.54
13:a:109:THR:HG23	13:a:126:ASP:HA	1.89	0.54
18:d:255:LEU:HD13	18:d:267:VAL:CG1	2.32	0.54
6:F:215:TRP:HZ3	6:F:227:VAL:HG23	1.73	0.54
12:L:13:LEU:O	12:L:24:ALA:N	2.39	0.54
17:c:113:ILE:O	17:c:120:LYS:HA	2.08	0.54
18:d:342:ILE:HB	18:d:347:ILE:HG23	1.88	0.54
19:e:184:PRO:HB2	19:e:306:LYS:HE3	1.89	0.54
27:m:15:PRO:HD2	27:m:143:TYR:CE1	2.43	0.54
27:m:104:MET:O	27:m:108:ALA:CB	2.56	0.54
1:A:127:ARG:O	7:G:127:GLN:NE2	2.41	0.54
4:D:161:THR:HG21	21:g:437:TYR:CB	2.38	0.54
6:F:227:VAL:HG11	6:F:232:ARG:HG2	1.89	0.54
13:M:105:PRO:HG2	13:M:107:TRP:HE1	1.73	0.54
2:P:174:MET:SD	2:P:199:LYS:NZ	2.73	0.54
9:W:146:TYR:O	9:W:149:CYS:N	2.41	0.54
13:a:105:PRO:HG2	13:a:107:TRP:HE1	1.73	0.54
17:c:157:ILE:HD12	17:c:161:VAL:HG12	1.89	0.54
17:c:165:GLN:N	17:c:238:ILE:HD13	2.23	0.54
17:c:327:LEU:HB3	17:c:332:MET:CE	2.38	0.54
18:d:270:LEU:CD1	18:d:282:VAL:CG2	2.85	0.54
18:d:387:LYS:HA	18:d:387:LYS:HE2	1.89	0.54
20:f:353:PHE:O	20:f:357:ALA:HB3	2.07	0.54
21:g:196:GLN:O	21:g:200:GLU:HB2	2.06	0.54
31:q:152:LYS:HB3	31:q:154:LYS:H	1.73	0.54
1:A:92:LEU:HD13	1:A:112:ARG:HB3	1.89	0.54
1:A:111:GLN:NE2	1:A:154:TYR:OH	2.36	0.54
16:S:215:VAL:HB	16:S:221:PHE:HD1	1.73	0.54
19:e:78:GLU:HA	31:q:152:LYS:HD2	1.89	0.54
20:f:36:LEU:O	20:f:40:TYR:CB	2.56	0.54
22:h:134:LEU:O	22:h:136:SER:N	2.40	0.54
23:i:569:SER:O	23:i:573:ASP:CB	2.56	0.54
29:o:131:VAL:HA	29:o:134:ALA:HB3	1.90	0.54
12:Z:28:ARG:HH11	12:Z:35:ILE:HG21	1.72	0.53
12:Z:28:ARG:NH2	12:Z:213:ASP:OXT	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:312:ILE:HG21	20:f:340:GLY:HA2	1.90	0.53
15:Q:47:LYS:CA	15:Q:207:GLU:OE1	2.50	0.53
18:d:254:GLU:O	18:d:266:LEU:HD22	2.08	0.53
20:f:64:LEU:C	20:f:69:PHE:HE1	2.14	0.53
21:g:369:HIS:ND1	21:g:397:LYS:HA	2.22	0.53
22:h:158:ILE:HA	22:h:161:ILE:HG22	1.90	0.53
23:i:497:LEU:O	23:i:501:LEU:CA	2.55	0.53
26:l:157:LEU:N	26:l:157:LEU:HD13	2.22	0.53
28:n:242:LEU:C	28:n:246:VAL:CB	2.80	0.53
9:I:146:TYR:O	9:I:149:CYS:N	2.41	0.53
12:L:166:LEU:HD23	12:L:171:ALA:HB2	1.91	0.53
17:c:157:ILE:O	17:c:161:VAL:HG13	2.08	0.53
18:d:230:THR:C	18:d:353:PHE:CE2	2.87	0.53
20:f:178:THR:C	35:g:501:ADP:N7	2.67	0.53
26:l:42:ALA:O	26:l:46:LYS:CB	2.57	0.53
1:A:67:ILE:N	1:A:71:ILE:O	2.34	0.53
2:B:49:ARG:NH1	2:B:211:VAL:O	2.41	0.53
5:E:34:ALA:HA	5:E:162:GLY:HA3	1.90	0.53
7:G:40:VAL:O	7:G:51:VAL:CG2	2.57	0.53
7:U:168:ALA:HB2	7:U:172:GLN:NE2	2.24	0.53
24:j:322:GLU:N	24:j:323:PRO:CD	2.71	0.53
3:C:50:VAL:C	3:C:54:GLN:HB2	2.34	0.53
4:D:20:ARG:HD2	4:D:20:ARG:N	2.24	0.53
1:O:118:GLN:HE21	2:P:85:VAL:HG21	1.73	0.53
7:U:139:ILE:HD13	7:U:153:LYS:HB2	1.91	0.53
11:Y:73:ARG:NH2	11:Y:104:TRP:O	2.42	0.53
17:c:336:ARG:O	17:c:337:LEU:CG	2.54	0.53
17:c:393:GLY:HA3	18:d:216:ILE:HG21	1.90	0.53
19:e:204:MET:HE3	19:e:310:ALA:HB2	1.90	0.53
6:T:186:CYS:HA	6:T:189:ILE:HG12	1.90	0.53
18:d:106:PRO:HB3	22:h:121:TYR:CD2	2.43	0.53
21:g:424:ILE:C	21:g:426:GLU:N	2.39	0.53
22:h:94:LYS:C	22:h:95:PHE:CD2	2.84	0.53
27:m:15:PRO:HD2	27:m:146:ARG:NH2	2.24	0.53
11:K:166:ARG:NH2	10:X:144:ASP:OD1	2.34	0.53
13:a:89:HIS:HB2	13:a:112:ILE:HD11	1.89	0.53
17:c:140:VAL:HG12	17:c:152:PRO:HA	1.91	0.53
17:c:178:GLY:O	17:c:354:ILE:HG22	2.09	0.53
17:c:306:LEU:HB3	17:c:336:ARG:CB	2.39	0.53
18:d:107:MET:HE2	18:d:151:LEU:CD1	2.32	0.53
19:e:104:GLY:HA2	19:e:110:ASN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:89:VAL:O	22:h:93:GLY:HA2	2.07	0.53
5:E:9:ASP:N	5:E:9:ASP:OD1	2.41	0.53
5:E:32:GLY:HA2	21:g:438:TYR:HB3	1.90	0.53
12:L:88:ILE:HG22	12:L:110:ILE:HD13	1.91	0.53
13:M:13:GLY:HA3	13:M:22:ILE:HG22	1.91	0.53
13:M:98:SER:O	13:M:102:LYS:NZ	2.41	0.53
15:Q:158:ALA:HB1	15:Q:172:LEU:HD13	1.90	0.53
17:c:299:MET:CE	17:c:331:LEU:CD1	2.86	0.53
18:d:237:LYS:HD3	18:d:283:PHE:CD1	2.44	0.53
18:d:271:PHE:O	18:d:275:GLU:HB2	2.09	0.53
19:e:376:ASN:O	19:e:380:GLN:HB3	2.09	0.53
19:e:386:ALA:HA	19:e:398:ASP:OD2	2.07	0.53
22:h:310:ARG:HH11	22:h:310:ARG:HG2	1.74	0.53
31:q:96:LEU:O	31:q:100:LYS:CB	2.56	0.53
4:D:41:GLN:HB3	4:D:166:ASP:HA	1.91	0.53
9:I:70:LEU:HD23	9:I:89:MET:HE1	1.91	0.53
8:V:2:THR:OG1	8:V:130:GLY:CA	2.57	0.53
8:V:2:THR:CB	8:V:130:GLY:HA3	2.39	0.53
17:c:293:ASN:O	17:c:296:GLN:HB2	2.09	0.53
22:h:92:GLU:OE1	22:h:92:GLU:HA	2.09	0.53
29:o:100:MET:C	29:o:102:PHE:N	2.66	0.53
29:o:123:THR:O	29:o:125:ASN:N	2.42	0.53
3:C:233:GLU:HA	3:C:233:GLU:OE1	2.08	0.53
7:G:29:PHE:CZ	19:e:416:PHE:CE1	2.96	0.53
9:I:52:LEU:HG	9:I:106:PRO:HB3	1.91	0.53
2:P:49:ARG:NH1	2:P:211:VAL:O	2.41	0.53
18:d:342:ILE:CA	18:d:347:ILE:CG2	2.85	0.53
22:h:244:SER:HB2	22:h:289:ILE:HG22	1.90	0.53
4:D:189:MET:HG3	4:D:191:LEU:H	1.74	0.52
9:W:52:LEU:HG	9:W:106:PRO:HB3	1.91	0.52
12:Z:166:LEU:HD23	12:Z:171:ALA:HB2	1.91	0.52
21:g:240:CYS:O	21:g:244:THR:OG1	2.26	0.52
22:h:68:GLU:OE1	22:h:68:GLU:N	2.42	0.52
22:h:167:LEU:HD11	27:m:94:ASN:HA	1.90	0.52
23:i:566:LEU:C	23:i:568:GLU:H	2.17	0.52
11:K:73:ARG:NH2	11:K:104:TRP:O	2.42	0.52
16:S:121:GLN:NE2	6:T:83:ASP:OD1	2.43	0.52
13:a:46:ASN:ND2	13:a:82:SER:OG	2.42	0.52
17:c:97:ARG:HA	17:c:139:ARG:HG2	1.90	0.52
19:e:122:GLU:CD	31:q:279:ASP:N	2.66	0.52
20:f:180:LYS:HB2	35:g:501:ADP:O3B	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:344:ARG:O	21:g:346:GLY:N	2.40	0.52
23:i:633:CYS:N	23:i:634:PRO:HD2	2.24	0.52
27:m:185:GLY:C	27:m:201:PHE:CZ	2.87	0.52
3:C:49:SER:CB	18:d:385:MET:HE3	2.39	0.52
4:D:81:LEU:HD12	4:D:84:ASP:HB2	1.91	0.52
17:c:163:MET:HE1	17:c:244:GLU:CB	2.36	0.52
19:e:121:ARG:O	31:q:275:VAL:HA	2.09	0.52
20:f:355:ILE:HG12	21:g:212:PHE:HD1	1.73	0.52
21:g:418:GLU:HA	21:g:421:MET:HB2	1.92	0.52
27:m:202:LEU:N	27:m:202:LEU:CD2	2.73	0.52
7:G:139:ILE:HD13	7:G:153:LYS:HB2	1.91	0.52
14:N:12:VAL:HG21	14:N:101:ALA:HB1	1.91	0.52
19:e:87:LEU:N	19:e:87:LEU:CD2	2.73	0.52
3:C:158:ALA:HB1	3:C:172:LEU:HD13	1.90	0.52
7:G:25:VAL:HG21	19:e:416:PHE:HE2	1.70	0.52
7:G:29:PHE:HZ	19:e:416:PHE:CE1	2.28	0.52
15:Q:31:THR:O	15:Q:45:VAL:HA	2.10	0.52
12:Z:43:CYS:HA	12:Z:52:ILE:O	2.10	0.52
17:c:350:GLY:O	17:c:353:HIS:HB2	2.10	0.52
18:d:232:LYS:HB3	18:d:235:LEU:HB2	1.91	0.52
19:e:169:GLY:O	19:e:340:GLN:NE2	2.42	0.52
19:e:263:PHE:CE2	19:e:265:ASP:CG	2.85	0.52
19:e:409:LYS:HG2	19:e:409:LYS:O	2.09	0.52
20:f:331:ILE:HG23	20:f:371:VAL:HG21	1.91	0.52
23:i:653:ALA:O	23:i:657:GLY:N	2.39	0.52
3:C:45:VAL:HG11	3:C:61:LYS:HB2	1.92	0.52
20:f:127:PRO:O	20:f:128:GLY:C	2.51	0.52
25:k:305:LEU:O	25:k:309:PHE:CB	2.58	0.52
27:m:78:GLU:O	27:m:82:LYS:CB	2.58	0.52
3:C:98:VAL:HG23	11:K:78:ALA:HB2	1.92	0.52
10:J:88:LEU:HD22	10:J:122:ALA:HB2	1.91	0.52
15:Q:98:VAL:HG23	11:Y:78:ALA:HB2	1.92	0.52
4:R:81:LEU:HD12	4:R:84:ASP:HB2	1.91	0.52
12:Z:88:ILE:HG22	12:Z:110:ILE:HD13	1.91	0.52
19:e:266:GLU:CG	20:f:258:MET:SD	2.90	0.52
20:f:181:THR:HG21	35:g:501:ADP:O1B	2.04	0.52
22:h:339:THR:HG23	22:h:341:GLY:H	1.75	0.52
6:F:94:GLU:OE2	6:F:114:ARG:NH1	2.43	0.52
12:L:27:THR:OG1	12:L:192:ALA:O	2.28	0.52
13:M:46:ASN:ND2	13:M:82:SER:OG	2.42	0.52
15:Q:192:ILE:HD11	15:Q:228:TYR:CA	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:94:GLU:OE2	6:T:114:ARG:NH1	2.43	0.52
7:U:40:VAL:C	7:U:167:ALA:HB2	2.33	0.52
12:Z:10:GLY:HA3	12:Z:42:LYS:HE3	1.92	0.52
14:b:12:VAL:HG21	14:b:101:ALA:HB1	1.91	0.52
19:e:366:ARG:HH11	19:e:368:ASP:HB2	1.74	0.52
22:h:332:HIS:HE1	35:h:401:ADP:O2'	1.93	0.52
26:l:166:LEU:O	26:l:170:GLN:CB	2.57	0.52
12:L:10:GLY:HA3	12:L:42:LYS:HE3	1.92	0.52
14:N:31:THR:O	14:N:175:ARG:NH1	2.42	0.52
1:O:110:VAL:HG22	1:O:135:ILE:HG13	1.92	0.52
13:a:11:VAL:HG21	13:a:53:ALA:H	1.75	0.52
17:c:354:ILE:CD1	17:c:382:GLY:HA2	2.39	0.52
19:e:323:ARG:CD	22:h:143:VAL:HG22	0.12	0.52
22:h:131:VAL:C	22:h:135:VAL:HG21	2.31	0.52
26:l:181:SER:OG	26:l:182:ASN:N	2.42	0.52
15:Q:87:ALA:HB2	15:Q:111:ILE:HD11	1.92	0.52
15:Q:116:GLN:NE2	4:R:84:ASP:OD1	2.42	0.52
17:c:193:THR:HG23	17:c:316:LYS:HE3	1.92	0.52
17:c:324:PRO:O	17:c:326:THR:N	2.36	0.52
19:e:245:ARG:HH22	20:f:78:ARG:HD2	1.74	0.52
20:f:316:HIS:HE1	35:g:501:ADP:C2	2.27	0.52
22:h:328:ILE:CD1	35:h:401:ADP:C5	2.92	0.52
15:Q:49:SER:O	15:Q:50:VAL:CB	2.56	0.51
16:S:34:ALA:HA	16:S:162:GLY:HA3	1.90	0.51
8:V:3:ILE:HG21	8:V:127:MET:HB2	1.92	0.51
12:Z:13:LEU:O	12:Z:24:ALA:N	2.39	0.51
17:c:101:ILE:HG13	17:c:111:TYR:HB3	1.91	0.51
19:e:68:LEU:O	19:e:72:PHE:CB	2.58	0.51
19:e:374:ASP:HB3	20:f:292:PRO:HG3	1.92	0.51
19:e:412:GLN:CA	19:e:412:GLN:NE2	2.73	0.51
7:G:42:VAL:CG2	7:G:194:THR:HG21	2.40	0.51
12:L:43:CYS:HA	12:L:52:ILE:O	2.10	0.51
13:M:11:VAL:HG21	13:M:53:ALA:H	1.75	0.51
2:P:49:ARG:NH2	2:P:212:GLU:OE1	2.44	0.51
15:Q:188:ILE:HG23	15:Q:228:TYR:CE2	2.40	0.51
10:X:88:LEU:HD22	10:X:122:ALA:HB2	1.91	0.51
13:a:13:GLY:HA3	13:a:22:ILE:HG22	1.91	0.51
14:b:31:THR:O	14:b:175:ARG:NH1	2.42	0.51
18:d:257:GLN:CD	18:d:266:LEU:HD12	2.34	0.51
18:d:265:LYS:HA	18:d:265:LYS:NZ	2.26	0.51
19:e:296:MET:SD	19:e:326:ARG:O	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:408:LYS:NZ	19:e:408:LYS:CB	2.73	0.51
20:f:155:ASN:HB3	20:f:158:LEU:HD13	1.92	0.51
1:A:110:VAL:HG22	1:A:135:ILE:HG13	1.92	0.51
10:J:19:ARG:NH1	10:J:193:ASN:OD1	2.43	0.51
12:L:139:GLY:N	12:L:142:SER:OG	2.36	0.51
15:Q:46:GLU:O	15:Q:47:LYS:O	2.28	0.51
7:U:230:LEU:HD22	7:U:234:GLU:HG3	1.93	0.51
18:d:301:GLY:N	18:d:304:GLU:OE1	2.44	0.51
18:d:341:LEU:CD1	18:d:341:LEU:N	2.73	0.51
20:f:83:CYS:SG	20:f:84:ARG:N	2.84	0.51
20:f:185:ARG:CZ	21:g:321:GLN:HG2	2.39	0.51
21:g:388:THR:HB	21:g:391:PHE:HE2	1.74	0.51
27:m:160:ASN:O	27:m:164:ALA:CB	2.59	0.51
27:m:291:HIS:O	27:m:295:TYR:CB	2.58	0.51
4:R:190:THR:OG1	4:R:192:LYS:NZ	2.34	0.51
9:W:70:LEU:HD23	9:W:89:MET:HE1	1.91	0.51
17:c:165:GLN:O	17:c:167:GLU:N	2.43	0.51
17:c:192:GLU:HB3	17:c:195:LEU:HD22	1.92	0.51
19:e:71:GLU:O	19:e:75:ALA:CB	2.57	0.51
19:e:267:ILE:C	19:e:269:ALA:N	2.68	0.51
22:h:357:ALA:C	22:h:359:VAL:N	2.65	0.51
27:m:17:LEU:O	27:m:18:ARG:C	2.54	0.51
3:C:87:ALA:HB2	3:C:111:ILE:HD11	1.92	0.51
19:e:208:PRO:HD2	19:e:335:LEU:HD12	1.91	0.51
19:e:267:ILE:C	19:e:269:ALA:H	2.19	0.51
19:e:403:TYR:O	19:e:407:ILE:CB	1.67	0.51
15:Q:206:ILE:HG22	15:Q:225:ILE:HG21	1.86	0.51
14:b:151:GLU:HA	14:b:154:GLN:HG2	1.93	0.51
17:c:156:LYS:HE3	18:d:122:ILE:HD12	1.93	0.51
17:c:163:MET:HG3	17:c:239:ARG:O	2.10	0.51
17:c:248:LYS:HB2	18:d:260:LEU:O	2.11	0.51
19:e:129:SER:HB3	19:e:252:ARG:HH12	1.74	0.51
21:g:222:GLY:C	21:g:348:LEU:HD13	2.35	0.51
35:h:401:ADP:N3	35:h:401:ADP:C2'	2.73	0.51
26:l:258:LYS:HD2	26:l:261:LEU:HD21	1.93	0.51
29:o:128:GLU:O	29:o:132:MET:N	2.40	0.51
1:O:38:LYS:HE3	1:O:143:PRO:HG2	1.93	0.51
15:Q:50:VAL:HA	15:Q:204:LYS:HD3	1.92	0.51
4:R:51:GLU:OE1	4:R:204:GLN:NE2	2.44	0.51
16:S:9:ASP:OD1	16:S:9:ASP:N	2.41	0.51
18:d:112:LEU:HD22	18:d:113:GLU:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:122:GLU:CG	31:q:278:GLN:CB	2.89	0.51
19:e:388:ARG:HH12	20:f:147:GLU:HG2	1.75	0.51
19:e:412:GLN:NE2	19:e:412:GLN:HA	2.25	0.51
20:f:179:GLY:H	35:g:501:ADP:H8	1.59	0.51
21:g:261:ILE:N	21:g:261:ILE:CD1	2.73	0.51
22:h:67:GLN:OE1	22:h:67:GLN:HA	2.11	0.51
24:j:339:ASN:O	24:j:342:VAL:N	2.40	0.51
11:K:127:SER:O	11:K:132:SER:OG	2.29	0.51
15:Q:51:ALA:HA	15:Q:54:GLN:HG2	1.92	0.51
17:c:327:LEU:C	17:c:332:MET:HE3	2.35	0.51
18:d:107:MET:CE	18:d:151:LEU:HD11	2.39	0.51
19:e:200:ARG:NH2	19:e:305:VAL:O	2.43	0.51
21:g:184:GLN:HG3	21:g:186:SER:H	1.76	0.51
22:h:99:VAL:HG22	22:h:123:LEU:HB2	1.91	0.51
22:h:114:VAL:HG13	22:h:127:LEU:CG	2.26	0.51
3:C:39:ASP:OD1	3:C:213:ARG:NE	2.43	0.51
15:Q:192:ILE:CG2	15:Q:228:TYR:HB3	2.40	0.51
18:d:105:THR:C	18:d:107:MET:H	2.07	0.51
19:e:385:LEU:HD23	19:e:398:ASP:OD1	2.10	0.51
20:f:257:LEU:O	20:f:261:LEU:HB2	2.11	0.51
20:f:264:MET:HG2	20:f:275:MET:HE3	1.93	0.51
26:l:417:LYS:O	26:l:421:LEU:CB	2.58	0.51
4:R:41:GLN:HB3	4:R:166:ASP:HA	1.91	0.51
10:X:182:VAL:HG23	10:X:191:LEU:CG	2.41	0.51
12:Z:139:GLY:N	12:Z:142:SER:OG	2.36	0.51
18:d:260:LEU:HD21	18:d:263:GLY:CA	2.31	0.51
21:g:235:LEU:HD13	35:g:502:ADP:H2'	1.93	0.51
28:n:263:ALA:C	28:n:265:LEU:N	2.37	0.51
2:P:162:THR:HA	2:P:172:VAL:HG21	1.93	0.50
15:Q:188:ILE:HG22	15:Q:228:TYR:CG	2.46	0.50
14:b:84:LYS:O	14:b:88:TYR:CB	2.60	0.50
20:f:249:ALA:HA	21:g:261:ILE:HD11	1.94	0.50
20:f:353:PHE:HZ	20:f:373:LYS:HD3	1.76	0.50
21:g:399:VAL:O	21:g:403:ALA:HB2	2.10	0.50
21:g:428:GLN:HG2	21:g:430:LYS:HE3	1.93	0.50
22:h:99:VAL:HG21	22:h:105:ILE:HD11	1.94	0.50
23:i:613:ASP:C	23:i:615:ARG:H	2.19	0.50
31:q:89:PRO:O	31:q:93:ALA:HB3	2.12	0.50
1:A:176:ARG:CD	26:l:160:MET:SD	2.99	0.50
12:L:13:LEU:HB3	12:L:24:ALA:HB3	1.93	0.50
13:M:114:GLY:HA2	13:M:192:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:VAL:HG12	1:O:46:ALA:HB3	1.94	0.50
15:Q:32:ALA:CB	15:Q:45:VAL:HG13	2.27	0.50
4:R:189:MET:HG3	4:R:191:LEU:H	1.74	0.50
18:d:247:PHE:HA	18:d:281:ILE:HG22	1.94	0.50
20:f:182:LEU:O	20:f:184:ALA:N	2.42	0.50
20:f:197:LYS:HA	20:f:231:PHE:HB3	1.93	0.50
22:h:117:ARG:HA	22:h:122:THR:N	2.25	0.50
22:h:132:ASP:CB	22:h:133:PRO:HD2	2.40	0.50
26:l:348:GLU:O	26:l:352:SER:CB	2.60	0.50
7:G:40:VAL:O	7:G:51:VAL:HG22	2.10	0.50
12:L:13:LEU:HD13	12:L:137:ALA:HB2	1.94	0.50
18:d:237:LYS:CD	18:d:283:PHE:CE1	2.58	0.50
18:d:264:PRO:O	18:d:265:LYS:HE2	2.11	0.50
21:g:195:ILE:O	21:g:199:VAL:HB	2.11	0.50
21:g:252:ALA:HB3	21:g:255:GLN:HG3	1.93	0.50
25:k:304:ASP:O	25:k:308:LEU:CB	2.60	0.50
27:m:17:LEU:C	27:m:19:ILE:N	2.68	0.50
28:n:75:LEU:O	28:n:79:TYR:CB	2.60	0.50
1:A:123:SER:HA	2:B:127:LYS:HE3	1.93	0.50
4:D:51:GLU:OE1	4:D:204:GLN:NE2	2.44	0.50
4:D:146:VAL:HG23	4:D:151:PRO:HG3	1.94	0.50
5:E:62:LYS:NZ	21:g:439:ALA:C	2.69	0.50
16:S:85:CYS:O	16:S:89:ARG:HB2	2.11	0.50
17:c:215:PHE:C	17:c:222:LYS:HE3	2.25	0.50
18:d:341:LEU:HD13	18:d:342:ILE:H	1.76	0.50
18:d:342:ILE:HD11	18:d:350:LYS:HZ3	1.75	0.50
19:e:394:VAL:HG22	19:e:399:PHE:CD1	2.46	0.50
20:f:60:VAL:HG13	20:f:60:VAL:O	2.12	0.50
20:f:238:ILE:HG22	20:f:257:LEU:HD23	1.92	0.50
26:l:224:ASP:HA	26:l:228:ALA:H	1.74	0.50
26:l:406:ASN:C	26:l:408:SER:H	2.18	0.50
12:L:185:ARG:HD3	8:V:26:VAL:HG13	1.94	0.50
14:N:84:LYS:O	14:N:88:TYR:CB	2.60	0.50
19:e:99:ASN:O	19:e:115:ILE:N	2.34	0.50
15:Q:220:LEU:CD1	15:Q:228:TYR:HE2	2.23	0.50
4:R:146:VAL:HG23	4:R:151:PRO:HG3	1.94	0.50
22:h:155:ASP:HA	22:h:158:ILE:HG12	1.93	0.50
26:l:403:THR:C	26:l:405:GLN:N	2.69	0.50
27:m:168:ILE:N	27:m:168:ILE:CD1	2.73	0.50
31:q:238:CYS:O	31:q:242:GLU:N	2.38	0.50
5:E:16:GLN:HG2	5:E:17:GLY:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:16:GLN:HG2	16:S:17:GLY:H	1.77	0.50
16:S:132:LEU:HB2	16:S:147:THR:HG22	1.94	0.50
6:T:67:PHE:HB2	6:T:75:MET:HB2	1.94	0.50
12:Z:13:LEU:HD13	12:Z:137:ALA:HB2	1.94	0.50
17:c:92:PRO:HB3	18:d:157:HIS:HB2	1.93	0.50
17:c:112:ILE:HG12	17:c:122:VAL:HG22	1.94	0.50
17:c:167:GLU:O	17:c:169:LYS:N	2.45	0.50
18:d:260:LEU:HD12	18:d:262:ASP:N	2.19	0.50
21:g:431:LYS:NZ	21:g:431:LYS:CB	2.73	0.50
7:G:230:LEU:HD22	7:G:234:GLU:HG3	1.93	0.50
14:N:151:GLU:HA	14:N:154:GLN:HG2	1.93	0.50
2:P:49:ARG:NH1	2:P:208:ALA:O	2.45	0.50
4:R:147:ASP:OD2	4:R:152:GLN:NE2	2.45	0.50
7:U:170:VAL:O	7:U:171:LYS:CB	2.59	0.50
7:U:232:GLU:O	7:U:236:ASP:CB	2.59	0.50
10:X:4:LEU:HD22	10:X:45:LEU:HD23	1.94	0.50
13:a:114:GLY:HA2	13:a:192:VAL:HG11	1.92	0.50
19:e:157:ASP:N	19:e:157:ASP:OD1	2.45	0.50
22:h:114:VAL:CG1	22:h:127:LEU:CA	2.90	0.50
26:l:137:TYR:HD1	26:l:142:ARG:HG3	1.76	0.50
4:D:121:LEU:HD23	5:E:126:ARG:HH21	1.76	0.50
7:U:49:VAL:HG23	7:U:219:VAL:HG12	1.93	0.50
14:b:144:ARG:HG3	14:b:145:GLU:H	1.77	0.50
17:c:327:LEU:CB	17:c:332:MET:HE3	2.41	0.50
17:c:354:ILE:HG13	17:c:385:ILE:HG21	1.93	0.50
18:d:149:SER:HG	18:d:163:LEU:HG	1.76	0.50
18:d:246:THR:CG2	18:d:280:SER:HB3	2.42	0.50
18:d:374:LEU:HA	18:d:414:VAL:HG12	1.94	0.50
19:e:208:PRO:HD3	19:e:335:LEU:HD12	1.94	0.50
19:e:377:SER:O	19:e:381:GLU:CB	2.60	0.50
20:f:135:ILE:CD1	20:f:182:LEU:HD21	2.41	0.50
20:f:193:CYS:HG	20:f:227:PRO:HG2	1.77	0.50
20:f:290:LEU:CD2	20:f:298:LYS:CD	2.82	0.50
21:g:428:GLN:CG	21:g:430:LYS:HE3	2.42	0.50
27:m:107:LYS:O	27:m:111:LEU:CB	2.60	0.50
2:B:49:ARG:NH1	2:B:208:ALA:O	2.45	0.49
2:B:49:ARG:NH2	2:B:212:GLU:OE1	2.44	0.49
4:D:18:GLU:CD	4:D:20:ARG:CZ	2.73	0.49
5:E:85:CYS:O	5:E:89:ARG:HB2	2.11	0.49
8:H:198:ARG:NH1	9:I:150:GLU:O	2.45	0.49
12:Z:13:LEU:HB3	12:Z:24:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:26:MET:HE1	13:a:202:PRO:HG3	1.94	0.49
17:c:299:MET:O	17:c:302:LEU:HB3	2.12	0.49
17:c:327:LEU:CB	17:c:332:MET:HE2	2.41	0.49
19:e:376:ASN:O	19:e:380:GLN:CB	2.60	0.49
26:l:153:LEU:HD12	26:l:166:LEU:HD23	1.94	0.49
33:s:54:ASN:O	33:s:58:ALA:HB2	2.12	0.49
6:F:227:VAL:HG13	6:F:229:LYS:HA	1.94	0.49
7:G:73:THR:HG23	7:G:75:ASN:H	1.78	0.49
8:H:32:SER:HB3	8:H:187:ARG:HH12	1.77	0.49
14:N:144:ARG:HG3	14:N:145:GLU:H	1.77	0.49
1:O:201:GLN:OE1	1:O:203:THR:OG1	2.28	0.49
15:Q:192:ILE:HG21	15:Q:228:TYR:CG	2.47	0.49
8:V:43:CYS:HA	8:V:100:LEU:HA	1.94	0.49
11:Y:127:SER:O	11:Y:132:SER:OG	2.29	0.49
18:d:105:THR:O	18:d:107:MET:HG2	2.11	0.49
18:d:361:LYS:HZ1	18:d:389:ASP:HA	1.76	0.49
23:i:633:CYS:N	23:i:634:PRO:CD	2.75	0.49
26:l:153:LEU:HD13	26:l:157:LEU:HG	1.94	0.49
26:l:165:LEU:C	26:l:165:LEU:CD1	2.85	0.49
7:G:49:VAL:HG23	7:G:219:VAL:HG12	1.93	0.49
6:T:227:VAL:HG13	6:T:229:LYS:HA	1.94	0.49
12:Z:15:ILE:O	12:Z:21:ALA:HA	2.12	0.49
17:c:236:CYS:SG	17:c:271:LEU:N	2.77	0.49
18:d:407:LEU:HD11	22:h:174:LEU:HD12	1.93	0.49
19:e:389:GLU:HG2	19:e:391:ARG:HB2	1.95	0.49
22:h:187:LEU:HB2	22:h:311:ILE:HG21	1.92	0.49
10:J:193:ASN:N	10:J:193:ASN:ND2	2.60	0.49
19:e:205:TYR:CZ	19:e:332:GLU:CA	2.96	0.49
20:f:61:LEU:CD1	20:f:72:LYS:CB	2.83	0.49
22:h:310:ARG:C	22:h:311:ILE:HD13	2.37	0.49
22:h:355:SER:O	22:h:356:GLY:C	2.52	0.49
26:l:403:THR:O	26:l:404:ILE:C	2.55	0.49
1:A:38:LYS:HE3	1:A:143:PRO:HG2	1.93	0.49
5:E:132:LEU:HB2	5:E:147:THR:HG22	1.94	0.49
10:J:4:LEU:HD22	10:J:45:LEU:HD23	1.94	0.49
18:d:103:ARG:NH2	18:d:138:PHE:HB3	2.28	0.49
19:e:408:LYS:NZ	19:e:408:LYS:CA	2.76	0.49
20:f:225:HIS:ND1	20:f:225:HIS:N	2.60	0.49
22:h:114:VAL:HG21	22:h:126:ILE:HA	1.95	0.49
22:h:270:GLN:OE1	22:h:270:GLN:HA	2.13	0.49
26:l:166:LEU:O	26:l:170:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:SER:OG	2:B:17:ARG:N	2.46	0.49
4:D:110:GLU:O	4:D:114:GLN:CB	2.59	0.49
11:K:166:ARG:NH1	9:W:33:MET:O	2.40	0.49
1:O:184:GLU:HG3	1:O:187:ILE:HD12	1.94	0.49
7:U:43:ARG:HD3	7:U:151:VAL:HG12	1.93	0.49
19:e:293:LEU:HD12	19:e:326:ARG:HD2	1.95	0.49
20:f:75:ASN:ND2	21:g:129:ARG:O	2.45	0.49
20:f:79:TYR:HE2	20:f:105:LEU:HD21	1.77	0.49
22:h:130:LYS:C	22:h:130:LYS:CD	2.85	0.49
1:O:106:THR:HB	1:O:144:TYR:HD2	1.77	0.49
15:Q:188:ILE:HG21	15:Q:228:TYR:HH	1.69	0.49
17:c:398:ARG:HH12	18:d:195:GLN:HE22	1.61	0.49
18:d:197:ILE:HB	18:d:351:ILE:HD11	1.94	0.49
18:d:220:LYS:O	18:d:348:ASP:OD1	2.29	0.49
18:d:249:ARG:HB2	18:d:283:PHE:HB3	1.95	0.49
18:d:264:PRO:HG3	18:d:308:THR:HA	1.95	0.49
18:d:407:LEU:HD22	22:h:178:LEU:HD11	1.87	0.49
20:f:125:GLU:CD	20:f:195:PHE:HD2	2.21	0.49
21:g:343:LEU:HD13	21:g:343:LEU:N	2.22	0.49
22:h:114:VAL:HG12	22:h:127:LEU:CD1	2.22	0.49
22:h:194:THR:HA	35:h:401:ADP:N7	2.28	0.49
27:m:53:TYR:O	27:m:57:LEU:N	2.45	0.49
27:m:188:CYS:HA	27:m:191:ILE:HG22	1.94	0.49
1:A:35:VAL:HG12	1:A:46:ALA:HB3	1.93	0.49
1:A:184:GLU:HG3	1:A:187:ILE:HD12	1.94	0.49
8:H:38:SER:HB3	8:H:41:ILE:HB	1.95	0.49
8:V:32:SER:HB3	8:V:187:ARG:HH12	1.77	0.49
13:a:98:SER:O	13:a:102:LYS:NZ	2.41	0.49
17:c:283:ALA:HB1	17:c:328:ASP:HB3	1.94	0.49
18:d:248:LEU:N	18:d:281:ILE:O	2.43	0.49
18:d:398:ILE:O	18:d:402:ALA:CB	2.61	0.49
21:g:88:TYR:HE1	21:g:161:LEU:HB2	1.77	0.49
26:l:406:ASN:O	26:l:407:MET:C	2.55	0.49
1:A:70:HIS:HA	1:A:217:PHE:H	1.78	0.49
4:D:147:ASP:OD2	4:D:152:GLN:NE2	2.45	0.49
6:F:140:TYR:HB3	6:F:146:ALA:HA	1.94	0.49
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.95	0.49
8:H:119:THR:H	14:N:53:GLN:NE2	2.11	0.49
10:J:59:TYR:HE2	10:J:87:ASN:HD21	1.59	0.49
14:N:29:ARG:HG3	14:N:30:VAL:HG22	1.95	0.49
8:V:37:ILE:HG23	8:V:60:SER:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:c:121:PHE:HB3	21:g:89:LEU:HD12	1.94	0.49
19:e:323:ARG:NH1	19:e:323:ARG:CB	2.73	0.49
19:e:377:SER:O	19:e:381:GLU:HB2	2.13	0.49
21:g:261:ILE:N	21:g:261:ILE:HD12	2.27	0.49
27:m:105:MET:HA	27:m:108:ALA:HB3	1.94	0.49
3:C:34:GLY:HA2	3:C:42:VAL:O	2.13	0.49
5:E:67:ASP:OD2	5:E:70:ILE:N	2.46	0.49
5:E:78:THR:HG22	21:g:439:ALA:HB2	1.95	0.49
6:F:67:PHE:HB2	6:F:75:MET:HB2	1.94	0.49
8:H:37:ILE:HG23	8:H:60:SER:HA	1.95	0.49
7:U:73:THR:HG23	7:U:75:ASN:H	1.77	0.49
9:W:59:VAL:O	9:W:63:ALA:HB2	2.13	0.49
10:X:59:TYR:HE2	10:X:87:ASN:HD21	1.59	0.49
18:d:401:GLU:OE2	18:d:425:ASN:ND2	2.45	0.49
19:e:323:ARG:NH1	19:e:323:ARG:CA	2.76	0.49
20:f:178:THR:HG22	20:f:301:ILE:HG22	1.94	0.49
23:i:516:LEU:O	23:i:520:MET:CB	2.61	0.49
25:k:288:HIS:CB	25:k:291:SER:CB	2.90	0.49
26:l:64:ALA:O	26:l:68:GLY:CA	2.54	0.49
27:m:192:ARG:HH12	27:m:291:HIS:HA	1.78	0.49
27:m:237:ARG:HH11	27:m:241:ILE:HD12	1.78	0.49
7:G:113:MET:HE2	8:H:70:THR:HG22	1.95	0.48
9:I:59:VAL:O	9:I:63:ALA:HB2	2.13	0.48
2:P:13:SER:OG	2:P:17:ARG:N	2.46	0.48
15:Q:47:LYS:HG2	15:Q:205:ASN:N	2.04	0.48
16:S:67:ASP:HB2	16:S:70:ILE:H	1.78	0.48
9:W:12:ALA:HA	9:W:20:ALA:O	2.13	0.48
10:X:164:LEU:HD12	10:X:194:ILE:HD12	1.95	0.48
12:Z:27:THR:OG1	12:Z:192:ALA:O	2.28	0.48
12:Z:44:TYR:HB2	12:Z:52:ILE:HG22	1.95	0.48
17:c:415:LYS:O	17:c:419:SER:OG	2.30	0.48
18:d:221:GLY:N	18:d:348:ASP:OD1	2.46	0.48
19:e:317:LEU:CD1	19:e:321:LEU:HD23	2.43	0.48
20:f:128:GLY:CA	21:g:321:GLN:NE2	2.53	0.48
21:g:437:TYR:O	21:g:439:ALA:N	2.46	0.48
22:h:196:LYS:CA	35:h:401:ADP:O1B	2.53	0.48
22:h:248:MET:HB2	22:h:293:MET:HA	1.95	0.48
27:m:124:PHE:HA	27:m:127:THR:HG22	1.95	0.48
9:I:12:ALA:HA	9:I:20:ALA:O	2.13	0.48
12:L:28:ARG:NH2	12:L:189:THR:OG1	2.46	0.48
15:Q:34:GLY:HA2	15:Q:42:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:44:GLY:HA3	7:U:47:CYS:O	2.12	0.48
18:d:234:LEU:HA	18:d:237:LYS:HG2	1.95	0.48
21:g:274:LEU:HD23	21:g:278:LYS:HG3	1.94	0.48
22:h:61:GLU:HA	22:h:64:GLN:HG3	1.95	0.48
22:h:88:LYS:HB3	22:h:94:LYS:HE3	1.95	0.48
22:h:137:LEU:CA	22:h:140:VAL:CG1	2.84	0.48
23:i:498:LYS:O	23:i:502:TYR:N	2.46	0.48
26:l:349:HIS:O	26:l:353:LEU:CB	2.61	0.48
3:C:115:LYS:HG2	3:C:127:PHE:HD2	1.78	0.48
8:H:43:CYS:HA	8:H:100:LEU:HA	1.94	0.48
17:c:192:GLU:O	17:c:197:HIS:ND1	2.46	0.48
25:k:70:VAL:O	25:k:74:CYS:CB	2.61	0.48
26:l:82:LYS:O	26:l:122:ARG:NH2	2.46	0.48
2:B:162:THR:HA	2:B:172:VAL:HG21	1.93	0.48
7:G:29:PHE:CE2	19:e:416:PHE:CZ	3.01	0.48
9:I:146:TYR:O	9:I:148:MET:N	2.46	0.48
9:I:150:GLU:OE1	12:Z:185:ARG:NE	2.46	0.48
10:J:182:VAL:CG2	10:J:191:LEU:HD11	2.43	0.48
12:L:15:ILE:O	12:L:21:ALA:HA	2.13	0.48
6:T:160:TYR:CG	6:T:163:CYS:HB3	2.49	0.48
9:W:146:TYR:O	9:W:148:MET:N	2.45	0.48
12:Z:28:ARG:NH2	12:Z:189:THR:OG1	2.46	0.48
14:b:29:ARG:HG3	14:b:30:VAL:HG22	1.95	0.48
18:d:361:LYS:O	18:d:365:PHE:HB2	2.14	0.48
22:h:94:LYS:O	22:h:95:PHE:CE2	2.62	0.48
25:k:319:THR:O	25:k:323:ASP:CB	2.61	0.48
5:E:67:ASP:HB2	5:E:70:ILE:H	1.79	0.48
15:Q:115:LYS:HG2	15:Q:127:PHE:HD2	1.78	0.48
15:Q:192:ILE:HD13	15:Q:228:TYR:HB3	0.50	0.48
18:d:250:VAL:HG21	18:d:270:LEU:CD1	2.44	0.48
19:e:214:MET:N	19:e:214:MET:SD	2.85	0.48
19:e:267:ILE:HD11	19:e:309:MET:CG	2.43	0.48
19:e:408:LYS:C	19:e:410:ASP:N	2.60	0.48
21:g:69:MET:O	21:g:73:ILE:CB	2.61	0.48
27:m:161:THR:HG22	27:m:184:GLN:HE22	1.78	0.48
3:C:89:VAL:HG22	10:J:66:LEU:HD11	1.95	0.48
4:D:85:ALA:HB2	4:D:139:VAL:HG21	1.95	0.48
9:I:202:ARG:HG2	12:Z:157:ASN:HD21	1.76	0.48
4:R:99:HIS:CD2	4:R:107:MET:HG2	2.49	0.48
10:X:193:ASN:N	10:X:193:ASN:ND2	2.60	0.48
18:d:135:ILE:HA	18:d:159:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:119:ILE:HD12	19:e:141:ASP:HA	1.95	0.48
20:f:204:VAL:HG22	21:g:261:ILE:CG2	2.37	0.48
22:h:134:LEU:HD21	22:h:237:MET:SD	2.54	0.48
22:h:141:GLU:HA	22:h:141:GLU:OE1	2.14	0.48
26:l:82:LYS:HE3	26:l:120:GLU:HG2	1.95	0.48
26:l:194:ARG:HH22	26:l:218:HIS:CE1	2.30	0.48
27:m:329:PHE:O	27:m:333:GLU:CB	2.61	0.48
29:o:104:ARG:C	29:o:106:ALA:H	2.19	0.48
3:C:141:THR:HG22	3:C:143:ARG:HG3	1.96	0.48
5:E:236:LEU:C	5:E:236:LEU:HD12	2.38	0.48
13:M:122:LEU:HG	13:M:137:LEU:HD12	1.96	0.48
14:N:152:CYS:HA	14:N:155:PHE:HB3	1.96	0.48
1:O:70:HIS:HA	1:O:217:PHE:H	1.78	0.48
15:Q:39:ASP:OD1	15:Q:213:ARG:NE	2.43	0.48
4:R:110:GLU:O	4:R:114:GLN:CB	2.59	0.48
16:S:85:CYS:O	16:S:89:ARG:CB	2.62	0.48
11:Y:19:ARG:NH1	11:Y:170:SER:O	2.47	0.48
11:Y:157:ARG:NH1	11:Y:190:ASP:OD2	2.47	0.48
18:d:246:THR:HG23	18:d:280:SER:HA	1.95	0.48
23:i:773:PHE:O	23:i:775:LEU:N	2.45	0.48
25:k:293:ASP:C	25:k:296:LEU:H	2.21	0.48
27:m:43:ALA:O	27:m:47:ASP:CB	2.62	0.48
27:m:208:PHE:HE2	27:m:211:TYR:O	1.96	0.48
4:D:99:HIS:CD2	4:D:107:MET:HG2	2.48	0.48
6:F:141:SER:HB2	6:F:144:ASP:HB2	1.96	0.48
16:S:67:ASP:OD2	16:S:70:ILE:N	2.46	0.48
7:U:112:ASP:N	7:U:112:ASP:OD1	2.46	0.48
8:V:107:GLY:O	8:V:109:HIS:ND1	2.46	0.48
20:f:70:ILE:N	20:f:70:ILE:CD1	2.77	0.48
20:f:210:GLU:OE2	20:f:213:ARG:NH2	2.34	0.48
20:f:271:HIS:O	20:f:272:ARG:NE	2.42	0.48
22:h:310:ARG:CG	22:h:310:ARG:NH1	2.73	0.48
23:i:665:ASN:C	23:i:667:GLU:N	2.72	0.48
29:o:104:ARG:C	29:o:106:ALA:N	2.69	0.48
8:H:204:CYS:SG	8:H:205:GLU:N	2.86	0.48
4:R:85:ALA:HB2	4:R:139:VAL:HG21	1.95	0.48
18:d:284:ILE:HG22	18:d:284:ILE:O	2.14	0.48
18:d:287:ILE:HG21	18:d:329:MET:HE3	1.95	0.48
19:e:88:VAL:HA	20:f:79:TYR:HB3	1.96	0.48
19:e:188:PHE:O	19:e:192:LYS:NZ	2.46	0.48
19:e:291:GLU:O	19:e:295:GLN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:89:VAL:HG13	22:h:91:PRO:HD2	1.96	0.48
22:h:297:ARG:HG2	22:h:299:ASP:H	1.79	0.48
6:F:160:TYR:CG	6:F:163:CYS:HB3	2.49	0.48
15:Q:221:ASN:HB2	15:Q:222:PRO:CD	2.42	0.48
6:T:141:SER:HB2	6:T:144:ASP:HB2	1.96	0.48
10:X:182:VAL:CG2	10:X:191:LEU:CD1	2.87	0.48
17:c:330:ALA:O	17:c:336:ARG:HD2	2.13	0.48
19:e:213:THR:HG23	35:e:501:ADP:O1B	2.13	0.48
20:f:172:LEU:O	20:f:180:LYS:NZ	2.40	0.48
1:A:106:THR:HB	1:A:144:TYR:HD2	1.78	0.47
5:E:85:CYS:O	5:E:89:ARG:CB	2.62	0.47
6:T:140:TYR:HB3	6:T:146:ALA:HA	1.94	0.47
8:V:38:SER:HB3	8:V:41:ILE:HB	1.95	0.47
12:Z:16:ALA:HB3	12:Z:134:SER:HA	1.96	0.47
18:d:403:GLY:O	18:d:407:LEU:HB2	2.13	0.47
20:f:64:LEU:O	20:f:66:GLU:CA	2.57	0.47
20:f:223:ARG:HH21	20:f:270:LEU:HD23	1.79	0.47
20:f:353:PHE:O	20:f:357:ALA:CB	2.62	0.47
11:K:157:ARG:NH1	11:K:190:ASP:OD2	2.47	0.47
15:Q:47:LYS:HD2	15:Q:47:LYS:H	1.78	0.47
19:e:370:ILE:HD13	19:e:375:ILE:HD11	1.96	0.47
20:f:61:LEU:CD1	20:f:61:LEU:N	2.77	0.47
22:h:131:VAL:C	22:h:135:VAL:CG2	2.87	0.47
25:k:139:GLU:O	25:k:143:ALA:CB	2.62	0.47
10:J:186:ASP:HB2	10:J:189:HIS:NE2	2.30	0.47
11:K:19:ARG:NH1	11:K:170:SER:O	2.47	0.47
12:L:16:ALA:HB3	12:L:134:SER:HA	1.96	0.47
12:L:36:HIS:HB3	13:M:132:TYR:CZ	2.49	0.47
8:V:137:VAL:HG21	8:V:158:ALA:HA	1.97	0.47
13:a:178:TYR:OH	13:a:208:ASN:N	2.46	0.47
20:f:61:LEU:N	20:f:61:LEU:HD12	2.29	0.47
20:f:127:PRO:O	20:f:189:SER:CB	2.47	0.47
22:h:347:ILE:O	22:h:351:MET:SD	2.72	0.47
23:i:478:SER:CB	23:i:514:LEU:CB	2.92	0.47
25:k:186:ILE:O	25:k:190:MET:CB	2.62	0.47
6:F:157:SER:H	7:G:88:ARG:NH2	2.12	0.47
7:G:42:VAL:HG11	7:G:198:ALA:HA	1.96	0.47
12:L:28:ARG:HG2	12:L:38:ARG:HG2	1.96	0.47
12:L:65:THR:O	12:L:69:GLU:HB2	2.14	0.47
15:Q:141:THR:HG22	15:Q:143:ARG:HG3	1.96	0.47
4:R:142:LEU:HD13	4:R:153:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:161:TRP:HB3	6:T:181:MET:HE2	1.96	0.47
10:X:186:ASP:HB2	10:X:189:HIS:HE1	1.80	0.47
13:a:122:LEU:HG	13:a:137:LEU:HD12	1.96	0.47
17:c:113:ILE:HG21	17:c:149:ILE:HD11	1.97	0.47
18:d:269:GLU:HA	18:d:272:ARG:HB3	1.96	0.47
18:d:334:ILE:HD12	18:d:337:LEU:HD21	1.95	0.47
18:d:341:LEU:N	18:d:341:LEU:HD13	2.29	0.47
20:f:310:LEU:HB3	20:f:332:VAL:HG21	1.95	0.47
22:h:384:GLU:O	22:h:388:ALA:CB	2.62	0.47
26:l:361:VAL:O	26:l:364:LYS:CB	2.62	0.47
4:D:71:ASP:HB2	4:D:96:THR:HG21	1.96	0.47
12:L:44:TYR:HB2	12:L:52:ILE:HG22	1.95	0.47
1:O:157:TRP:HA	2:P:57:ASP:H	1.79	0.47
15:Q:68:ASN:HA	15:Q:211:MET:HE2	1.96	0.47
7:U:44:GLY:C	7:U:46:ASP:H	2.22	0.47
18:d:247:PHE:HA	18:d:281:ILE:CG2	2.44	0.47
18:d:341:LEU:H	18:d:341:LEU:HD12	1.79	0.47
19:e:385:LEU:C	19:e:398:ASP:CG	2.81	0.47
21:g:437:TYR:C	21:g:439:ALA:N	2.69	0.47
22:h:106:ASN:HD22	22:h:106:ASN:C	2.18	0.47
22:h:127:LEU:HB3	22:h:128:PRO:CD	2.28	0.47
22:h:141:GLU:O	22:h:141:GLU:HG3	2.14	0.47
26:l:129:LEU:O	26:l:133:LEU:CB	2.62	0.47
26:l:323:LEU:O	26:l:327:TYR:CB	2.63	0.47
27:m:208:PHE:C	27:m:209:THR:HG22	2.39	0.47
6:F:161:TRP:HB3	6:F:181:MET:HE2	1.96	0.47
7:G:232:GLU:O	7:G:236:ASP:CB	2.59	0.47
10:J:81:ALA:HB1	10:J:124:LEU:HD11	1.97	0.47
2:P:86:LEU:HA	2:P:89:GLU:HB2	1.97	0.47
4:R:71:ASP:HB2	4:R:96:THR:HG21	1.96	0.47
19:e:87:LEU:HD12	19:e:131:ALA:HB1	1.97	0.47
20:f:130:VAL:HG11	20:f:185:ARG:HB3	1.97	0.47
22:h:114:VAL:HG13	22:h:127:LEU:CB	2.42	0.47
25:k:363:ILE:O	25:k:367:ALA:CB	2.63	0.47
26:l:159:LYS:HA	26:l:159:LYS:HD3	1.54	0.47
6:F:87:LEU:HA	6:F:90:ILE:HG13	1.96	0.47
6:F:97:ASN:O	6:F:101:ASN:CB	2.63	0.47
6:T:175:GLU:HA	6:T:178:LYS:HG2	1.97	0.47
14:b:152:CYS:HA	14:b:155:PHE:HB3	1.95	0.47
17:c:179:GLY:C	17:c:180:CYS:SG	2.92	0.47
17:c:328:ASP:N	17:c:328:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:d:106:PRO:CB	22:h:121:TYR:CD2	2.98	0.47
18:d:311:GLU:O	18:d:315:GLN:CB	2.61	0.47
19:e:412:GLN:O	19:e:413:GLU:C	2.57	0.47
20:f:148:VAL:HG21	20:f:297:ARG:HD3	1.96	0.47
20:f:222:ALA:HB1	20:f:273:VAL:HG11	1.97	0.47
21:g:383:GLU:HA	21:g:386:ARG:HG2	1.97	0.47
22:h:105:ILE:HD12	22:h:108:VAL:CG2	2.45	0.47
22:h:136:SER:C	22:h:140:VAL:CG1	2.76	0.47
27:m:127:THR:O	27:m:131:THR:OG1	2.32	0.47
27:m:211:TYR:HB2	27:m:214:MET:HB3	1.96	0.47
29:o:105:PRO:O	29:o:106:ALA:C	2.54	0.47
12:Z:24:ALA:HA	12:Z:195:ILE:HG22	1.96	0.47
12:Z:65:THR:O	12:Z:69:GLU:HB2	2.14	0.47
18:d:255:LEU:HG	18:d:308:THR:CG2	2.45	0.47
19:e:213:THR:CB	35:e:501:ADP:O1B	2.62	0.47
20:f:84:ARG:HH21	20:f:87:LEU:HA	1.80	0.47
20:f:118:LEU:CD1	20:f:121:ASN:HD22	2.27	0.47
21:g:234:THR:HG23	35:g:502:ADP:O1B	2.14	0.47
22:h:384:GLU:O	22:h:388:ALA:HB3	2.14	0.47
26:l:182:ASN:HB3	26:l:184:PRO:HD2	1.96	0.47
2:B:34:CYS:SG	2:B:75:SER:OG	2.67	0.47
2:B:50:ARG:NH1	2:B:51:ASN:OD1	2.48	0.47
3:C:68:ASN:HA	3:C:211:MET:HE2	1.96	0.47
15:Q:180:ALA:HB1	15:Q:187:THR:HG22	1.97	0.47
11:Y:84:ALA:O	11:Y:88:TYR:HB2	2.15	0.47
18:d:415:THR:HG22	18:d:418:ASP:H	1.79	0.47
19:e:109:SER:HB3	22:h:91:PRO:HD3	1.97	0.47
19:e:281:ALA:HA	20:f:208:ILE:HG21	1.97	0.47
21:g:235:LEU:O	21:g:239:ALA:CB	2.63	0.47
6:F:175:GLU:HA	6:F:178:LYS:HG2	1.97	0.47
18:d:145:GLU:N	18:d:145:GLU:CD	2.73	0.47
18:d:271:PHE:CE1	18:d:282:VAL:HG11	2.49	0.47
19:e:353:ASN:HB3	19:e:393:ILE:HG22	1.97	0.47
20:f:228:CYS:SG	20:f:229:ILE:N	2.88	0.47
22:h:350:LEU:HD11	22:h:387:VAL:HG21	1.97	0.47
27:m:198:ALA:HB2	27:m:226:VAL:HG13	1.97	0.47
6:F:112:ALA:O	6:F:116:ALA:HB2	2.15	0.46
6:F:143:ASN:HD21	14:N:106:GLN:HG3	1.79	0.46
11:K:84:ALA:O	11:K:88:TYR:HB2	2.15	0.46
12:L:2:PHE:HE1	13:M:127:MET:HE2	1.80	0.46
15:Q:188:ILE:CD1	15:Q:228:TYR:HH	2.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:220:LEU:CD1	15:Q:224:GLU:HB3	2.41	0.46
17:c:383:ALA:HA	35:c:501:ADP:H1'	1.39	0.46
18:d:338:ASP:O	18:d:341:LEU:HD12	2.15	0.46
20:f:168:LYS:HE3	20:f:275:MET:HE1	1.97	0.46
23:i:680:VAL:CB	23:i:683:VAL:CB	2.93	0.46
29:o:131:VAL:O	29:o:135:LEU:CB	2.63	0.46
13:M:110:MET:SD	13:M:110:MET:N	2.87	0.46
6:T:87:LEU:HA	6:T:90:ILE:HG13	1.97	0.46
18:d:364:ILE:HD12	35:d:501:ADP:N6	2.30	0.46
20:f:63:GLN:C	20:f:65:THR:N	2.63	0.46
20:f:179:GLY:CA	20:f:182:LEU:HD22	2.45	0.46
21:g:391:PHE:CE1	21:g:427:VAL:HG11	2.50	0.46
22:h:99:VAL:HG11	22:h:105:ILE:HG12	1.97	0.46
22:h:106:ASN:ND2	22:h:106:ASN:C	2.73	0.46
27:m:160:ASN:O	27:m:164:ALA:HB2	2.15	0.46
9:W:57:THR:O	9:W:61:THR:OG1	2.25	0.46
14:b:95:MET:HG3	14:b:116:MET:HE3	1.97	0.46
17:c:240:VAL:HG11	17:c:260:LEU:HD21	1.96	0.46
19:e:268:ASP:N	19:e:268:ASP:OD1	2.45	0.46
24:j:178:THR:O	24:j:182:LEU:CB	2.63	0.46
2:B:123:GLN:NE2	3:C:124:ARG:O	2.47	0.46
4:D:208:GLU:OE2	4:D:211:ASN:ND2	2.49	0.46
5:E:14:SER:HB2	5:E:18:ARG:HB3	1.98	0.46
6:F:15:SER:OG	6:F:19:ARG:N	2.48	0.46
12:L:24:ALA:HA	12:L:195:ILE:HG22	1.96	0.46
14:N:95:MET:HG3	14:N:116:MET:HE3	1.97	0.46
16:S:14:SER:HB2	16:S:18:ARG:HB3	1.98	0.46
6:T:97:ASN:O	6:T:101:ASN:CB	2.63	0.46
17:c:184:ILE:O	17:c:188:ARG:N	2.46	0.46
18:d:341:LEU:CD2	18:d:347:ILE:HG21	2.42	0.46
19:e:70:LYS:HA	28:n:185:GLY:HA3	1.97	0.46
19:e:223:THR:HB	19:e:225:ALA:HB3	1.98	0.46
19:e:373:ALA:C	20:f:292:PRO:HG2	2.40	0.46
19:e:377:SER:HB2	20:f:292:PRO:HB2	1.98	0.46
20:f:182:LEU:CG	20:f:183:LEU:N	2.79	0.46
20:f:344:ARG:HH22	21:g:218:GLN:HG2	1.80	0.46
21:g:343:LEU:CD1	21:g:343:LEU:N	2.73	0.46
22:h:142:LYS:HD3	22:h:142:LYS:H	1.77	0.46
27:m:167:LEU:C	27:m:167:LEU:HD23	2.40	0.46
29:o:100:MET:O	29:o:102:PHE:N	2.48	0.46
12:L:94:THR:O	12:L:98:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:202:GLY:H	15:Q:229:VAL:HG21	1.81	0.46
17:c:384:GLU:OE1	17:c:385:ILE:CA	2.63	0.46
21:g:96:LEU:HD22	21:g:145:LEU:HD12	1.98	0.46
2:B:240:HIS:CE1	2:B:243:GLU:HB3	2.49	0.46
4:D:142:LEU:HD13	4:D:153:LEU:HD13	1.97	0.46
7:G:112:ASP:N	7:G:112:ASP:OD1	2.46	0.46
2:P:50:ARG:NH1	2:P:51:ASN:OD1	2.48	0.46
2:B:86:LEU:HA	2:B:89:GLU:HB2	1.97	0.46
3:C:92:GLN:HB3	10:J:62:LYS:HG3	1.97	0.46
9:I:163:PHE:O	9:I:197:ARG:NH2	2.49	0.46
4:R:38:ILE:HD13	4:R:197:SER:HB2	1.98	0.46
6:T:15:SER:OG	6:T:19:ARG:N	2.48	0.46
8:V:3:ILE:CG2	8:V:127:MET:HB2	2.45	0.46
9:W:163:PHE:O	9:W:197:ARG:NH2	2.49	0.46
12:Z:2:PHE:HE1	13:a:127:MET:HE2	1.80	0.46
12:Z:94:THR:O	12:Z:98:SER:HB3	2.16	0.46
17:c:223:THR:O	17:c:226:ALA:HB3	2.16	0.46
22:h:305:LEU:HD12	22:h:311:ILE:HD11	1.98	0.46
26:l:368:MET:O	26:l:370:LEU:N	2.43	0.46
27:m:87:GLU:HA	27:m:90:ASP:HB3	1.96	0.46
31:q:266:THR:N	31:q:267:PRO:HD3	2.29	0.46
1:A:134:LEU:HA	1:A:147:GLN:HA	1.98	0.46
6:F:28:LYS:HD3	6:F:31:GLU:HB2	1.98	0.46
8:H:1:THR:CA	8:H:33:LYS:NZ	2.79	0.46
9:I:14:LYS:HE3	9:I:133:ASP:HA	1.98	0.46
4:R:43:SER:OG	4:R:44:GLU:OE1	2.32	0.46
16:S:169:ARG:O	16:S:173:GLU:N	2.48	0.46
17:c:420:TYR:O	17:c:424:SER:OG	2.31	0.46
20:f:60:VAL:O	20:f:62:LYS:N	2.43	0.46
25:k:141:GLU:O	25:k:145:LEU:CB	2.64	0.46
3:C:180:ALA:HB1	3:C:187:THR:HG22	1.97	0.46
9:I:1:SER:OG	9:I:2:ILE:N	2.48	0.46
15:Q:146:GLN:NE2	15:Q:147:THR:O	2.49	0.46
6:T:112:ALA:O	6:T:116:ALA:HB2	2.15	0.46
17:c:280:ILE:HG22	17:c:295:VAL:HG13	1.98	0.46
18:d:363:ARG:HD2	18:d:366:GLN:HE21	1.80	0.46
22:h:385:MET:HB3	26:l:195:THR:HG22	1.98	0.46
26:l:163:LYS:HD3	26:l:163:LYS:HA	1.84	0.46
29:o:99:GLU:O	29:o:102:PHE:CB	2.64	0.46
7:G:17:SER:OG	7:G:20:GLY:O	2.32	0.46
9:I:169:ALA:O	9:I:173:ALA:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:26:MET:CE	13:M:202:PRO:HG3	2.45	0.46
1:O:67:ILE:N	1:O:71:ILE:O	2.34	0.46
9:W:1:SER:OG	9:W:2:ILE:N	2.48	0.46
9:W:14:LYS:HE3	9:W:133:ASP:HA	1.98	0.46
12:Z:28:ARG:HG2	12:Z:38:ARG:HG2	1.96	0.46
17:c:300:LEU:HD21	21:g:287:GLU:HB3	1.98	0.46
19:e:114:ARG:NE	22:h:66:LEU:HD12	2.26	0.46
20:f:167:PRO:O	20:f:274:LYS:NZ	2.38	0.46
20:f:212:ALA:HA	20:f:215:ILE:HG22	1.98	0.46
27:m:124:PHE:HD2	27:m:144:LEU:HD13	1.81	0.46
16:S:14:SER:N	16:S:18:ARG:O	2.43	0.45
16:S:121:GLN:HB3	6:T:122:TYR:OH	2.15	0.45
7:U:17:SER:OG	7:U:20:GLY:O	2.32	0.45
17:c:383:ALA:N	35:c:501:ADP:C8	2.84	0.45
21:g:342:LEU:O	21:g:342:LEU:HD23	2.15	0.45
22:h:210:THR:HG21	22:h:241:HIS:CD2	2.44	0.45
25:k:142:ARG:O	25:k:146:THR:CB	2.64	0.45
27:m:208:PHE:CE2	27:m:211:TYR:CB	2.98	0.45
1:A:134:LEU:HB3	1:A:162:MET:HE1	1.98	0.45
9:I:204:ASP:HB3	11:Y:192:VAL:HG11	1.99	0.45
10:J:64:VAL:HG13	10:J:75:LEU:HD12	1.98	0.45
6:T:30:VAL:HG11	6:T:134:SER:H	1.81	0.45
7:U:141:ILE:HD12	7:U:220:VAL:HG22	1.98	0.45
10:X:66:LEU:O	10:X:70:ARG:HB2	2.17	0.45
18:d:249:ARG:HA	18:d:283:PHE:HB3	1.97	0.45
20:f:69:PHE:HE2	20:f:92:LEU:HD12	1.82	0.45
20:f:122:MET:HB3	20:f:196:LEU:HD21	1.97	0.45
21:g:224:LEU:HA	21:g:330:ALA:HB3	1.97	0.45
21:g:342:LEU:O	21:g:343:LEU:HD13	1.79	0.45
26:l:165:LEU:HD22	26:l:169:VAL:HG23	1.98	0.45
9:I:18:CYS:HA	9:I:189:ILE:O	2.16	0.45
9:I:146:TYR:HB3	12:Z:185:ARG:HG2	1.97	0.45
14:N:127:ILE:HG12	14:N:132:SER:HB2	1.98	0.45
1:O:134:LEU:HA	1:O:147:GLN:HA	1.98	0.45
15:Q:188:ILE:HG22	15:Q:228:TYR:CE2	2.41	0.45
15:Q:221:ASN:C	15:Q:223:GLU:H	2.25	0.45
10:X:64:VAL:HG13	10:X:75:LEU:HD12	1.98	0.45
13:a:110:MET:N	13:a:110:MET:SD	2.87	0.45
19:e:267:ILE:HD11	19:e:309:MET:CB	2.46	0.45
21:g:234:THR:OG1	35:g:502:ADP:O1A	2.29	0.45
22:h:157:GLN:HA	22:h:315:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:140:THR:HG23	26:l:142:ARG:HG2	1.98	0.45
31:q:89:PRO:O	31:q:93:ALA:CB	2.65	0.45
6:F:105:ASN:HD22	6:F:106:ILE:H	1.64	0.45
8:H:107:GLY:O	8:H:109:HIS:ND1	2.46	0.45
8:H:137:VAL:HG21	8:H:158:ALA:HA	1.97	0.45
11:K:97:MET:H	11:K:116:SER:HB2	1.82	0.45
12:L:145:LEU:HD22	12:L:178:VAL:HB	1.98	0.45
9:W:169:ALA:O	9:W:173:ALA:CB	2.64	0.45
10:X:81:ALA:HB1	10:X:124:LEU:HD11	1.97	0.45
14:b:84:LYS:O	14:b:88:TYR:HB2	2.16	0.45
18:d:380:LEU:HA	18:d:383:LEU:HB2	1.98	0.45
19:e:245:ARG:HH12	20:f:78:ARG:HD2	1.81	0.45
26:l:415:TYR:O	26:l:420:LYS:N	2.45	0.45
27:m:144:LEU:HD12	27:m:147:ILE:HD11	1.97	0.45
3:C:146:GLN:NE2	3:C:147:THR:O	2.49	0.45
15:Q:79:ASP:HB3	15:Q:127:PHE:HD1	1.82	0.45
6:T:28:LYS:HD3	6:T:31:GLU:HB2	1.98	0.45
11:Y:97:MET:H	11:Y:116:SER:HB2	1.82	0.45
17:c:126:SER:OG	17:c:149:ILE:O	2.28	0.45
19:e:323:ARG:NH1	19:e:323:ARG:HA	2.31	0.45
21:g:248:PHE:HD1	21:g:282:ILE:HG13	1.81	0.45
27:m:194:PHE:HD2	27:m:229:ILE:HG21	1.81	0.45
4:D:38:ILE:HD13	4:D:197:SER:HB2	1.98	0.45
5:E:196:ARG:HH22	5:E:235:GLY:HA3	1.81	0.45
6:F:30:VAL:HG11	6:F:134:SER:H	1.81	0.45
6:F:106:ILE:HD12	6:F:107:PRO:HD2	1.98	0.45
7:G:141:ILE:HD12	7:G:220:VAL:HG22	1.98	0.45
12:L:4:PRO:O	13:M:100:ARG:NH2	2.37	0.45
12:L:191:ASP:O	12:L:210:LEU:N	2.49	0.45
14:N:84:LYS:O	14:N:88:TYR:HB2	2.16	0.45
15:Q:192:ILE:HD12	15:Q:228:TYR:CB	2.25	0.45
6:T:105:ASN:HD22	6:T:106:ILE:H	1.64	0.45
7:U:164:LYS:NZ	7:U:164:LYS:CB	2.73	0.45
12:Z:191:ASP:O	12:Z:210:LEU:N	2.49	0.45
14:b:127:ILE:HG12	14:b:132:SER:HB2	1.98	0.45
20:f:342:ASP:OD1	21:g:345:SER:OG	2.34	0.45
21:g:81:LYS:HA	21:g:84:LYS:HG3	1.97	0.45
22:h:78:ARG:HB2	22:h:110:PRO:CD	2.38	0.45
11:K:18:SER:OG	11:K:173:ALA:N	2.46	0.45
4:R:114:GLN:OE1	16:S:82:ARG:NH1	2.50	0.45
18:d:270:LEU:O	18:d:274:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:e:90:GLY:HA3	19:e:105:SER:HA	1.99	0.45
22:h:375:ARG:NH2	22:h:382:ASP:OD2	2.49	0.45
26:l:284:THR:O	26:l:288:LYS:CB	2.64	0.45
27:m:108:ALA:HB1	27:m:124:PHE:HE1	1.81	0.45
12:L:188:TYR:HE1	8:V:167:LEU:HD13	1.82	0.45
1:O:220:LEU:HD12	1:O:224:GLU:HG2	1.99	0.45
2:P:72:MET:HE2	2:P:72:MET:HB3	1.86	0.45
17:c:223:THR:O	17:c:224:LEU:C	2.59	0.45
18:d:170:LEU:HD13	18:d:173:VAL:HG11	1.98	0.45
18:d:194:ILE:O	18:d:198:LYS:HB2	2.17	0.45
18:d:271:PHE:HA	18:d:274:ALA:HB3	1.99	0.45
21:g:196:GLN:O	21:g:200:GLU:CB	2.65	0.45
22:h:141:GLU:OE1	22:h:143:VAL:HG23	2.16	0.45
22:h:355:SER:HB3	22:h:358:GLU:HB2	1.99	0.45
31:q:90:VAL:O	31:q:94:LYS:CB	2.64	0.45
1:A:220:LEU:HD12	1:A:224:GLU:HG2	1.99	0.45
12:L:158:MET:HG3	8:V:208:THR:HG23	1.98	0.45
4:R:208:GLU:OE2	4:R:211:ASN:ND2	2.49	0.45
16:S:104:PRO:HB3	13:a:81:HIS:CE1	2.52	0.45
18:d:196:GLU:HB3	18:d:349:ARG:HH22	1.81	0.45
18:d:249:ARG:CB	18:d:283:PHE:HB3	2.47	0.45
20:f:313:LEU:O	20:f:317:ALA:CB	2.65	0.45
22:h:99:VAL:HA	22:h:123:LEU:HB2	1.98	0.45
26:l:163:LYS:HG3	26:l:167:VAL:HG12	1.89	0.45
27:m:14:ASN:CA	27:m:146:ARG:HH22	2.29	0.45
1:O:178:ASN:HD22	1:O:179:GLU:H	1.64	0.45
17:c:163:MET:O	17:c:164:MET:C	2.60	0.45
17:c:327:LEU:O	17:c:332:MET:CE	2.52	0.45
18:d:249:ARG:NH2	22:h:279:GLN:OE1	2.50	0.45
21:g:418:GLU:O	21:g:422:GLU:CB	2.47	0.45
22:h:100:ASP:OD1	22:h:123:LEU:O	2.35	0.45
3:C:50:VAL:CB	3:C:54:GLN:HB2	2.42	0.44
3:C:79:ASP:HB3	3:C:127:PHE:HD1	1.82	0.44
11:K:157:ARG:O	11:K:161:TYR:HB2	2.17	0.44
1:O:192:LEU:HA	1:O:195:LYS:HB3	1.98	0.44
9:W:67:LYS:O	9:W:71:ASN:HB2	2.17	0.44
13:a:50:MET:HB3	13:a:50:MET:HE2	1.78	0.44
17:c:166:VAL:HG22	17:c:239:ARG:CG	2.47	0.44
17:c:345:LEU:CD2	17:c:381:THR:CG2	2.77	0.44
17:c:387:SER:O	17:c:391:GLU:CB	2.65	0.44
19:e:205:TYR:CD2	19:e:205:TYR:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:161:ARG:NH1	25:k:174:TYR:O	2.38	0.44
23:i:678:ASP:CB	23:i:679:PRO:CD	2.95	0.44
27:m:112:CYS:HA	27:m:120:ALA:HB2	1.98	0.44
27:m:208:PHE:O	27:m:209:THR:HG23	2.14	0.44
1:A:70:HIS:HD2	1:A:138:TRP:H	1.65	0.44
4:D:41:GLN:NE2	4:D:151:PRO:O	2.50	0.44
11:K:84:ALA:O	11:K:88:TYR:CB	2.65	0.44
13:M:99:ARG:HG3	13:M:105:PRO:HA	2.00	0.44
2:P:8:ARG:HH22	4:R:9:ASP:N	2.15	0.44
13:a:186:ARG:HD3	13:a:202:PRO:HB3	1.98	0.44
18:d:143:LEU:HD12	18:d:162:VAL:HG21	1.94	0.44
18:d:270:LEU:O	18:d:274:ALA:CB	2.65	0.44
19:e:205:TYR:O	19:e:205:TYR:CG	2.70	0.44
21:g:128:THR:HG23	21:g:130:GLN:HG2	1.98	0.44
21:g:224:LEU:HB2	21:g:348:LEU:HG	1.99	0.44
21:g:340:PRO:HA	21:g:343:LEU:HB2	1.99	0.44
23:i:555:VAL:CB	23:i:563:ALA:CB	2.95	0.44
26:l:252:LYS:O	26:l:256:LEU:HB2	2.16	0.44
1:A:178:ASN:HD22	1:A:179:GLU:H	1.64	0.44
3:C:224:GLU:O	3:C:228:TYR:CD1	2.70	0.44
13:M:99:ARG:NE	13:M:104:ASN:O	2.50	0.44
1:O:94:GLN:HG3	8:V:65:LEU:HD12	1.99	0.44
15:Q:222:PRO:HA	15:Q:225:ILE:HG13	2.00	0.44
4:R:148:GLU:OE2	4:R:149:LYS:NZ	2.50	0.44
7:U:168:ALA:HA	7:U:172:GLN:HG3	1.98	0.44
8:V:68:LEU:HD23	8:V:68:LEU:HA	1.83	0.44
10:X:138:LEU:HD21	10:X:171:PHE:HB2	1.99	0.44
17:c:248:LYS:CG	18:d:262:ASP:CG	2.89	0.44
22:h:84:LYS:HA	22:h:84:LYS:HD2	1.73	0.44
22:h:152:GLY:HA3	22:h:328:ILE:HB	1.99	0.44
5:E:169:ARG:O	5:E:173:GLU:N	2.48	0.44
1:O:134:LEU:HB3	1:O:162:MET:HE1	1.99	0.44
2:P:50:ARG:NH1	2:P:51:ASN:O	2.51	0.44
16:S:196:ARG:HH22	16:S:235:GLY:HA3	1.83	0.44
9:W:18:CYS:HA	9:W:189:ILE:O	2.16	0.44
11:Y:84:ALA:O	11:Y:88:TYR:CB	2.65	0.44
19:e:85:ILE:HA	19:e:86:PRO:HA	1.70	0.44
22:h:105:ILE:HD12	22:h:108:VAL:HG21	2.00	0.44
26:l:236:PHE:CZ	26:l:247:ALA:HA	2.53	0.44
10:J:66:LEU:O	10:J:70:ARG:HB2	2.17	0.44
16:S:101:ARG:NH1	13:a:74:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:106:ILE:HD12	6:T:107:PRO:HD2	1.98	0.44
17:c:309:PHE:H	21:g:238:ARG:HH22	1.64	0.44
18:d:265:LYS:HE2	18:d:265:LYS:CA	2.46	0.44
19:e:412:GLN:C	19:e:412:GLN:NE2	2.73	0.44
22:h:145:ASP:O	22:h:146:SER:C	2.59	0.44
26:l:265:GLU:O	26:l:269:ALA:CB	2.66	0.44
27:m:108:ALA:O	27:m:112:CYS:CB	2.66	0.44
2:B:50:ARG:NH1	2:B:51:ASN:O	2.51	0.44
13:M:178:TYR:OH	13:M:208:ASN:N	2.46	0.44
16:S:63:ILE:HD11	16:S:223:ILE:HG23	2.00	0.44
11:Y:148:GLU:HG2	11:Y:151:GLN:HE22	1.83	0.44
18:d:281:ILE:HB	18:d:326:LYS:HG3	1.44	0.44
19:e:87:LEU:HD12	19:e:140:VAL:HG21	1.99	0.44
28:n:263:ALA:O	28:n:266:ILE:N	2.50	0.44
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.86	0.44
1:A:192:LEU:HA	1:A:195:LYS:HB3	1.98	0.44
2:B:239:LYS:HD2	2:B:239:LYS:HA	1.55	0.44
2:B:241:GLU:CD	2:B:242:GLU:N	2.75	0.44
1:O:189:THR:HA	1:O:192:LEU:HG	2.00	0.44
9:W:143:GLU:HA	9:W:146:TYR:HB2	2.00	0.44
12:Z:139:GLY:H	12:Z:142:SER:HG	1.61	0.44
12:Z:145:LEU:HD22	12:Z:178:VAL:HB	1.98	0.44
17:c:165:GLN:HG2	17:c:238:ILE:CD1	2.48	0.44
17:c:172:VAL:O	17:c:231:ASN:ND2	2.47	0.44
18:d:407:LEU:HD13	22:h:178:LEU:HG	1.99	0.44
21:g:435:LEU:HD12	21:g:437:TYR:CE1	2.53	0.44
7:G:25:VAL:CG2	19:e:416:PHE:HE2	2.28	0.44
8:H:126:THR:HB	8:H:131:SER:HA	2.00	0.44
10:J:61:GLN:O	10:J:65:GLN:HB2	2.18	0.44
2:P:91:ARG:HD3	9:W:75:LEU:HB3	2.00	0.44
15:Q:51:ALA:HA	15:Q:54:GLN:HG3	1.98	0.44
4:R:41:GLN:NE2	4:R:151:PRO:O	2.50	0.44
9:W:59:VAL:O	9:W:63:ALA:CB	2.66	0.44
19:e:112:TYR:HB3	22:h:71:SER:HB2	2.00	0.44
19:e:155:THR:HA	19:e:228:ILE:HG22	2.00	0.44
19:e:210:CYS:O	35:e:501:ADP:O1A	2.36	0.44
19:e:374:ASP:HA	20:f:292:PRO:HG3	1.99	0.44
19:e:399:PHE:CD1	19:e:399:PHE:N	2.84	0.44
19:e:411:GLU:O	19:e:412:GLN:HB2	2.18	0.44
20:f:149:ILE:HD13	20:f:149:ILE:HA	1.82	0.44
20:f:289:LEU:C	20:f:289:LEU:CD2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:h:347:ILE:HG12	22:h:383:PHE:HB3	1.99	0.44
27:m:149:LEU:HD13	27:m:186:LEU:HD12	1.99	0.44
9:I:59:VAL:O	9:I:63:ALA:CB	2.66	0.44
8:V:2:THR:HB	8:V:130:GLY:HA3	2.00	0.44
18:d:100:ASP:OD1	18:d:103:ARG:O	2.36	0.44
19:e:323:ARG:HG3	22:h:143:VAL:HG23	1.95	0.44
6:F:83:ASP:HB3	6:F:131:PHE:HD1	1.83	0.43
8:H:42:TYR:HE2	8:H:185:PHE:HB2	1.83	0.43
9:W:13:MET:HG2	9:W:166:ILE:HD12	2.00	0.43
14:b:80:ALA:HB2	14:b:100:ILE:HD11	2.00	0.43
17:c:164:MET:C	17:c:238:ILE:CD1	2.91	0.43
19:e:207:PRO:HA	19:e:208:PRO:HA	1.74	0.43
19:e:384:MET:HE1	20:f:148:VAL:HA	1.99	0.43
1:A:38:LYS:HB3	1:A:158:LYS:HA	2.00	0.43
1:A:52:LYS:CB	19:e:413:GLU:OE2	2.66	0.43
2:B:72:MET:HE2	2:B:72:MET:HB3	1.86	0.43
8:H:135:MET:HE3	13:a:179:ARG:HH21	1.83	0.43
9:I:176:ARG:HA	11:Y:26:ILE:HD11	1.99	0.43
6:T:83:ASP:HB3	6:T:131:PHE:HD1	1.83	0.43
17:c:121:PHE:HB2	21:g:89:LEU:HA	1.99	0.43
17:c:157:ILE:CD1	17:c:161:VAL:HG12	2.48	0.43
18:d:260:LEU:CD1	18:d:262:ASP:N	2.44	0.43
19:e:289:LEU:O	19:e:293:LEU:HB2	2.18	0.43
20:f:181:THR:OG1	35:g:501:ADP:O1B	2.31	0.43
20:f:196:LEU:HD23	20:f:228:CYS:SG	2.58	0.43
24:j:328:HIS:C	24:j:330:ARG:H	2.26	0.43
1:A:158:LYS:HB3	1:A:177:TYR:CZ	2.54	0.43
7:U:93:ARG:HE	7:U:121:ILE:HG21	1.84	0.43
9:W:169:ALA:O	9:W:173:ALA:HB2	2.19	0.43
13:a:50:MET:N	13:a:113:GLY:O	2.44	0.43
17:c:383:ALA:CB	35:c:501:ADP:C8	2.96	0.43
20:f:37:THR:O	20:f:41:GLU:CB	2.66	0.43
20:f:113:ARG:HH21	20:f:224:ASP:HB2	1.84	0.43
20:f:170:CYS:H	20:f:276:ILE:HG22	1.83	0.43
26:l:362:GLU:O	26:l:365:LEU:CB	2.65	0.43
27:m:15:PRO:HA	27:m:16:ASP:HA	1.56	0.43
3:C:139:ASP:OD1	3:C:139:ASP:N	2.52	0.43
9:I:67:LYS:O	9:I:71:ASN:HB2	2.17	0.43
9:I:169:ALA:O	9:I:173:ALA:HB2	2.19	0.43
10:J:184:ASP:OD1	10:J:189:HIS:ND1	2.52	0.43
14:N:107:GLU:HG2	14:N:110:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:122:THR:HG23	15:Q:125:ARG:HH22	1.82	0.43
15:Q:139:ASP:OD1	15:Q:139:ASP:N	2.52	0.43
16:S:47:VAL:HG12	16:S:195:LEU:HD22	2.01	0.43
16:S:120:THR:HG22	6:T:129:ARG:HH21	1.83	0.43
7:U:41:ALA:N	7:U:167:ALA:HB2	2.32	0.43
18:d:251:VAL:HG13	18:d:285:ASP:O	2.18	0.43
19:e:323:ARG:NH1	19:e:324:PRO:CD	2.79	0.43
21:g:291:ILE:H	21:g:291:ILE:HG13	1.65	0.43
1:A:189:THR:HA	1:A:192:LEU:HG	2.00	0.43
2:B:149:GLN:HB3	2:B:159:TRP:CD1	2.54	0.43
9:I:143:GLU:HA	9:I:146:TYR:HB2	2.00	0.43
11:K:148:GLU:HG2	11:K:151:GLN:HE22	1.83	0.43
11:K:157:ARG:O	11:K:161:TYR:CB	2.67	0.43
1:O:38:LYS:HB3	1:O:158:LYS:HA	2.00	0.43
1:O:64:VAL:HG23	1:O:219:ARG:HE	1.84	0.43
2:P:77:ALA:HB2	2:P:164:ILE:HD12	2.00	0.43
7:U:195:VAL:HG12	7:U:238:HIS:CD2	2.53	0.43
8:V:42:TYR:HE2	8:V:185:PHE:HB2	1.83	0.43
13:a:99:ARG:NE	13:a:104:ASN:O	2.50	0.43
13:a:99:ARG:HG3	13:a:105:PRO:HA	2.00	0.43
17:c:248:LYS:HB3	18:d:261:GLY:HA3	1.92	0.43
18:d:392:GLY:O	18:d:395:ILE:HG13	2.19	0.43
20:f:46:ASP:O	20:f:50:LEU:CB	2.57	0.43
22:h:142:LYS:CD	22:h:142:LYS:H	2.32	0.43
28:n:258:VAL:O	28:n:259:VAL:C	2.61	0.43
1:A:83:ARG:HD2	7:G:116:LYS:HG3	2.01	0.43
5:E:63:ILE:HD11	5:E:223:ILE:HG23	2.00	0.43
7:G:195:VAL:HG12	7:G:238:HIS:CD2	2.53	0.43
9:I:160:ASP:O	9:I:163:PHE:HB3	2.18	0.43
13:M:211:ILE:HD11	14:b:29:ARG:HD3	1.99	0.43
14:N:80:ALA:HB2	14:N:100:ILE:HD11	2.00	0.43
8:V:19:ARG:H	8:V:33:LYS:HZ1	1.66	0.43
11:Y:157:ARG:O	11:Y:161:TYR:HB2	2.17	0.43
17:c:130:ALA:HB3	17:c:133:ASP:HB2	1.99	0.43
19:e:86:PRO:HG3	20:f:105:LEU:HB3	2.00	0.43
19:e:384:MET:HE1	20:f:148:VAL:HG23	2.01	0.43
20:f:238:ILE:HG21	20:f:260:LEU:HD13	2.01	0.43
21:g:398:ALA:O	21:g:400:CYS:N	2.51	0.43
22:h:88:LYS:HB2	22:h:93:GLY:C	2.37	0.43
27:m:207:THR:O	27:m:207:THR:HG22	2.17	0.43
6:F:231:ILE:HA	6:F:234:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:138:LEU:HD21	10:J:171:PHE:HB2	1.99	0.43
1:O:70:HIS:HD2	1:O:138:TRP:H	1.65	0.43
1:O:134:LEU:HD12	1:O:145:LEU:HD21	2.01	0.43
9:W:158:ASP:N	9:W:158:ASP:OD1	2.52	0.43
10:X:61:GLN:O	10:X:65:GLN:HB2	2.18	0.43
11:Y:18:SER:OG	11:Y:173:ALA:N	2.46	0.43
18:d:267:VAL:HA	18:d:270:LEU:HB3	2.01	0.43
19:e:210:CYS:SG	19:e:211:GLY:N	2.91	0.43
20:f:172:LEU:HD23	20:f:299:ILE:HB	2.00	0.43
6:F:217:GLY:H	6:F:220:THR:HG1	1.64	0.43
13:M:61:GLN:HA	13:M:64:LYS:HG2	2.01	0.43
12:Z:184:GLU:OE2	12:Z:211:ARG:NH1	2.51	0.43
18:d:250:VAL:CG2	18:d:270:LEU:CD1	2.96	0.43
19:e:326:ARG:NH1	19:e:326:ARG:CG	2.73	0.43
19:e:408:LYS:HZ3	19:e:408:LYS:CA	2.26	0.43
20:f:231:PHE:CZ	20:f:233:ASP:HB3	2.54	0.43
24:j:159:THR:O	24:j:163:ALA:HB2	2.19	0.43
27:m:377:LEU:O	27:m:381:GLN:N	2.43	0.43
3:C:50:VAL:O	3:C:54:GLN:N	2.47	0.43
5:E:148:CYS:SG	5:E:150:SER:OG	2.64	0.43
7:G:93:ARG:HE	7:G:121:ILE:HG21	1.84	0.43
11:K:160:ILE:HA	11:K:163:ALA:HB3	2.01	0.43
15:Q:88:ARG:HH11	10:X:70:ARG:HG3	1.84	0.43
15:Q:188:ILE:CG2	15:Q:228:TYR:CD2	2.96	0.43
6:T:217:GLY:H	6:T:220:THR:HG1	1.63	0.43
9:W:11:MET:HB3	9:W:145:MET:HE2	2.01	0.43
10:X:29:LYS:HD3	11:Y:123:GLY:HA2	2.01	0.43
21:g:291:ILE:HG22	21:g:306:VAL:HG13	2.01	0.43
22:h:143:VAL:CG1	22:h:213:ARG:NH1	2.82	0.43
3:C:88:ARG:HH11	10:J:70:ARG:HG3	1.83	0.43
4:D:114:GLN:OE1	5:E:82:ARG:NH1	2.51	0.43
12:L:184:GLU:OE2	12:L:211:ARG:NH1	2.52	0.43
8:V:173:ILE:O	8:V:189:TYR:N	2.43	0.43
9:W:57:THR:O	10:X:85:ARG:NH2	2.52	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.43
11:Y:160:ILE:HA	11:Y:163:ALA:HB3	2.01	0.43
18:d:153:ASN:HD22	18:d:154:HIS:H	1.66	0.43
19:e:94:GLU:HB3	19:e:102:ILE:HD11	2.01	0.43
19:e:293:LEU:HD23	22:h:140:VAL:HG23	2.01	0.43
19:e:387:VAL:HG11	20:f:159:PHE:HE1	1.84	0.43
19:e:412:GLN:O	19:e:413:GLU:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:e:501:ADP:H5'2	20:f:291:ARG:HE	1.84	0.43
20:f:64:LEU:HD13	20:f:69:PHE:HE1	1.18	0.43
21:g:70:LYS:O	21:g:74:LYS:CB	2.67	0.43
21:g:251:LEU:HD11	21:g:256:LEU:HD21	2.00	0.43
27:m:257:ARG:HG2	27:m:261:PHE:HE1	1.84	0.43
1:A:10:THR:HG23	1:A:20:GLN:HB2	2.01	0.42
2:B:77:ALA:HB2	2:B:164:ILE:HD12	2.00	0.42
10:J:169:LYS:O	10:X:27:GLN:NE2	2.51	0.42
4:R:53:ARG:NH2	4:R:172:SER:OG	2.52	0.42
12:Z:49:LYS:HD3	12:Z:113:LEU:HD11	2.01	0.42
17:c:93:LEU:O	18:d:132:TYR:N	2.41	0.42
18:d:174:MET:HG3	18:d:176:VAL:HG22	2.01	0.42
18:d:364:ILE:HG21	35:d:501:ADP:N1	2.34	0.42
19:e:160:PRO:HB2	19:e:217:LYS:HG3	2.00	0.42
19:e:267:ILE:H	19:e:267:ILE:HG12	1.54	0.42
26:l:193:ALA:O	26:l:197:ALA:HB2	2.19	0.42
2:P:149:GLN:HB3	2:P:159:TRP:CD1	2.54	0.42
7:U:40:VAL:HB	7:U:51:VAL:HG23	2.01	0.42
18:d:192:ASN:O	18:d:196:GLU:HG2	2.19	0.42
18:d:194:ILE:HA	18:d:197:ILE:HG22	2.01	0.42
19:e:266:GLU:O	19:e:267:ILE:C	2.61	0.42
20:f:61:LEU:CD1	20:f:72:LYS:HB2	2.39	0.42
22:h:127:LEU:N	22:h:127:LEU:HD23	2.34	0.42
28:n:279:LYS:O	28:n:283:ARG:CB	2.67	0.42
31:q:37:ALA:O	31:q:41:MET:CB	2.67	0.42
1:A:220:LEU:HD13	1:A:220:LEU:HA	1.92	0.42
6:F:34:SER:HG	6:F:65:ARG:HH12	1.61	0.42
9:I:11:MET:HB3	9:I:145:MET:HE2	2.01	0.42
15:Q:188:ILE:HB	15:Q:228:TYR:CE1	2.54	0.42
8:V:2:THR:HG1	8:V:130:GLY:C	2.21	0.42
10:X:35:MET:HG2	10:X:45:LEU:HG	2.01	0.42
14:b:17:ASP:OD2	14:b:170:SER:OG	2.30	0.42
14:b:107:GLU:HG2	14:b:110:GLN:HE21	1.83	0.42
19:e:263:PHE:HD1	19:e:308:ILE:HG13	1.83	0.42
20:f:172:LEU:HD22	20:f:301:ILE:HD11	2.01	0.42
20:f:259:GLU:OE2	20:f:263:GLN:NE2	2.52	0.42
22:h:328:ILE:HD11	35:h:401:ADP:C4	2.55	0.42
27:m:233:ARG:HH22	27:m:264:TYR:HD1	1.67	0.42
3:C:125:ARG:HA	3:C:126:PRO:HD2	1.91	0.42
9:I:13:MET:HG2	9:I:166:ILE:HD12	2.00	0.42
12:L:189:THR:OG1	12:L:190:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:148:CYS:HG	16:S:150:SER:HG	1.57	0.42
7:U:50:ILE:HB	7:U:218:GLY:O	2.20	0.42
9:W:160:ASP:O	9:W:163:PHE:HB3	2.18	0.42
11:Y:98:GLY:HA2	11:Y:115:ASP:HA	2.02	0.42
11:Y:157:ARG:O	11:Y:161:TYR:CB	2.67	0.42
17:c:191:VAL:HG13	17:c:192:GLU:HG3	2.00	0.42
18:d:281:ILE:HA	18:d:326:LYS:HB2	1.80	0.42
20:f:181:THR:HG1	35:g:501:ADP:PA	2.42	0.42
20:f:308:ALA:O	20:f:312:ILE:HG12	2.19	0.42
21:g:348:LEU:HD13	21:g:348:LEU:HA	1.66	0.42
23:i:673:GLU:CB	23:i:674:PRO:HD3	2.49	0.42
25:k:294:LYS:O	25:k:297:GLU:CB	2.66	0.42
26:l:127:GLN:NE2	26:l:156:GLU:OE1	2.46	0.42
26:l:190:LEU:HD21	26:l:214:SER:HA	2.00	0.42
1:A:64:VAL:HG23	1:A:219:ARG:HE	1.84	0.42
1:A:94:GLN:NE2	8:H:64:GLU:OE2	2.53	0.42
3:C:50:VAL:C	3:C:54:GLN:CB	2.92	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42
11:K:58:LEU:HD11	11:K:61:ARG:HH21	1.84	0.42
13:a:61:GLN:HA	13:a:64:LYS:HG2	2.01	0.42
13:a:195:LYS:HB2	13:a:195:LYS:HE3	1.81	0.42
17:c:398:ARG:HH12	18:d:195:GLN:NE2	2.17	0.42
18:d:149:SER:OG	18:d:149:SER:O	2.29	0.42
18:d:173:VAL:O	18:d:175:LYS:N	2.52	0.42
18:d:260:LEU:HG	18:d:263:GLY:HA3	1.43	0.42
19:e:338:ARG:HD3	19:e:367:PRO:HG3	2.01	0.42
19:e:373:ALA:HB2	35:e:501:ADP:C5'	2.41	0.42
20:f:61:LEU:CD1	20:f:72:LYS:HB3	2.45	0.42
20:f:184:ALA:HB1	20:f:195:PHE:HZ	1.85	0.42
21:g:318:ASP:HB3	21:g:347:ARG:HG3	2.02	0.42
21:g:399:VAL:O	21:g:403:ALA:CB	2.67	0.42
22:h:90:HIS:N	22:h:91:PRO:HD2	2.33	0.42
4:D:28:ILE:HG21	21:g:434:ASN:ND2	2.31	0.42
8:H:1:THR:CA	8:H:33:LYS:HZ1	2.32	0.42
8:H:202:TYR:OH	12:Z:177:ASP:OD2	2.38	0.42
14:N:115:PRO:HG3	14:N:119:MET:HE2	2.02	0.42
2:P:86:LEU:O	2:P:89:GLU:HB2	2.20	0.42
15:Q:8:THR:HG22	15:Q:16:LEU:HD11	2.02	0.42
15:Q:220:LEU:CD1	15:Q:228:TYR:CE2	3.02	0.42
8:V:2:THR:OG1	8:V:130:GLY:O	2.32	0.42
12:Z:210:LEU:HB3	12:Z:211:ARG:H	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:115:PRO:HG3	14:b:119:MET:HE2	2.02	0.42
17:c:180:CYS:HB3	17:c:183:GLN:HG2	2.01	0.42
17:c:195:LEU:HB3	17:c:196:LEU:H	1.67	0.42
18:d:263:GLY:C	18:d:265:LYS:N	2.78	0.42
19:e:111:TYR:OH	19:e:137:ASN:OD1	2.29	0.42
19:e:267:ILE:O	19:e:270:ILE:N	2.38	0.42
20:f:261:LEU:CD1	20:f:294:ARG:HE	2.33	0.42
21:g:73:ILE:O	21:g:77:SER:CB	2.67	0.42
22:h:143:VAL:N	22:h:144:PRO:CD	2.82	0.42
27:m:203:ASP:OD1	27:m:203:ASP:N	2.39	0.42
29:o:105:PRO:C	29:o:107:ASN:N	2.67	0.42
1:O:10:THR:HG23	1:O:20:GLN:HB2	2.01	0.42
2:P:208:ALA:HA	2:P:211:VAL:HG12	2.02	0.42
17:c:350:GLY:HA2	17:c:353:HIS:HD2	1.85	0.42
19:e:79:VAL:HG12	22:h:63:LEU:HB3	2.00	0.42
19:e:214:MET:HE2	35:e:501:ADP:C2'	2.30	0.42
31:q:152:LYS:HE2	31:q:152:LYS:HB2	1.89	0.42
5:E:47:VAL:HG12	5:E:195:LEU:HD22	2.01	0.42
13:M:78:GLY:O	13:M:80:GLY:N	2.53	0.42
14:N:29:ARG:HD2	13:a:179:ARG:NH1	2.25	0.42
1:O:229:LEU:HD23	1:O:229:LEU:HA	1.89	0.42
16:S:107:ARG:HH12	13:a:81:HIS:HB3	1.84	0.42
6:T:120:HIS:NE2	7:U:86:ASP:OD1	2.42	0.42
12:Z:159:GLN:HB3	12:Z:160:ASN:H	1.70	0.42
13:a:78:GLY:O	13:a:80:GLY:N	2.53	0.42
18:d:342:ILE:HG12	18:d:344:PRO:HD3	1.95	0.42
20:f:291:ARG:O	20:f:292:PRO:O	2.37	0.42
21:g:369:HIS:ND1	21:g:397:LYS:CA	2.82	0.42
22:h:308:PRO:HA	22:h:309:GLY:HA2	1.34	0.42
31:q:248:MET:O	31:q:252:ALA:CB	2.67	0.42
1:A:71:ILE:HG21	1:A:109:LEU:HD23	2.02	0.42
2:B:36:GLY:HA2	2:B:44:LEU:O	2.19	0.42
3:C:231:GLU:OE1	3:C:231:GLU:N	2.53	0.42
8:H:179:SER:OG	8:H:182:LYS:O	2.33	0.42
10:J:35:MET:HG2	10:J:45:LEU:HG	2.01	0.42
7:U:138:MET:HB3	7:U:140:LEU:HD23	2.02	0.42
17:c:195:LEU:O	17:c:198:PRO:HD2	2.20	0.42
17:c:410:LEU:HA	17:c:413:VAL:HG12	2.00	0.42
18:d:232:LYS:HE3	22:h:278:ASN:ND2	2.35	0.42
19:e:373:ALA:HB1	20:f:292:PRO:O	2.20	0.42
22:h:152:GLY:N	35:h:401:ADP:HN62	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:m:140:ILE:O	27:m:144:LEU:N	2.50	0.42
1:A:134:LEU:HD12	1:A:145:LEU:HD21	2.01	0.42
3:C:182:GLU:OE2	3:C:185:ASP:N	2.53	0.42
11:K:98:GLY:HA2	11:K:115:ASP:HA	2.02	0.42
15:Q:156:TRP:CD1	4:R:59:MET:HB2	2.55	0.42
15:Q:227:LYS:HE2	15:Q:227:LYS:HB3	1.50	0.42
12:Z:189:THR:OG1	12:Z:190:GLY:N	2.53	0.42
17:c:169:LYS:HG3	17:c:231:ASN:HA	2.00	0.42
19:e:323:ARG:HD3	22:h:143:VAL:HG23	1.47	0.42
24:j:318:TYR:O	24:j:319:SER:CB	2.68	0.42
26:l:163:LYS:HB2	26:l:196:THR:HB	2.00	0.42
27:m:134:LEU:HD11	27:m:169:GLU:HB2	1.31	0.42
1:A:90:ARG:NH2	8:H:68:LEU:O	2.53	0.41
2:B:86:LEU:O	2:B:89:GLU:HB2	2.20	0.41
5:E:26:MET:SD	5:E:148:CYS:HB2	2.60	0.41
13:M:50:MET:HB3	13:M:50:MET:HE2	1.78	0.41
2:P:36:GLY:HA2	2:P:44:LEU:O	2.19	0.41
16:S:26:MET:SD	16:S:148:CYS:HB2	2.60	0.41
6:T:157:SER:H	7:U:88:ARG:NH2	2.18	0.41
11:Y:58:LEU:HD11	11:Y:61:ARG:HH21	1.84	0.41
17:c:353:HIS:O	17:c:356:LYS:HB3	2.19	0.41
20:f:50:LEU:HD21	21:g:80:ILE:HG21	2.01	0.41
20:f:60:VAL:C	20:f:62:LYS:N	2.66	0.41
20:f:168:LYS:NZ	20:f:269:THR:O	2.44	0.41
7:G:50:ILE:HB	7:G:218:GLY:O	2.20	0.41
15:Q:71:MET:HB3	15:Q:133:ILE:HD13	2.02	0.41
15:Q:225:ILE:H	15:Q:225:ILE:HG12	1.42	0.41
17:c:327:LEU:HB3	17:c:332:MET:HE2	2.01	0.41
17:c:384:GLU:O	17:c:386:ARG:C	2.62	0.41
18:d:109:VAL:HA	18:d:151:LEU:HA	2.02	0.41
18:d:343:ARG:C	18:d:345:GLY:H	2.27	0.41
20:f:55:GLN:O	21:g:133:PHE:N	2.51	0.41
20:f:64:LEU:O	20:f:69:PHE:HE1	2.02	0.41
26:l:170:GLN:NE2	26:l:189:ALA:O	2.54	0.41
26:l:251:LEU:HA	26:l:254:MET:HE3	2.01	0.41
26:l:261:LEU:HD12	26:l:263:THR:H	1.85	0.41
31:q:274:ASN:O	31:q:276:GLY:C	2.61	0.41
2:B:176:LYS:CD	3:C:52:LYS:CG	2.68	0.41
9:I:62:VAL:HA	9:I:65:ARG:HB3	2.03	0.41
4:R:59:MET:HE1	4:R:61:PRO:HB3	2.03	0.41
6:T:7:TYR:CD2	6:T:16:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:33:ASN:ND2	7:U:169:GLY:O	2.53	0.41
13:a:74:GLU:HA	13:a:77:LEU:HD23	2.02	0.41
19:e:205:TYR:HE2	19:e:332:GLU:HG2	1.85	0.41
19:e:397:LYS:HB3	19:e:401:LYS:CG	2.50	0.41
20:f:181:THR:N	35:g:501:ADP:O1A	2.50	0.41
26:l:202:CYS:HB2	26:l:207:GLN:HB2	2.01	0.41
27:m:77:ASN:O	27:m:81:LEU:CB	2.68	0.41
27:m:290:PRO:O	27:m:294:TYR:CB	2.68	0.41
1:A:5:TYR:HD1	1:A:5:TYR:HA	1.76	0.41
3:C:203:GLY:HA2	3:C:226:GLU:OE2	2.21	0.41
5:E:14:SER:N	5:E:18:ARG:O	2.43	0.41
12:L:49:LYS:HD3	12:L:113:LEU:HD11	2.01	0.41
13:M:74:GLU:HA	13:M:77:LEU:HD23	2.02	0.41
13:M:200:GLU:O	13:M:203:LEU:CD1	2.68	0.41
6:T:231:ILE:HA	6:T:234:GLU:HB3	2.01	0.41
8:V:5:GLY:HA2	8:V:13:VAL:O	2.21	0.41
8:V:126:THR:HB	8:V:131:SER:HA	2.00	0.41
11:Y:19:ARG:NH2	11:Y:26:ILE:HG21	2.36	0.41
11:Y:21:THR:HG22	11:Y:26:ILE:HG22	2.02	0.41
11:Y:155:LEU:O	11:Y:159:ALA:CB	2.68	0.41
18:d:223:ILE:HG13	18:d:329:MET:HB2	2.02	0.41
19:e:274:ARG:HH12	20:f:244:SER:HB3	1.86	0.41
21:g:369:HIS:ND1	21:g:397:LYS:CG	2.84	0.41
22:h:105:ILE:HD12	22:h:105:ILE:HA	1.61	0.41
22:h:134:LEU:CD2	22:h:237:MET:CB	2.89	0.41
22:h:334:ARG:HH21	27:m:176:ARG:HE	1.68	0.41
23:i:555:VAL:CB	23:i:563:ALA:HB1	2.50	0.41
26:l:163:LYS:HD2	26:l:166:LEU:N	2.35	0.41
9:I:158:ASP:OD1	9:I:158:ASP:N	2.52	0.41
1:O:71:ILE:HG21	1:O:109:LEU:HD23	2.02	0.41
14:b:99:ILE:HG22	14:b:113:SER:HA	2.02	0.41
19:e:98:GLN:O	19:e:100:THR:N	2.54	0.41
19:e:274:ARG:O	20:f:251:ARG:NH1	2.53	0.41
20:f:71:VAL:HG21	20:f:100:LEU:HD21	2.02	0.41
20:f:204:VAL:HG21	21:g:261:ILE:HG21	2.01	0.41
20:f:320:ILE:HD12	21:g:217:ILE:HD13	2.02	0.41
25:k:139:GLU:O	25:k:143:ALA:HB2	2.21	0.41
1:A:158:LYS:NZ	2:B:56:LEU:H	2.18	0.41
2:B:208:ALA:HA	2:B:211:VAL:HG12	2.02	0.41
3:C:71:MET:HB3	3:C:133:ILE:HD13	2.03	0.41
3:C:88:ARG:NH1	10:J:70:ARG:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:ARG:HH22	17:c:431:THR:HB	1.85	0.41
4:D:206:MET:HG3	17:c:376:LEU:HD21	2.02	0.41
4:D:232:GLU:HA	4:D:235:GLU:HG2	2.02	0.41
7:G:172:GLN:O	7:G:175:SER:OG	2.36	0.41
8:H:5:GLY:HA2	8:H:13:VAL:O	2.21	0.41
13:M:110:MET:HB3	13:M:110:MET:HE3	1.78	0.41
2:P:34:CYS:SG	2:P:75:SER:OG	2.67	0.41
16:S:19:ILE:H	16:S:19:ILE:HG22	1.59	0.41
6:T:117:MET:HE1	7:U:92:GLN:HG3	2.02	0.41
18:d:107:MET:CG	22:h:96:VAL:HB	2.45	0.41
21:g:341:ALA:O	21:g:347:ARG:HD2	2.20	0.41
1:A:66:PRO:HB3	1:A:217:PHE:HD2	1.86	0.41
2:B:70:GLU:H	2:B:70:GLU:HG3	1.71	0.41
10:J:66:LEU:O	10:J:70:ARG:CB	2.69	0.41
12:L:159:GLN:HB3	12:L:160:ASN:H	1.70	0.41
13:M:50:MET:N	13:M:113:GLY:O	2.44	0.41
14:N:59:VAL:HG21	14:N:83:PHE:CZ	2.55	0.41
6:T:33:SER:O	6:T:167:LYS:N	2.54	0.41
7:U:82:GLY:HA3	7:U:136:CYS:HA	2.03	0.41
8:V:3:ILE:HG22	8:V:127:MET:O	2.21	0.41
12:Z:209:SER:OG	12:Z:210:LEU:N	2.54	0.41
17:c:81:ALA:N	18:d:137:SER:OG	2.51	0.41
18:d:273:VAL:HA	18:d:276:GLU:HG2	2.03	0.41
19:e:194:ILE:HD12	22:h:371:LEU:HD23	2.03	0.41
19:e:414:HIS:HA	19:e:415:GLU:N	2.36	0.41
20:f:291:ARG:NH1	20:f:294:ARG:HH12	2.18	0.41
20:f:365:GLU:HA	20:f:368:MET:HB3	2.02	0.41
21:g:209:LYS:O	21:g:213:GLU:N	2.45	0.41
21:g:222:GLY:O	21:g:348:LEU:HD13	2.15	0.41
26:l:233:TYR:HA	26:l:236:PHE:HB3	2.01	0.41
1:A:73:LEU:HD11	1:A:86:VAL:HG22	2.03	0.41
7:G:138:MET:HB3	7:G:140:LEU:HD23	2.02	0.41
8:H:83:LEU:O	8:H:87:LEU:CB	2.69	0.41
10:J:162:LYS:HB3	11:Y:141:ARG:HD3	2.02	0.41
11:K:19:ARG:NH2	11:K:26:ILE:HG21	2.36	0.41
14:N:99:ILE:HG22	14:N:113:SER:HA	2.02	0.41
1:O:66:PRO:HA	1:O:72:GLY:HA2	2.03	0.41
2:P:11:ILE:HG23	15:Q:18:GLN:HE22	1.85	0.41
14:b:59:VAL:HG21	14:b:83:PHE:CZ	2.55	0.41
19:e:352:MET:HE2	20:f:164:ILE:HB	2.03	0.41
22:h:152:GLY:H	35:h:401:ADP:N6	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:602:LEU:O	23:i:606:ALA:N	2.49	0.41
23:i:619:VAL:O	23:i:655:ALA:HB1	2.11	0.41
26:l:308:ASP:N	26:l:311:ALA:HB2	2.35	0.41
27:m:314:LEU:O	27:m:354:VAL:N	2.43	0.41
3:C:8:THR:HG22	3:C:16:LEU:HD11	2.02	0.41
3:C:11:SER:OG	3:C:15:HIS:O	2.31	0.41
4:D:59:MET:HE1	4:D:61:PRO:HB3	2.03	0.41
4:D:161:THR:OG1	21:g:437:TYR:HB2	2.21	0.41
6:F:7:TYR:CD2	6:F:16:PRO:HD3	2.55	0.41
7:G:29:PHE:CE2	19:e:416:PHE:HZ	2.39	0.41
7:G:40:VAL:HB	7:G:51:VAL:HG23	2.01	0.41
7:G:106:GLY:HA2	8:H:81:ARG:HE	1.85	0.41
10:J:101:ASN:OD1	10:J:101:ASN:N	2.54	0.41
12:L:209:SER:OG	12:L:210:LEU:N	2.54	0.41
13:M:107:TRP:CD1	13:M:127:MET:HE3	2.56	0.41
2:P:163:CYS:SG	2:P:164:ILE:N	2.94	0.41
4:R:70:ILE:HD11	4:R:89:ILE:HD12	2.03	0.41
7:U:231:THR:N	7:U:234:GLU:OE2	2.46	0.41
8:V:34:ILE:HB	8:V:185:PHE:HE1	1.86	0.41
11:Y:130:SER:OG	11:Y:131:GLY:N	2.53	0.41
12:Z:113:LEU:HA	12:Z:119:GLY:HA2	2.03	0.41
13:a:107:TRP:CD1	13:a:127:MET:HE3	2.56	0.41
14:b:136:TYR:O	14:b:140:ASP:CB	2.69	0.41
14:b:201:THR:HB	14:b:202:LEU:H	1.58	0.41
17:c:165:GLN:HA	17:c:165:GLN:NE2	2.33	0.41
18:d:225:TYR:CZ	18:d:352:GLU:HG2	2.55	0.41
18:d:342:ILE:HD12	18:d:350:LYS:HE2	2.02	0.41
18:d:361:LYS:O	18:d:365:PHE:CB	2.69	0.41
19:e:122:GLU:CD	31:q:278:GLN:CA	2.88	0.41
19:e:206:GLY:N	19:e:212:LYS:HZ1	2.07	0.41
20:f:50:LEU:HD11	21:g:80:ILE:HD13	2.01	0.41
20:f:157:GLU:HG2	20:f:158:LEU:HD12	2.03	0.41
21:g:137:ILE:HG21	21:g:159:LEU:HD12	2.03	0.41
21:g:228:PRO:HB2	21:g:229:PRO:HD2	1.31	0.41
22:h:94:LYS:HB3	22:h:94:LYS:HE2	1.34	0.41
22:h:139:MET:O	22:h:139:MET:SD	2.79	0.41
22:h:180:ILE:HA	22:h:180:ILE:HD12	1.78	0.41
24:j:207:SER:O	24:j:209:MET:N	2.53	0.41
27:m:97:GLU:O	27:m:101:ARG:CB	2.69	0.41
6:F:105:ASN:HD22	6:F:106:ILE:N	2.19	0.41
6:F:120:HIS:CE1	7:G:86:ASP:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:VAL:O	13:M:75:GLU:CB	2.64	0.41
13:M:74:GLU:OE1	13:M:83:TYR:OH	2.28	0.41
18:d:232:LYS:HE3	22:h:278:ASN:HD21	1.86	0.41
18:d:246:THR:HG23	18:d:280:SER:HB3	2.00	0.41
22:h:186:VAL:HG22	22:h:313:ARG:HB3	2.03	0.41
1:A:66:PRO:HA	1:A:72:GLY:HA2	2.03	0.40
2:B:163:CYS:SG	2:B:164:ILE:N	2.94	0.40
4:D:70:ILE:HD11	4:D:89:ILE:HD12	2.03	0.40
6:F:33:SER:O	6:F:167:LYS:N	2.54	0.40
8:H:18:THR:OG1	8:H:172:ASN:OD1	2.38	0.40
8:H:34:ILE:HB	8:H:185:PHE:HE1	1.86	0.40
8:H:83:LEU:O	8:H:87:LEU:HB3	2.20	0.40
9:I:57:THR:O	9:I:61:THR:OG1	2.25	0.40
15:Q:40:ILE:HD11	15:Q:210:VAL:HB	2.03	0.40
15:Q:59:VAL:O	15:Q:59:VAL:HG13	2.20	0.40
6:T:34:SER:OG	6:T:65:ARG:NH1	2.33	0.40
7:U:42:VAL:HG23	7:U:49:VAL:H	1.86	0.40
17:c:387:SER:O	17:c:391:GLU:HB2	2.21	0.40
20:f:313:LEU:O	20:f:317:ALA:HB3	2.21	0.40
21:g:235:LEU:O	21:g:239:ALA:HB2	2.20	0.40
23:i:634:PRO:HB3	23:i:667:GLU:CB	2.51	0.40
24:j:320:THR:O	28:n:251:LEU:CA	2.25	0.40
8:H:1:THR:HA	8:H:33:LYS:HZ1	1.85	0.40
8:H:212:LEU:HD12	9:I:200:LYS:HB2	2.03	0.40
8:V:1:THR:O	8:V:1:THR:OG1	2.32	0.40
8:V:83:LEU:O	8:V:87:LEU:HB3	2.20	0.40
9:W:164:GLU:O	9:W:167:SER:OG	2.29	0.40
11:Y:4:LEU:HD12	11:Y:135:ALA:HB1	2.04	0.40
13:a:110:MET:HE3	13:a:110:MET:HB3	1.78	0.40
17:c:248:LYS:HG2	18:d:262:ASP:CG	2.46	0.40
20:f:118:LEU:HA	20:f:121:ASN:HB2	2.03	0.40
20:f:148:VAL:HG13	20:f:149:ILE:HG12	2.03	0.40
22:h:101:LYS:HE2	22:h:101:LYS:HA	2.04	0.40
24:j:320:THR:CB	28:n:251:LEU:O	2.35	0.40
25:k:119:PRO:HB2	25:k:120:ILE:H	1.68	0.40
27:m:144:LEU:HG	27:m:160:ASN:HD21	1.85	0.40
27:m:185:GLY:HA3	27:m:201:PHE:CE1	2.56	0.40
27:m:208:PHE:C	27:m:209:THR:CG2	2.93	0.40
5:E:31:GLN:NE2	21:g:432:LYS:HG3	2.23	0.40
7:G:43:ARG:NH1	7:G:149:PRO:O	2.53	0.40
15:Q:51:ALA:O	15:Q:54:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:83:LEU:O	8:V:87:LEU:CB	2.69	0.40
17:c:238:ILE:HB	17:c:272:ILE:HG13	2.02	0.40
17:c:279:ALA:O	18:d:307:ARG:NE	2.54	0.40
17:c:327:LEU:HD23	17:c:331:LEU:CD2	2.51	0.40
19:e:161:ASP:HA	19:e:221:HIS:CE1	2.56	0.40
19:e:374:ASP:CB	20:f:292:PRO:HG3	2.51	0.40
22:h:76:VAL:HG12	22:h:87:VAL:HA	2.04	0.40
22:h:134:LEU:CD2	22:h:237:MET:SD	3.10	0.40
22:h:196:LYS:HE3	22:h:317:PHE:HD2	1.86	0.40
26:l:243:ASP:OD1	26:l:245:PRO:HD2	2.20	0.40
27:m:199:GLU:O	27:m:202:LEU:HG	2.20	0.40
27:m:208:PHE:CE2	27:m:211:TYR:HB2	2.57	0.40
2:B:5:TYR:CG	7:G:13:ILE:HD11	2.56	0.40
10:J:15:VAL:HG21	10:J:45:LEU:HD11	2.03	0.40
10:J:29:LYS:HD3	11:K:123:GLY:HA2	2.03	0.40
10:J:181:ARG:HG2	10:J:190:ASN:CB	2.31	0.40
13:M:26:MET:HE1	13:M:202:PRO:HG2	1.98	0.40
13:M:27:LEU:HD13	13:M:184:TYR:HB2	2.04	0.40
2:P:47:ALA:HB1	2:P:64:LYS:HG2	2.04	0.40
15:Q:31:THR:HB	15:Q:46:GLU:CG	2.51	0.40
15:Q:220:LEU:CB	15:Q:224:GLU:HB3	2.35	0.40
15:Q:221:ASN:O	15:Q:224:GLU:N	2.54	0.40
11:Y:103:GLY:HA2	11:Y:179:VAL:HG21	2.03	0.40
14:b:133:SER:HA	14:b:136:TYR:CE2	2.57	0.40
18:d:133:VAL:HG12	18:d:157:HIS:HB3	2.03	0.40
18:d:143:LEU:HB2	18:d:162:VAL:CG2	2.52	0.40
18:d:227:PRO:CA	18:d:230:THR:HG21	2.52	0.40
18:d:390:LEU:CD1	18:d:395:ILE:CG2	2.65	0.40
19:e:89:ILE:HG13	20:f:78:ARG:O	2.22	0.40
20:f:97:ARG:NH1	21:g:95:GLU:OE2	2.50	0.40
21:g:375:VAL:HG22	21:g:415:LEU:HD11	2.04	0.40
23:i:650:TYR:O	23:i:653:ALA:HB3	2.21	0.40
25:k:283:GLN:O	25:k:287:VAL:N	2.53	0.40
26:l:242:ILE:H	26:l:242:ILE:HG13	1.40	0.40
27:m:17:LEU:C	27:m:19:ILE:H	2.28	0.40
3:C:182:GLU:HG2	3:C:186:LEU:HD23	2.04	0.40
6:F:112:ALA:O	6:F:116:ALA:CB	2.70	0.40
7:G:237:ALA:HA	7:G:240:VAL:HG22	2.04	0.40
11:K:21:THR:HG22	11:K:26:ILE:HG22	2.02	0.40
11:K:130:SER:OG	11:K:131:GLY:N	2.53	0.40
15:Q:166:LYS:HA	15:Q:169:ARG:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:191:LYS:HZ2	6:T:238:TYR:HH	1.62	0.40
7:U:45:LYS:HD3	7:U:190:THR:HB	2.02	0.40
10:X:15:VAL:HG21	10:X:45:LEU:HD11	2.03	0.40
11:Y:115:ASP:OD2	11:Y:119:ASN:ND2	2.55	0.40
18:d:393:ALA:O	18:d:394:ASP:C	2.62	0.40
19:e:144:PRO:HA	19:e:145:PRO:HD3	1.95	0.40
19:e:397:LYS:HB3	19:e:401:LYS:HG2	2.03	0.40
21:g:225:MET:HG2	21:g:352:ILE:HD11	2.03	0.40
21:g:229:PRO:HB2	21:g:392:ASN:HD22	1.87	0.40
22:h:88:LYS:HA	22:h:94:LYS:HA	2.03	0.40
22:h:271:ARG:O	22:h:275:GLU:N	2.55	0.40
26:l:266:ASP:O	26:l:270:LEU:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
1	O	228/234 (97%)	197 (86%)	31 (14%)	0	100	100
2	B	228/261 (87%)	195 (86%)	30 (13%)	3 (1%)	9	38
2	P	242/261 (93%)	203 (84%)	35 (14%)	4 (2%)	7	34
3	C	232/234 (99%)	191 (82%)	38 (16%)	3 (1%)	9	38
4	D	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
4	R	231/241 (96%)	199 (86%)	32 (14%)	0	100	100
5	E	232/234 (99%)	190 (82%)	41 (18%)	1 (0%)	30	62
6	F	228/255 (89%)	195 (86%)	31 (14%)	2 (1%)	14	45
6	T	238/255 (93%)	202 (85%)	34 (14%)	2 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	229/246 (93%)	206 (90%)	21 (9%)	2 (1%)	14	45
7	U	239/246 (97%)	213 (89%)	25 (10%)	1 (0%)	30	62
8	H	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
8	V	219/277 (79%)	208 (95%)	11 (5%)	0	100	100
9	I	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	12	43
9	W	202/205 (98%)	182 (90%)	18 (9%)	2 (1%)	12	43
10	J	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
10	X	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
11	K	198/204 (97%)	174 (88%)	24 (12%)	0	100	100
11	Y	199/204 (98%)	175 (88%)	24 (12%)	0	100	100
12	L	212/241 (88%)	184 (87%)	28 (13%)	0	100	100
12	Z	211/241 (88%)	184 (87%)	27 (13%)	0	100	100
13	M	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	24	57
13	a	214/264 (81%)	192 (90%)	21 (10%)	1 (0%)	24	57
14	N	199/239 (83%)	179 (90%)	20 (10%)	0	100	100
14	b	201/239 (84%)	179 (89%)	21 (10%)	1 (0%)	24	57
15	Q	233/235 (99%)	186 (80%)	38 (16%)	9 (4%)	2	20
16	S	236/238 (99%)	195 (83%)	39 (16%)	2 (1%)	16	48
17	c	343/433 (79%)	256 (75%)	74 (22%)	13 (4%)	2	21
18	d	329/428 (77%)	251 (76%)	59 (18%)	19 (6%)	1	15
19	e	355/418 (85%)	279 (79%)	63 (18%)	13 (4%)	2	21
20	f	346/379 (91%)	285 (82%)	51 (15%)	10 (3%)	3	25
21	g	359/439 (82%)	292 (81%)	60 (17%)	7 (2%)	6	32
22	h	324/355 (91%)	248 (76%)	59 (18%)	17 (5%)	1	17
23	i	224/953 (24%)	173 (77%)	31 (14%)	20 (9%)	0	9
24	j	147/534 (28%)	111 (76%)	32 (22%)	4 (3%)	4	27
25	k	354/456 (78%)	272 (77%)	77 (22%)	5 (1%)	9	37
26	l	411/422 (97%)	341 (83%)	62 (15%)	8 (2%)	6	32
27	m	373/389 (96%)	318 (85%)	51 (14%)	4 (1%)	11	41
28	n	200/324 (62%)	147 (74%)	46 (23%)	7 (4%)	3	23
29	o	73/376 (19%)	56 (77%)	12 (16%)	5 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	p	90/377 (24%)	78 (87%)	11 (12%)	1 (1%)	11	41
31	q	253/310 (82%)	191 (76%)	54 (21%)	8 (3%)	3	24
32	r	4/350 (1%)	4 (100%)	0	0	100	100
33	s	24/70 (34%)	19 (79%)	5 (21%)	0	100	100
All	All	10342/13680 (76%)	8678 (84%)	1487 (14%)	177 (2%)	9	34

All (177) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	69	HIS
6	F	227	VAL
6	F	228	PRO
7	G	69	LEU
13	M	79	ASP
2	P	241	GLU
15	Q	47	LYS
15	Q	50	VAL
15	Q	222	PRO
16	S	69	HIS
16	S	237	GLU
6	T	227	VAL
6	T	228	PRO
7	U	69	LEU
13	a	79	ASP
14	b	202	LEU
17	c	164	MET
17	c	167	GLU
17	c	337	LEU
17	c	385	ILE
18	d	146	PRO
18	d	149	SER
18	d	233	THR
18	d	251	VAL
18	d	260	LEU
18	d	279	PRO
18	d	344	PRO
18	d	349	ARG
19	e	207	PRO
19	e	324	PRO
19	e	408	LYS
19	e	409	LYS

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Mol	Chain	Res	Type
19	e	412	GLN
19	e	413	GLU
19	e	416	PHE
20	f	64	LEU
20	f	65	THR
20	f	129	ASN
21	g	229	PRO
21	g	345	SER
21	g	425	LEU
22	h	84	LYS
22	h	117	ARG
22	h	131	VAL
22	h	133	PRO
22	h	142	LYS
22	h	243	PRO
22	h	354	ALA
23	i	506	ALA
23	i	540	GLN
23	i	586	VAL
23	i	614	VAL
23	i	625	ILE
23	i	626	LEU
23	i	630	PRO
23	i	631	GLU
23	i	666	LYS
23	i	680	VAL
24	j	208	LEU
24	j	340	MET
25	k	413	ILE
26	l	241	SER
26	l	244	SER
26	l	370	LEU
26	l	407	MET
27	m	18	ARG
28	n	243	GLN
28	n	264	SER
29	o	106	ALA
29	o	124	VAL
31	q	51	MET
31	q	232	GLN
31	q	233	ASP
31	q	267	PRO

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Mol	Chain	Res	Type
2	B	55	LEU
3	C	77	THR
7	G	45	LYS
9	I	146	TYR
9	I	147	GLY
2	P	55	LEU
15	Q	49	SER
15	Q	52	LYS
15	Q	77	THR
9	W	146	TYR
9	W	147	GLY
17	c	166	VAL
17	c	168	GLU
17	c	180	CYS
17	c	325	ASP
18	d	389	ASP
18	d	391	SER
19	e	98	GLN
19	e	99	ASN
19	e	268	ASP
20	f	66	GLU
20	f	128	GLY
20	f	271	HIS
22	h	108	VAL
22	h	129	ASN
22	h	358	GLU
23	i	560	MET
23	i	567	ILE
25	k	119	PRO
26	l	369	ILE
26	l	404	ILE
27	m	48	ASN
28	n	114	ARG
28	n	179	ILE
31	q	231	LEU
31	q	275	VAL
17	c	169	LYS
17	c	380	SER
18	d	106	PRO
18	d	264	PRO
18	d	285	ASP
20	f	86	GLN

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Mol	Chain	Res	Type
20	f	123	SER
20	f	292	PRO
21	g	349	ASP
22	h	138	MET
23	i	521	LEU
23	i	538	GLU
23	i	661	ALA
26	l	82	LYS
28	n	178	ASP
29	o	101	THR
30	p	56	ASN
15	Q	46	GLU
18	d	104	GLY
18	d	145	GLU
18	d	188	GLY
18	d	355	LEU
19	e	417	TYR
22	h	106	ASN
23	i	543	LYS
23	i	549	ALA
23	i	627	PHE
24	j	262	SER
27	m	206	SER
28	n	177	ARG
29	o	107	ASN
31	q	175	ARG
2	P	160	LYS
2	P	172	VAL
17	c	324	PRO
22	h	66	LEU
22	h	121	TYR
25	k	200	ILE
26	l	395	LYS
29	o	123	THR
2	B	160	LYS
2	B	186	LEU
3	C	199	VAL
17	c	195	LEU
20	f	61	LEU
21	g	399	VAL
22	h	105	ILE
23	i	568	GLU

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Mol	Chain	Res	Type
25	k	198	ASP
27	m	205	VAL
31	q	272	ILE
18	d	345	GLY
18	d	356	PRO
22	h	195	GLY
22	h	351	MET
24	j	193	ILE
25	k	412	ILE
3	C	125	ARG
15	Q	125	ARG
21	g	228	PRO
23	i	550	VAL
28	n	184	VAL
15	Q	199	VAL
17	c	177	VAL
19	e	303	VAL
21	g	280	PRO
19	e	86	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/191 (95%)	180 (99%)	1 (1%)	78	79
1	O	181/191 (95%)	180 (99%)	1 (1%)	78	79
2	B	195/221 (88%)	187 (96%)	8 (4%)	27	51
2	P	194/221 (88%)	189 (97%)	5 (3%)	40	60
3	C	179/197 (91%)	172 (96%)	7 (4%)	28	52
4	D	189/203 (93%)	187 (99%)	2 (1%)	65	73
4	R	192/203 (95%)	191 (100%)	1 (0%)	81	81
5	E	192/200 (96%)	190 (99%)	2 (1%)	68	74
6	F	190/212 (90%)	189 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	197/212 (93%)	196 (100%)	1 (0%)	81	81
7	G	197/210 (94%)	195 (99%)	2 (1%)	68	74
7	U	196/210 (93%)	192 (98%)	4 (2%)	48	65
8	H	181/228 (79%)	180 (99%)	1 (1%)	78	79
8	V	173/228 (76%)	170 (98%)	3 (2%)	53	67
9	I	173/174 (99%)	171 (99%)	2 (1%)	63	72
9	W	172/174 (99%)	170 (99%)	2 (1%)	63	72
10	J	163/166 (98%)	160 (98%)	3 (2%)	51	67
10	X	164/166 (99%)	162 (99%)	2 (1%)	63	72
11	K	154/159 (97%)	149 (97%)	5 (3%)	34	56
11	Y	156/159 (98%)	151 (97%)	5 (3%)	34	56
12	L	175/199 (88%)	173 (99%)	2 (1%)	65	73
12	Z	175/199 (88%)	173 (99%)	2 (1%)	65	73
13	M	179/215 (83%)	177 (99%)	2 (1%)	65	73
13	a	177/215 (82%)	175 (99%)	2 (1%)	65	73
14	N	157/181 (87%)	156 (99%)	1 (1%)	78	79
14	b	157/181 (87%)	156 (99%)	1 (1%)	78	79
15	Q	182/199 (92%)	171 (94%)	11 (6%)	17	43
16	S	194/202 (96%)	193 (100%)	1 (0%)	81	81
17	c	297/372 (80%)	280 (94%)	17 (6%)	18	44
18	d	281/375 (75%)	257 (92%)	24 (8%)	10	33
19	e	289/366 (79%)	266 (92%)	23 (8%)	11	36
20	f	287/331 (87%)	276 (96%)	11 (4%)	29	53
21	g	291/379 (77%)	272 (94%)	19 (6%)	15	42
22	h	266/307 (87%)	238 (90%)	28 (10%)	6	26
23	i	8/816 (1%)	8 (100%)	0	100	100
24	j	5/460 (1%)	5 (100%)	0	100	100
25	k	5/416 (1%)	5 (100%)	0	100	100
26	l	148/362 (41%)	141 (95%)	7 (5%)	23	48
27	m	154/344 (45%)	144 (94%)	10 (6%)	15	42
28	n	5/295 (2%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	o	2/336 (1%)	2 (100%)	0	100	100
30	p	3/312 (1%)	3 (100%)	0	100	100
31	q	14/268 (5%)	14 (100%)	0	100	100
32	r	1/294 (0%)	1 (100%)	0	100	100
All	All	7071/11549 (61%)	6852 (97%)	219 (3%)	36	57

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
2	B	35	LEU
2	B	52	ILE
2	B	70	GLU
2	B	132	VAL
2	B	147	LEU
2	B	186	LEU
2	B	239	LYS
2	B	241	GLU
3	C	45	VAL
3	C	90	GLU
3	C	100	ASP
3	C	172	LEU
3	C	179	ASP
3	C	231	GLU
3	C	235	GLU
4	D	20	ARG
4	D	210	LEU
5	E	56	LEU
5	E	77	LEU
6	F	89	ASP
7	G	43	ARG
7	G	232	GLU
8	H	28	ASP
9	I	120	ILE
9	I	125	LEU
10	J	190	ASN
10	J	191	LEU
10	J	192	GLU
11	K	12	VAL
11	K	13	ILE
11	K	72	GLU

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Mol	Chain	Res	Type
11	K	174	VAL
11	K	179	VAL
12	L	26	ASP
12	L	131	GLN
13	M	195	LYS
13	M	200	GLU
14	N	69	GLU
1	O	48	GLU
2	P	35	LEU
2	P	70	GLU
2	P	132	VAL
2	P	147	LEU
2	P	186	LEU
15	Q	45	VAL
15	Q	46	GLU
15	Q	47	LYS
15	Q	90	GLU
15	Q	100	ASP
15	Q	172	LEU
15	Q	179	ASP
15	Q	223	GLU
15	Q	224	GLU
15	Q	225	ILE
15	Q	227	LYS
4	R	210	LEU
16	S	56	LEU
6	T	89	ASP
7	U	43	ARG
7	U	164	LYS
7	U	166	THR
7	U	232	GLU
8	V	1	THR
8	V	2	THR
8	V	28	ASP
9	W	120	ILE
9	W	125	LEU
10	X	190	ASN
10	X	192	GLU
11	Y	12	VAL
11	Y	13	ILE
11	Y	72	GLU
11	Y	174	VAL

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Mol	Chain	Res	Type
11	Y	179	VAL
12	Z	26	ASP
12	Z	131	GLN
13	a	167	ASP
13	a	195	LYS
14	b	69	GLU
17	c	149	ILE
17	c	157	ILE
17	c	161	VAL
17	c	163	MET
17	c	164	MET
17	c	165	GLN
17	c	167	GLU
17	c	168	GLU
17	c	177	VAL
17	c	204	LEU
17	c	220	THR
17	c	222	LYS
17	c	280	ILE
17	c	331	LEU
17	c	332	MET
17	c	333	ARG
17	c	381	THR
18	d	105	THR
18	d	142	ASP
18	d	144	LEU
18	d	145	GLU
18	d	163	LEU
18	d	199	GLU
18	d	230	THR
18	d	235	LEU
18	d	256	ILE
18	d	257	GLN
18	d	258	LYS
18	d	260	LEU
18	d	265	LYS
18	d	266	LEU
18	d	275	GLU
18	d	276	GLU
18	d	281	ILE
18	d	327	VAL
18	d	341	LEU

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Mol	Chain	Res	Type
18	d	342	ILE
18	d	374	LEU
18	d	387	LYS
18	d	389	ASP
18	d	390	LEU
19	e	85	ILE
19	e	87	LEU
19	e	154	LEU
19	e	231	VAL
19	e	266	GLU
19	e	267	ILE
19	e	311	THR
19	e	321	LEU
19	e	322	LEU
19	e	323	ARG
19	e	326	ARG
19	e	327	LEU
19	e	398	ASP
19	e	399	PHE
19	e	407	ILE
19	e	408	LYS
19	e	409	LYS
19	e	410	ASP
19	e	411	GLU
19	e	412	GLN
19	e	415	GLU
19	e	416	PHE
19	e	417	TYR
20	f	63	GLN
20	f	64	LEU
20	f	65	THR
20	f	68	LYS
20	f	70	ILE
20	f	182	LEU
20	f	185	ARG
20	f	225	HIS
20	f	289	LEU
20	f	290	LEU
20	f	291	ARG
21	g	261	ILE
21	g	263	ASP
21	g	277	GLU

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Mol	Chain	Res	Type
21	g	291	ILE
21	g	332	THR
21	g	342	LEU
21	g	343	LEU
21	g	347	ARG
21	g	348	LEU
21	g	396	CYS
21	g	397	LYS
21	g	421	MET
21	g	425	LEU
21	g	430	LYS
21	g	431	LYS
21	g	432	LYS
21	g	435	LEU
21	g	436	GLN
21	g	437	TYR
22	h	63	LEU
22	h	66	LEU
22	h	69	GLN
22	h	92	GLU
22	h	94	LYS
22	h	99	VAL
22	h	105	ILE
22	h	112	CYS
22	h	113	ARG
22	h	114	VAL
22	h	116	LEU
22	h	118	ASN
22	h	127	LEU
22	h	130	LYS
22	h	135	VAL
22	h	137	LEU
22	h	140	VAL
22	h	142	LYS
22	h	145	ASP
22	h	178	LEU
22	h	180	ILE
22	h	196	LYS
22	h	235	PHE
22	h	239	ARG
22	h	271	ARG
22	h	310	ARG

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Mol	Chain	Res	Type
22	h	349	GLU
22	h	350	LEU
26	l	157	LEU
26	l	159	LYS
26	l	160	MET
26	l	163	LYS
26	l	165	LEU
26	l	240	ASP
26	l	242	ILE
27	m	138	LEU
27	m	141	VAL
27	m	167	LEU
27	m	168	ILE
27	m	169	GLU
27	m	199	GLU
27	m	202	LEU
27	m	204	THR
27	m	207	THR
27	m	208	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	108	GLN
1	A	111	GLN
1	A	118	GLN
1	A	178	ASN
1	A	206	ASN
2	B	69	ASN
2	B	84	ASN
2	B	88	ASN
2	B	102	GLN
2	B	146	GLN
2	B	240	HIS
3	C	120	GLN
3	C	146	GLN
3	C	154	HIS
4	D	41	GLN
4	D	97	GLN
4	D	99	HIS
4	D	104	ASN

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Mol	Chain	Res	Type
4	D	182	GLN
4	D	204	GLN
5	E	21	GLN
5	E	31	GLN
5	E	68	ASN
5	E	166	GLN
6	F	105	ASN
6	F	170	GLN
6	F	201	HIS
7	G	68	HIS
7	G	75	ASN
8	H	66	HIS
8	H	116	HIS
8	H	165	ASN
9	I	172	ASN
10	J	71	ASN
10	J	99	HIS
11	K	70	ASN
12	L	8	ASN
12	L	151	ASN
12	L	157	ASN
13	M	38	ASN
13	M	47	ASN
13	M	89	HIS
13	M	104	ASN
13	M	208	ASN
14	N	53	GLN
1	O	70	HIS
1	O	108	GLN
1	O	111	GLN
1	O	118	GLN
1	O	178	ASN
1	O	206	ASN
2	P	69	ASN
2	P	102	GLN
2	P	146	GLN
2	P	198	ASN
15	Q	92	GLN
15	Q	122	ASN
15	Q	146	GLN
15	Q	175	ASN
4	R	41	GLN

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Mol	Chain	Res	Type
4	R	97	GLN
4	R	99	HIS
4	R	104	ASN
4	R	182	GLN
4	R	204	GLN
16	S	21	GLN
16	S	68	ASN
16	S	166	GLN
16	S	203	GLN
6	T	22	GLN
6	T	105	ASN
6	T	201	HIS
7	U	12	HIS
7	U	24	GLN
7	U	33	ASN
7	U	68	HIS
7	U	75	ASN
8	V	116	HIS
9	W	168	GLN
10	X	61	GLN
10	X	71	ASN
10	X	189	HIS
12	Z	8	ASN
12	Z	157	ASN
13	a	47	ASN
13	a	89	HIS
13	a	104	ASN
13	a	208	ASN
13	a	213	HIS
17	c	91	GLN
17	c	150	HIS
17	c	247	GLN
17	c	293	ASN
17	c	296	GLN
17	c	433	ASN
18	d	153	ASN
18	d	195	GLN
18	d	241	ASN
18	d	315	GLN
18	d	416	ASN
19	e	412	GLN
20	f	254	GLN

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Mol	Chain	Res	Type
20	f	280	ASN
20	f	316	HIS
20	f	359	HIS
21	g	130	GLN
21	g	321	GLN
21	g	323	ASN
21	g	434	ASN
22	h	106	ASN
22	h	278	ASN
22	h	332	HIS
22	h	337	ASN
22	h	377	HIS
26	l	170	GLN
26	l	178	HIS
26	l	218	HIS
26	l	322	HIS
27	m	178	ASN
27	m	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	7C9	u	2	34	5,6,7	0.60	0	2,6,8	0.26	0
34	6V9	u	1	34	7,8,9	1.16	1 (14%)	7,10,12	4.49	7 (100%)
34	7C9	t	2	34	5,6,7	0.52	0	2,6,8	0.38	0
34	7C9	t	3	34	5,6,7	0.57	0	2,6,8	0.29	0
34	7C9	u	3	34	5,6,7	0.58	0	2,6,8	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	6V9	t	1	34	7,8,9	1.27	1 (14%)	7,10,12	4.66	7 (100%)

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	7C9	u	2	34	-	2/3/5/7	-
34	6V9	u	1	34	-	2/2/2/4	0/1/1/1
34	7C9	t	2	34	-	2/3/5/7	-
34	7C9	t	3	34	-	0/3/5/7	-
34	7C9	u	3	34	-	0/3/5/7	-
34	6V9	t	1	34	-	2/2/2/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	t	1	6V9	C-C3	2.83	1.49	1.45
34	u	1	6V9	C-C3	2.50	1.48	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	1	6V9	C21-C3-C	6.23	134.35	127.15
34	u	1	6V9	C21-C3-C	5.96	134.04	127.15
34	t	1	6V9	S-C1-N	-5.70	110.75	114.63
34	u	1	6V9	S-C1-N	-5.48	110.91	114.63
34	t	1	6V9	C2-C1-N	4.68	133.54	123.75
34	u	1	6V9	C2-C1-N	4.62	133.42	123.75
34	u	1	6V9	C-C3-S	-4.38	115.97	121.31
34	t	1	6V9	C-C3-S	-4.29	116.09	121.31
34	t	1	6V9	C1-S-C3	4.19	92.07	89.63
34	u	1	6V9	C1-S-C3	3.63	91.74	89.63
34	t	1	6V9	O-C-C3	-3.54	118.73	124.98
34	u	1	6V9	O-C-C3	-3.38	119.02	124.98
34	u	1	6V9	C2-C1-S	-3.19	115.67	122.51
34	t	1	6V9	C2-C1-S	-3.17	115.70	122.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	t	1	6V9	O-C-C3-S
34	t	1	6V9	O-C-C3-C21
34	u	1	6V9	O-C-C3-S
34	u	1	6V9	O-C-C3-C21
34	t	2	7C9	O20-C19-CA-N
34	t	2	7C9	O20-C19-CA-C
34	u	2	7C9	O20-C19-CA-N
34	u	2	7C9	O20-C19-CA-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
35	ADP	c	501	-	28,29,29	1.37	5 (17%)	43,45,45	1.80	10 (23%)
35	ADP	g	501	-	28,29,29	1.34	5 (17%)	43,45,45	1.79	8 (18%)
35	ADP	h	401	-	28,29,29	1.34	5 (17%)	43,45,45	1.81	8 (18%)
35	ADP	d	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.89	10 (23%)
35	ADP	e	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	9 (20%)
35	ADP	g	502	-	28,29,29	1.33	5 (17%)	43,45,45	1.82	8 (18%)

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
35	ADP	c	501	-	-	3/16/32/32	0/3/3/3
35	ADP	g	501	-	-	6/16/32/32	0/3/3/3
35	ADP	h	401	-	-	3/16/32/32	0/3/3/3
35	ADP	d	501	-	-	4/16/32/32	0/3/3/3
35	ADP	e	501	-	-	5/16/32/32	0/3/3/3
35	ADP	g	502	-	-	4/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	501	ADP	C5-C4	4.72	1.47	1.39
35	d	501	ADP	C5-C4	4.45	1.47	1.39
35	g	501	ADP	C5-C4	4.41	1.47	1.39
35	h	401	ADP	C5-C4	4.35	1.46	1.39
35	c	501	ADP	C5-C4	4.25	1.46	1.39
35	g	502	ADP	C5-C4	4.21	1.46	1.39
35	g	502	ADP	C5-N7	-2.78	1.34	1.39
35	e	501	ADP	C5-C6	2.76	1.48	1.41
35	c	501	ADP	C5-N7	-2.61	1.34	1.39
35	d	501	ADP	C5-C6	2.59	1.48	1.41
35	h	401	ADP	C5-N7	-2.56	1.34	1.39
35	g	501	ADP	C5-N7	-2.54	1.34	1.39
35	c	501	ADP	C4-N9	-2.49	1.32	1.37
35	c	501	ADP	C5-C6	2.47	1.47	1.41
35	d	501	ADP	C5-N7	-2.46	1.34	1.39
35	h	401	ADP	C5-C6	2.38	1.47	1.41
35	e	501	ADP	C8-N7	2.34	1.36	1.31
35	g	501	ADP	C5-C6	2.34	1.47	1.41
35	d	501	ADP	C8-N7	2.25	1.36	1.31
35	g	502	ADP	C5-C6	2.25	1.47	1.41
35	h	401	ADP	C8-N7	2.24	1.36	1.31
35	c	501	ADP	C8-N7	2.22	1.36	1.31
35	g	501	ADP	C8-N7	2.20	1.35	1.31
35	e	501	ADP	C5-N7	-2.20	1.35	1.39
35	g	502	ADP	C4-N9	-2.19	1.33	1.37
35	h	401	ADP	C4-N9	-2.16	1.33	1.37
35	g	501	ADP	C4-N9	-2.12	1.33	1.37
35	g	502	ADP	C8-N7	2.11	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	501	ADP	C5-C4-N3	-6.03	118.42	126.72
35	e	501	ADP	C5-C4-N3	-5.84	118.68	126.72
35	g	502	ADP	C5-C4-N3	-5.80	118.73	126.72
35	h	401	ADP	C5-C4-N3	-5.62	118.98	126.72
35	g	501	ADP	C5-C4-N3	-5.50	119.14	126.72
35	c	501	ADP	C5-C4-N3	-5.32	119.39	126.72
35	g	502	ADP	N3-C4-N9	4.66	135.10	127.17
35	d	501	ADP	N3-C4-N9	4.65	135.07	127.17
35	e	501	ADP	N3-C4-N9	4.61	135.01	127.17
35	h	401	ADP	N3-C4-N9	4.47	134.77	127.17
35	g	501	ADP	N3-C4-N9	4.36	134.58	127.17
35	c	501	ADP	N3-C4-N9	3.99	133.96	127.17
35	d	501	ADP	C4-C5-N7	-3.75	106.30	110.58
35	e	501	ADP	C2-N3-C4	3.70	120.87	111.83
35	d	501	ADP	C2-N3-C4	3.69	120.84	111.83
35	c	501	ADP	C4-C5-N7	-3.68	106.38	110.58
35	g	502	ADP	C2-N3-C4	3.59	120.60	111.83
35	h	401	ADP	C2-N3-C4	3.55	120.51	111.83
35	g	501	ADP	C2-N3-C4	3.51	120.41	111.83
35	e	501	ADP	C4-C5-N7	-3.46	106.63	110.58
35	c	501	ADP	C2-N3-C4	3.36	120.05	111.83
35	g	502	ADP	C4-C5-N7	-3.32	106.78	110.58
35	h	401	ADP	C4-C5-N7	-3.30	106.81	110.58
35	g	501	ADP	N3-C2-N1	-3.26	123.65	128.58
35	g	501	ADP	C4-C5-N7	-3.24	106.88	110.58
35	e	501	ADP	N3-C2-N1	-3.21	123.72	128.58
35	h	401	ADP	N3-C2-N1	-3.17	123.78	128.58
35	g	502	ADP	N3-C2-N1	-3.15	123.82	128.58
35	d	501	ADP	N3-C2-N1	-3.10	123.89	128.58
35	c	501	ADP	N3-C2-N1	-2.95	124.11	128.58
35	g	502	ADP	C4-N9-C8	2.82	108.70	105.74
35	c	501	ADP	C4-N9-C8	2.78	108.65	105.74
35	h	401	ADP	C4-N9-C8	2.77	108.65	105.74
35	d	501	ADP	C5-N7-C8	2.75	107.77	103.45
35	c	501	ADP	C2'-C1'-N9	-2.69	106.62	113.30
35	d	501	ADP	C4-N9-C8	2.63	108.50	105.74
35	g	501	ADP	C4-N9-C8	2.60	108.47	105.74
35	e	501	ADP	C4-N9-C8	2.59	108.45	105.74
35	c	501	ADP	C5-N7-C8	2.56	107.47	103.45
35	g	502	ADP	C5-N7-C8	2.54	107.44	103.45
35	e	501	ADP	C5-N7-C8	2.51	107.40	103.45
35	e	501	ADP	C3'-C2'-C1'	2.49	106.17	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	501	ADP	O4'-C1'-N9	2.44	112.78	108.09
35	h	401	ADP	C5-N7-C8	2.44	107.28	103.45
35	g	501	ADP	C5-N7-C8	2.37	107.18	103.45
35	c	501	ADP	N9-C8-N7	-2.18	110.84	113.94
35	g	502	ADP	N9-C8-N7	-2.14	110.90	113.94
35	d	501	ADP	N9-C8-N7	-2.13	110.92	113.94
35	g	501	ADP	C3'-C2'-C1'	2.11	105.46	101.46
35	c	501	ADP	C6-C5-N7	2.11	136.16	132.09
35	h	401	ADP	N9-C8-N7	-2.06	111.02	113.94
35	e	501	ADP	C6-C5-N7	2.05	136.05	132.09
35	d	501	ADP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (25) torsion outliers are listed below:

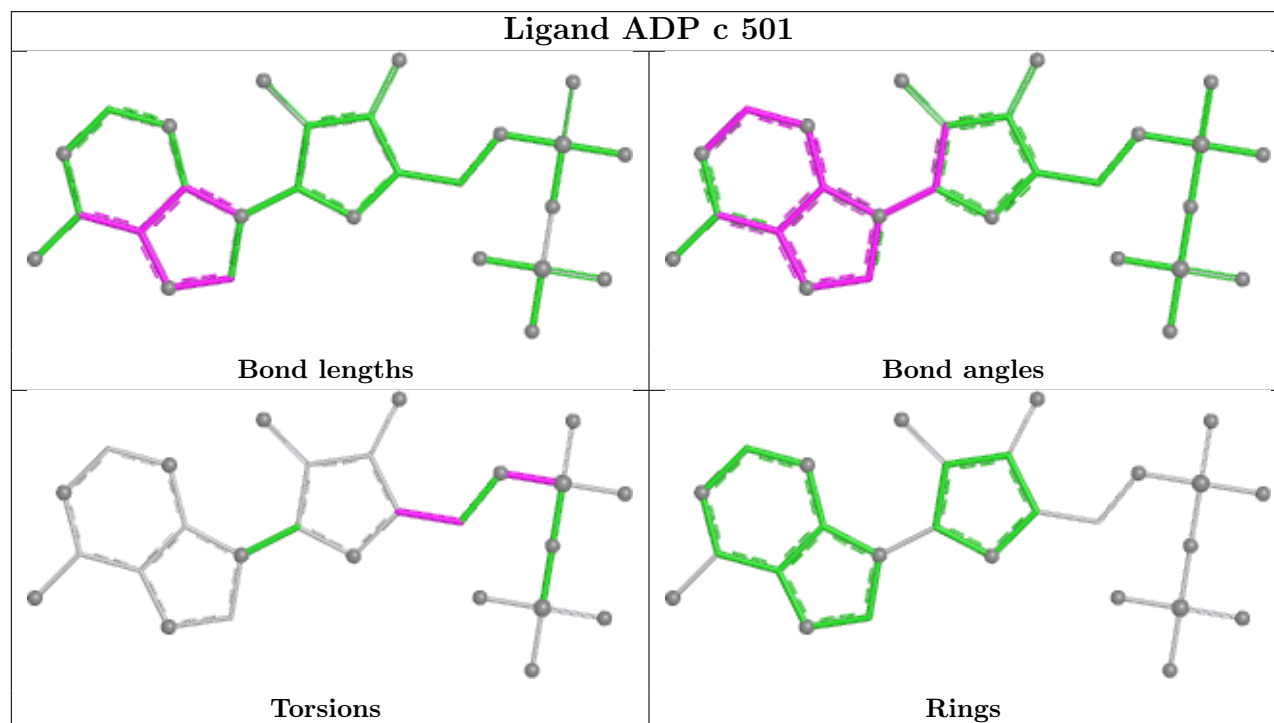
Mol	Chain	Res	Type	Atoms
35	c	501	ADP	C5'-O5'-PA-O1A
35	d	501	ADP	C4'-C5'-O5'-PA
35	e	501	ADP	C5'-O5'-PA-O1A
35	e	501	ADP	C5'-O5'-PA-O2A
35	e	501	ADP	C5'-O5'-PA-O3A
35	g	501	ADP	C5'-O5'-PA-O1A
35	g	502	ADP	C5'-O5'-PA-O2A
35	g	502	ADP	C5'-O5'-PA-O3A
35	h	401	ADP	C5'-O5'-PA-O1A
35	c	501	ADP	C3'-C4'-C5'-O5'
35	c	501	ADP	O4'-C4'-C5'-O5'
35	e	501	ADP	O4'-C4'-C5'-O5'
35	g	501	ADP	C2'-C1'-N9-C4
35	h	401	ADP	C2'-C1'-N9-C4
35	h	401	ADP	C2'-C1'-N9-C8
35	e	501	ADP	C3'-C4'-C5'-O5'
35	d	501	ADP	C2'-C1'-N9-C8
35	g	501	ADP	C2'-C1'-N9-C8
35	g	501	ADP	C4'-C5'-O5'-PA
35	g	502	ADP	C2'-C1'-N9-C4
35	g	502	ADP	C2'-C1'-N9-C8
35	d	501	ADP	PB-O3A-PA-O2A
35	g	501	ADP	PB-O3A-PA-O2A
35	d	501	ADP	O4'-C1'-N9-C8
35	g	501	ADP	PB-O3A-PA-O1A

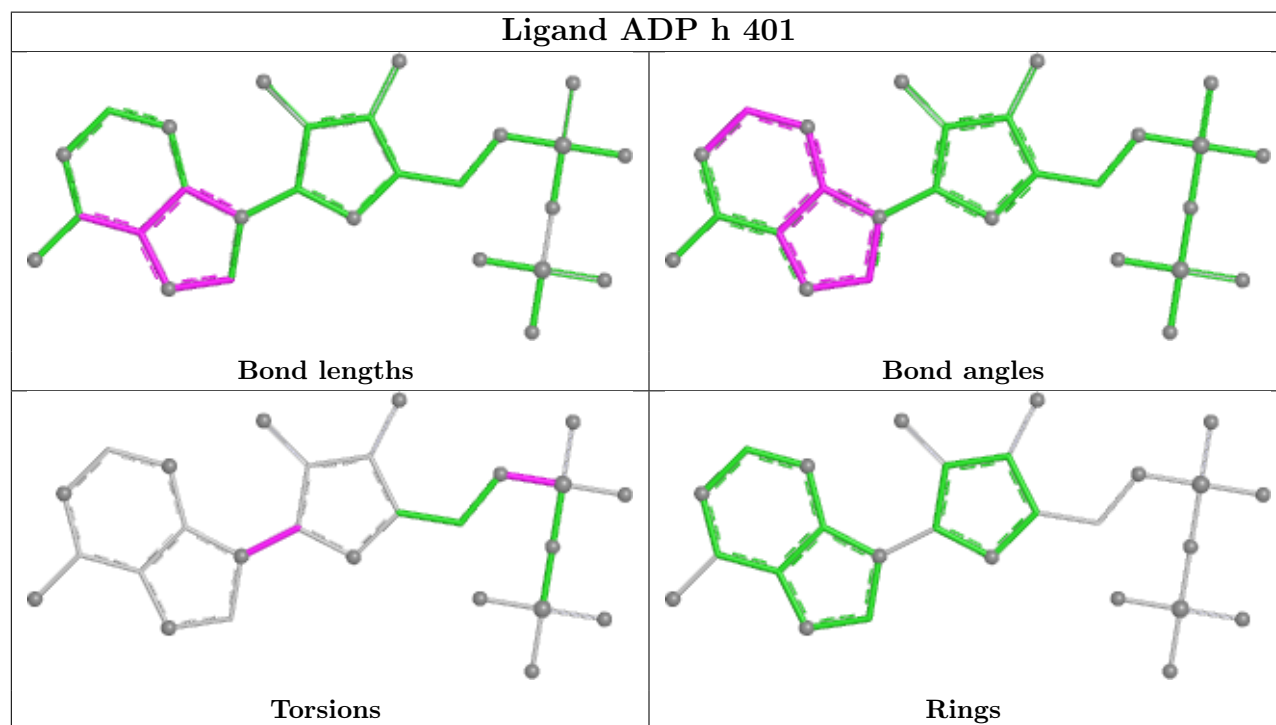
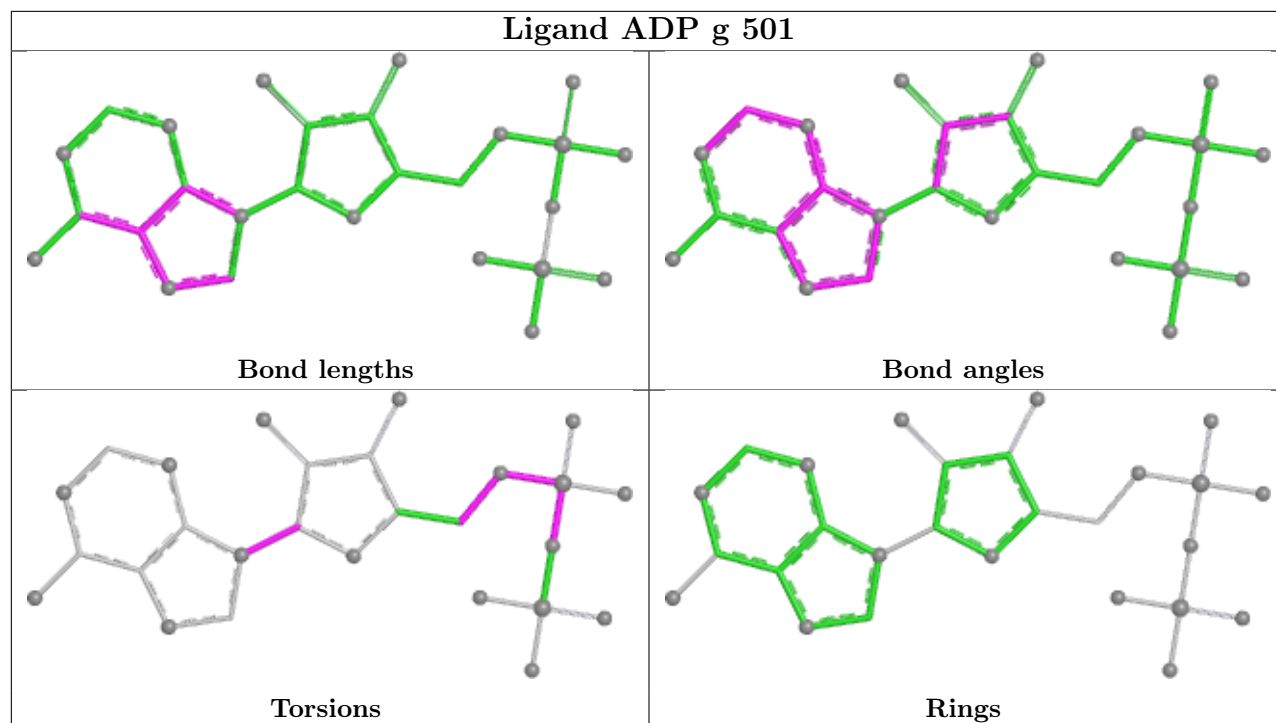
There are no ring outliers.

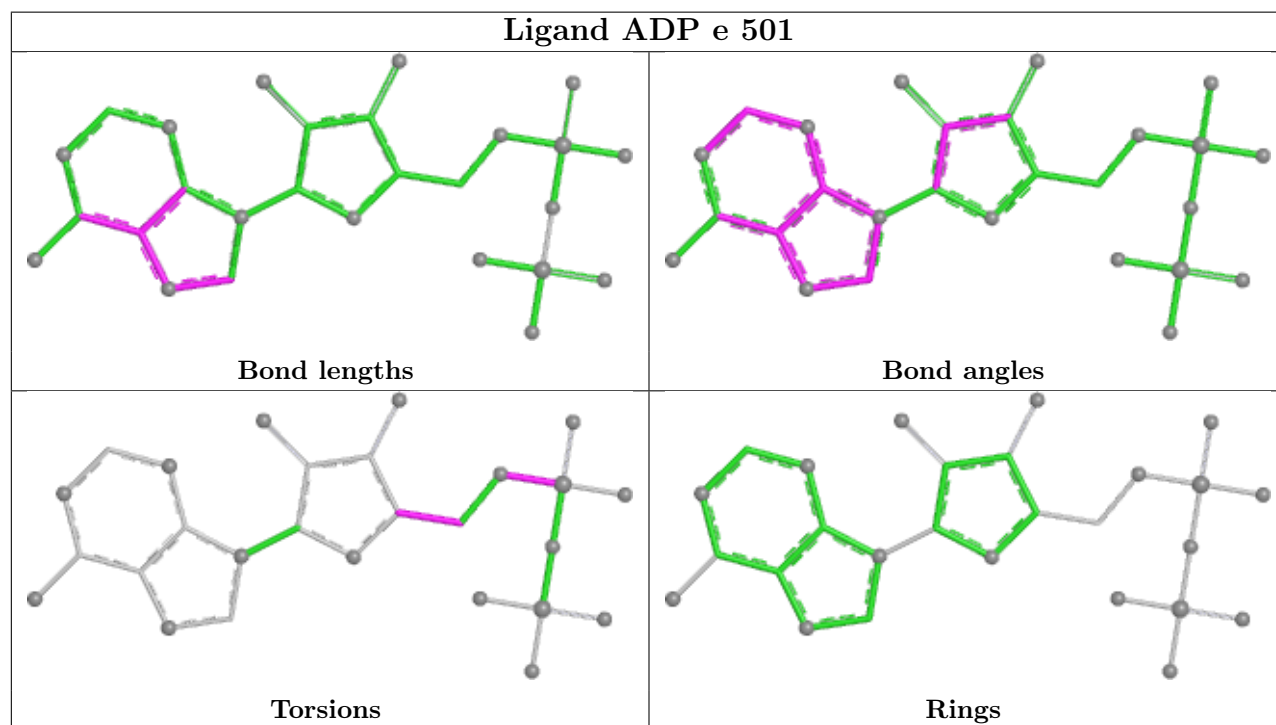
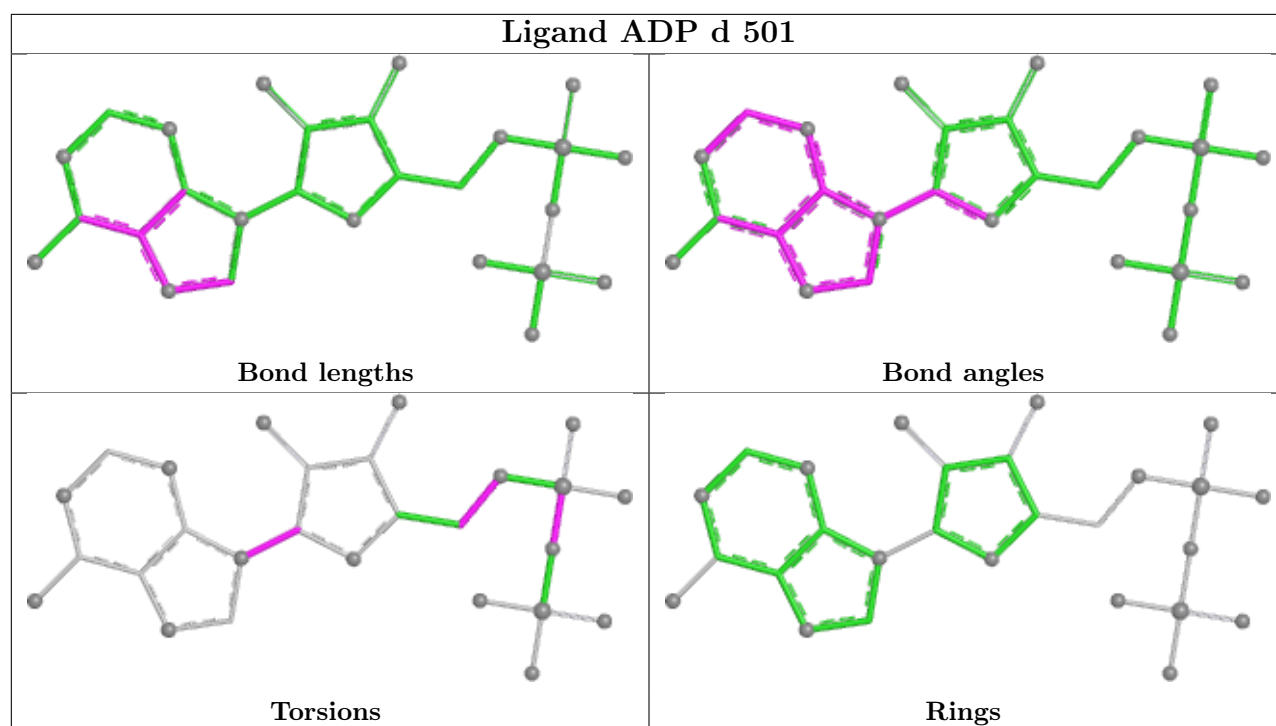
6 monomers are involved in 81 short contacts:

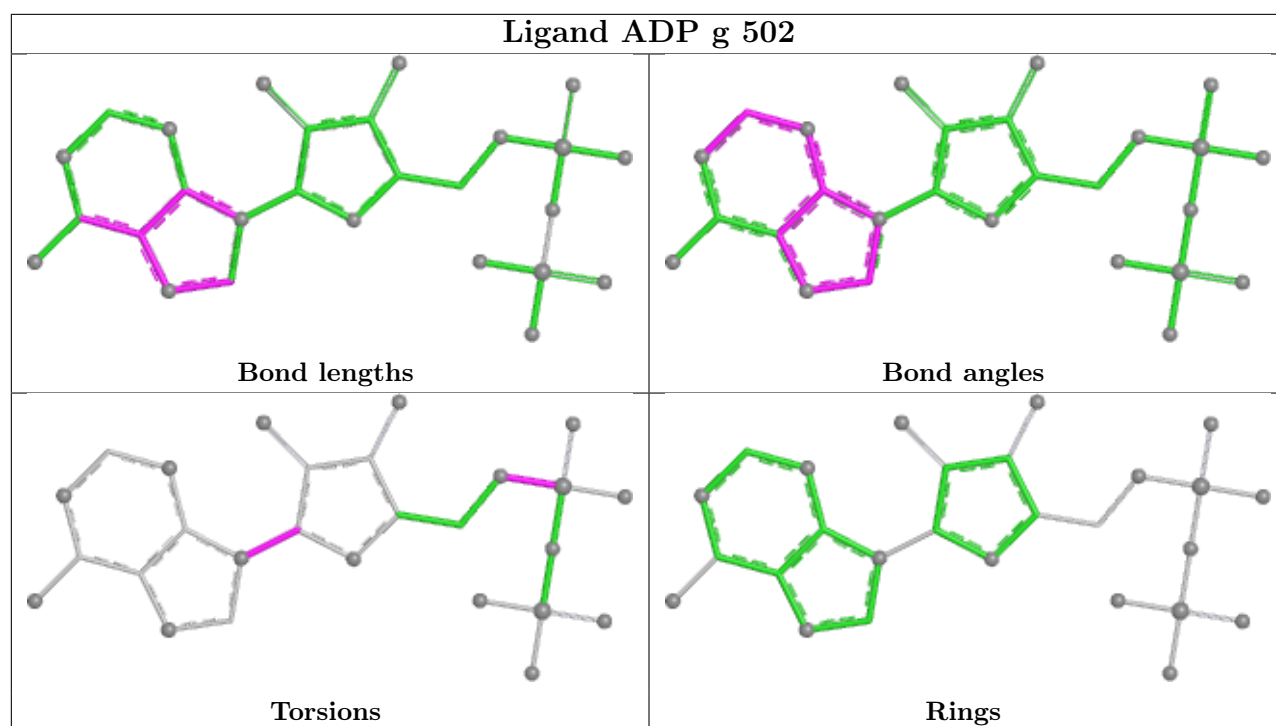
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	c	501	ADP	7	0
35	g	501	ADP	14	0
35	h	401	ADP	22	0
35	d	501	ADP	11	0
35	e	501	ADP	19	0
35	g	502	ADP	8	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	e	1
15	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	414:HIS	C	415:GLU	N	4.11
1	Q	45:VAL	C	46:GLU	N	0.63

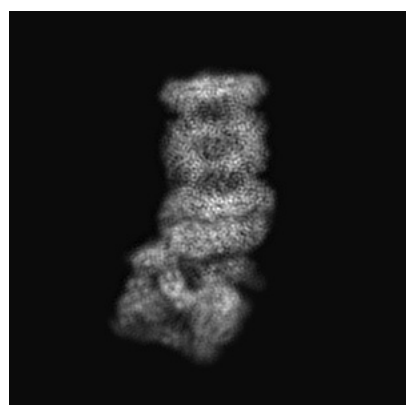
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4146. These allow visual inspection of the internal detail of the map and identification of artifacts.

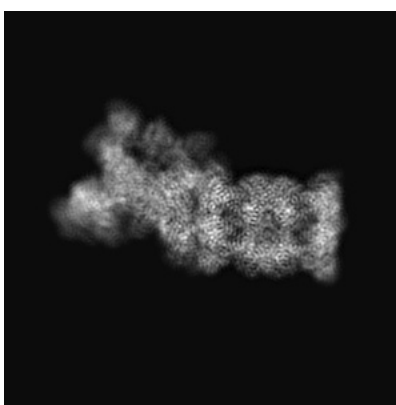
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

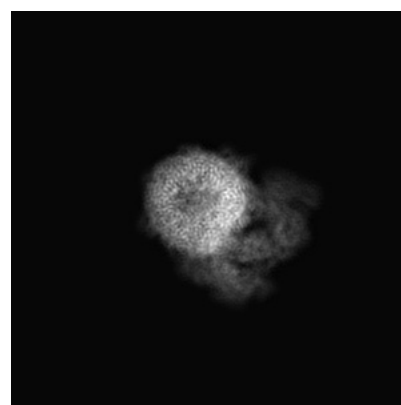
6.1.1 Primary map



X



Y

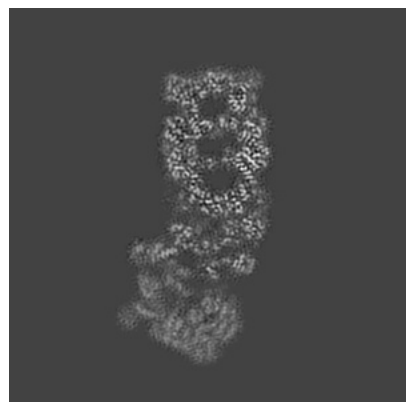


Z

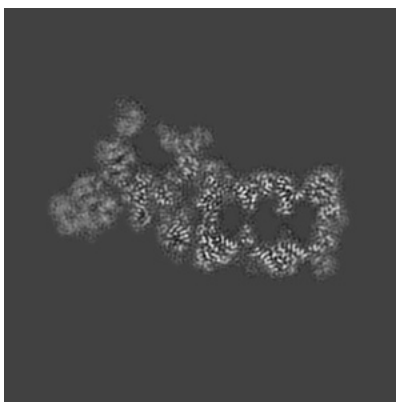
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

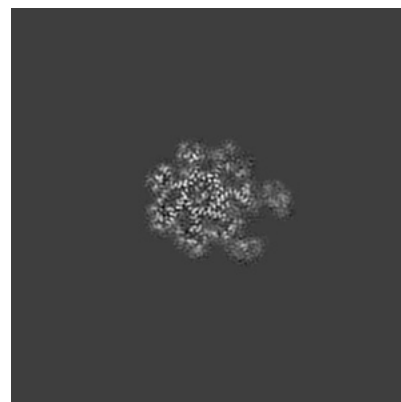
6.2.1 Primary map



X Index: 168



Y Index: 168

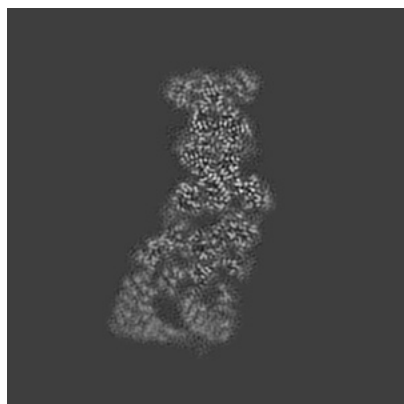


Z Index: 168

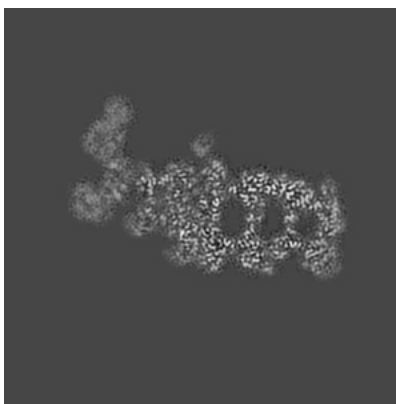
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

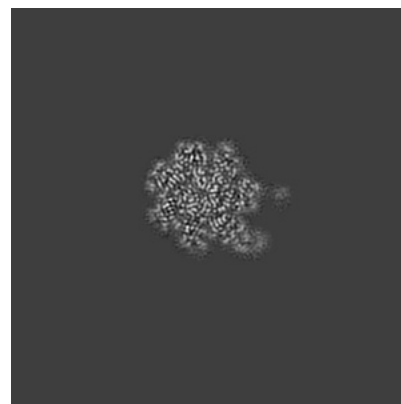
6.3.1 Primary map



X Index: 181



Y Index: 186

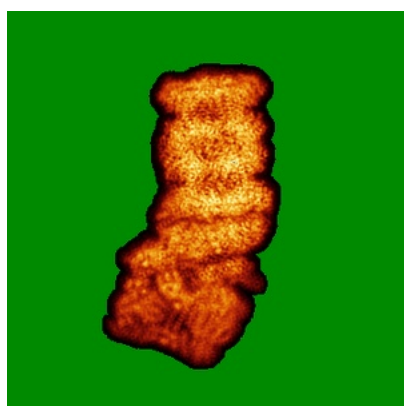


Z Index: 176

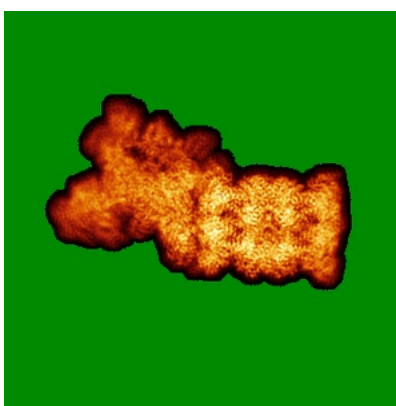
The images above show the largest variance slices of the map in three orthogonal directions.

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

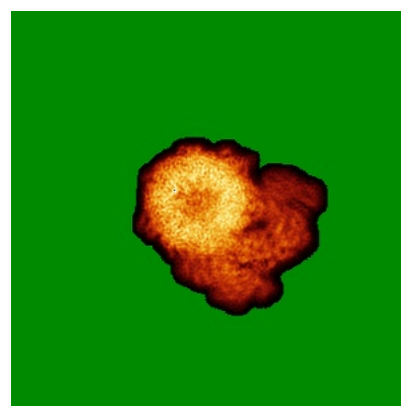
6.4.1 Primary map



X



Y

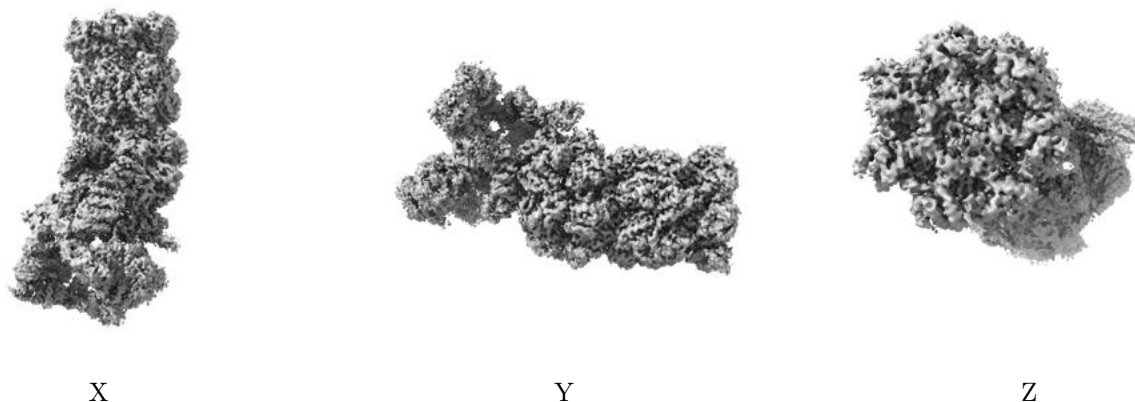


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

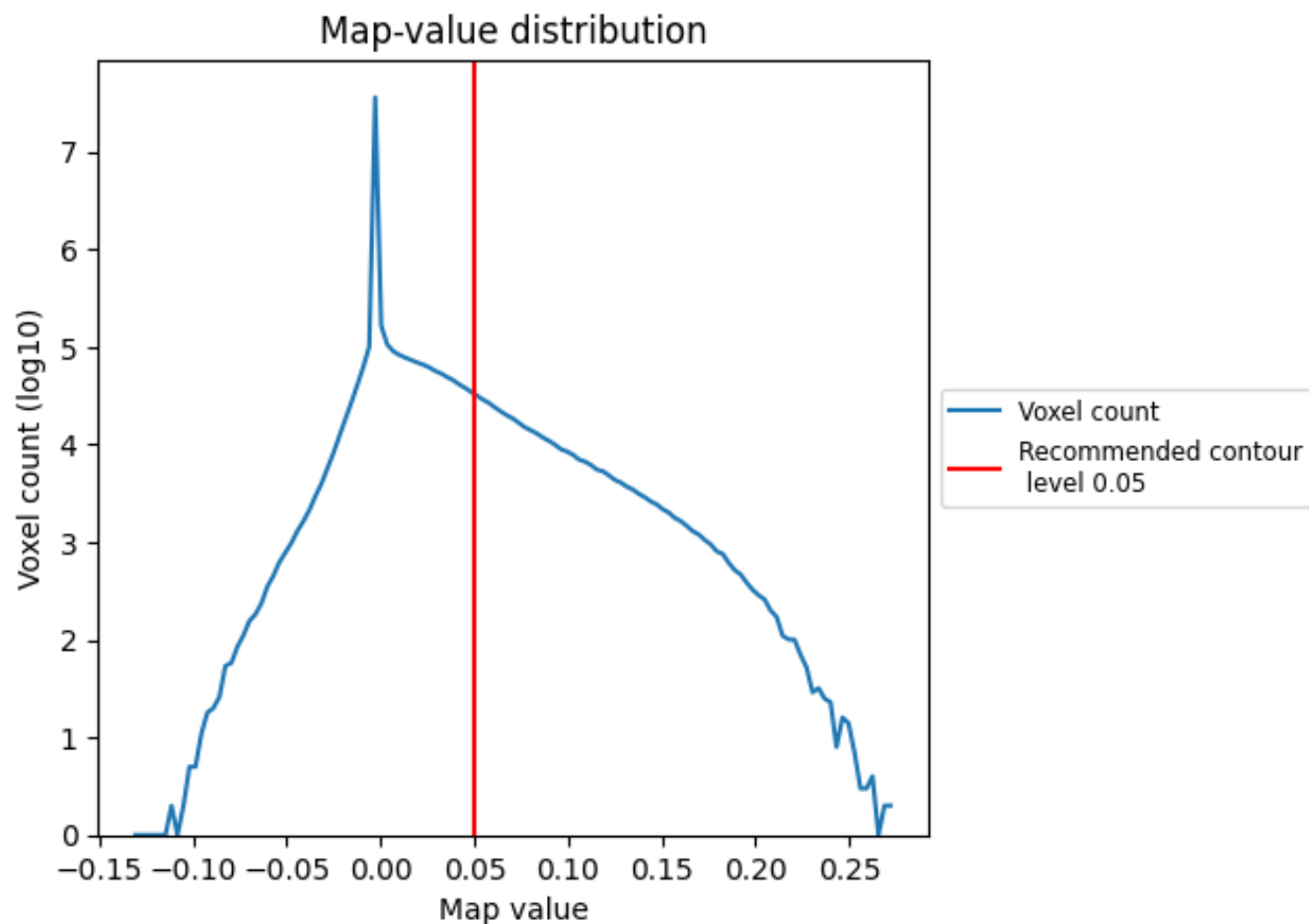
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

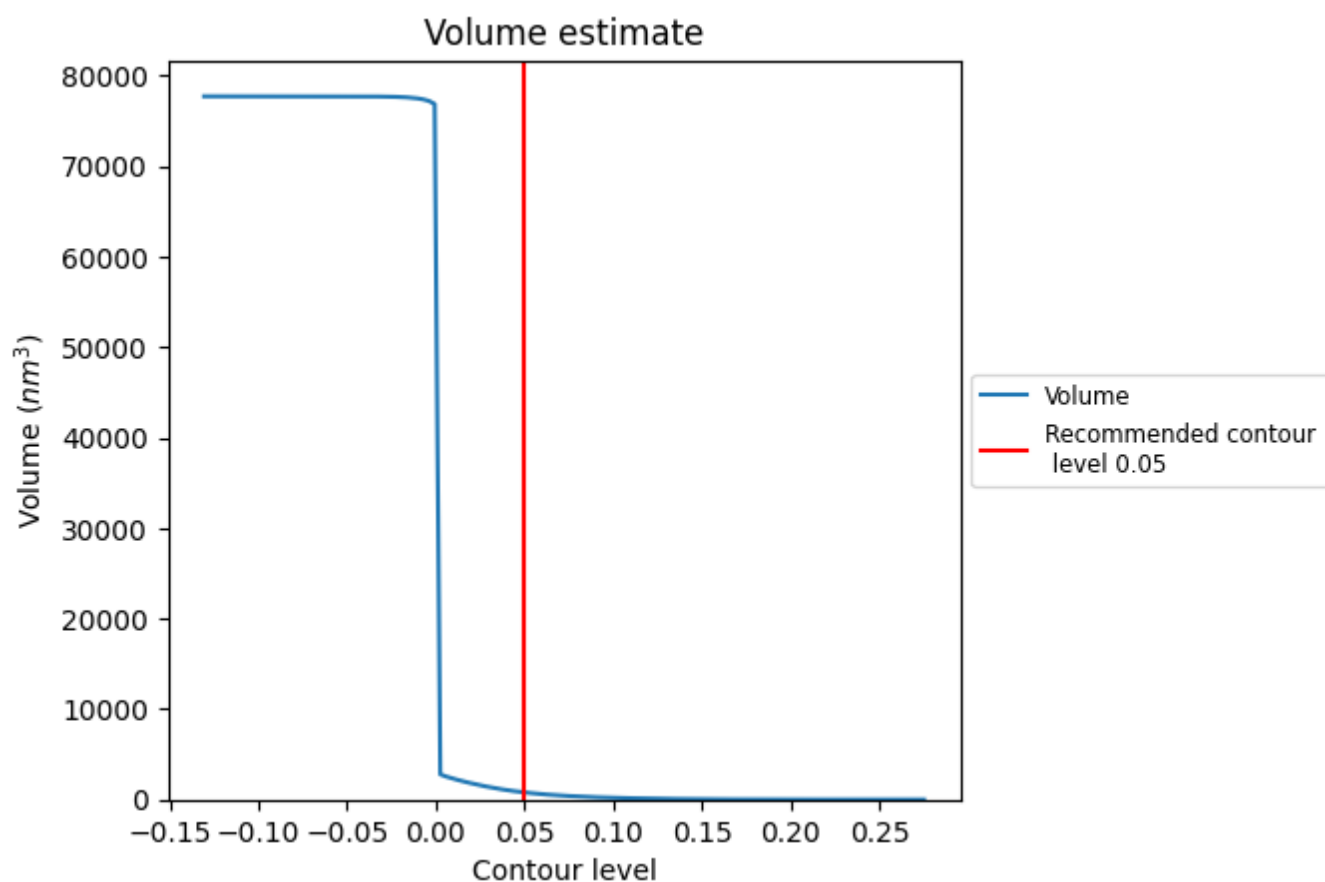
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

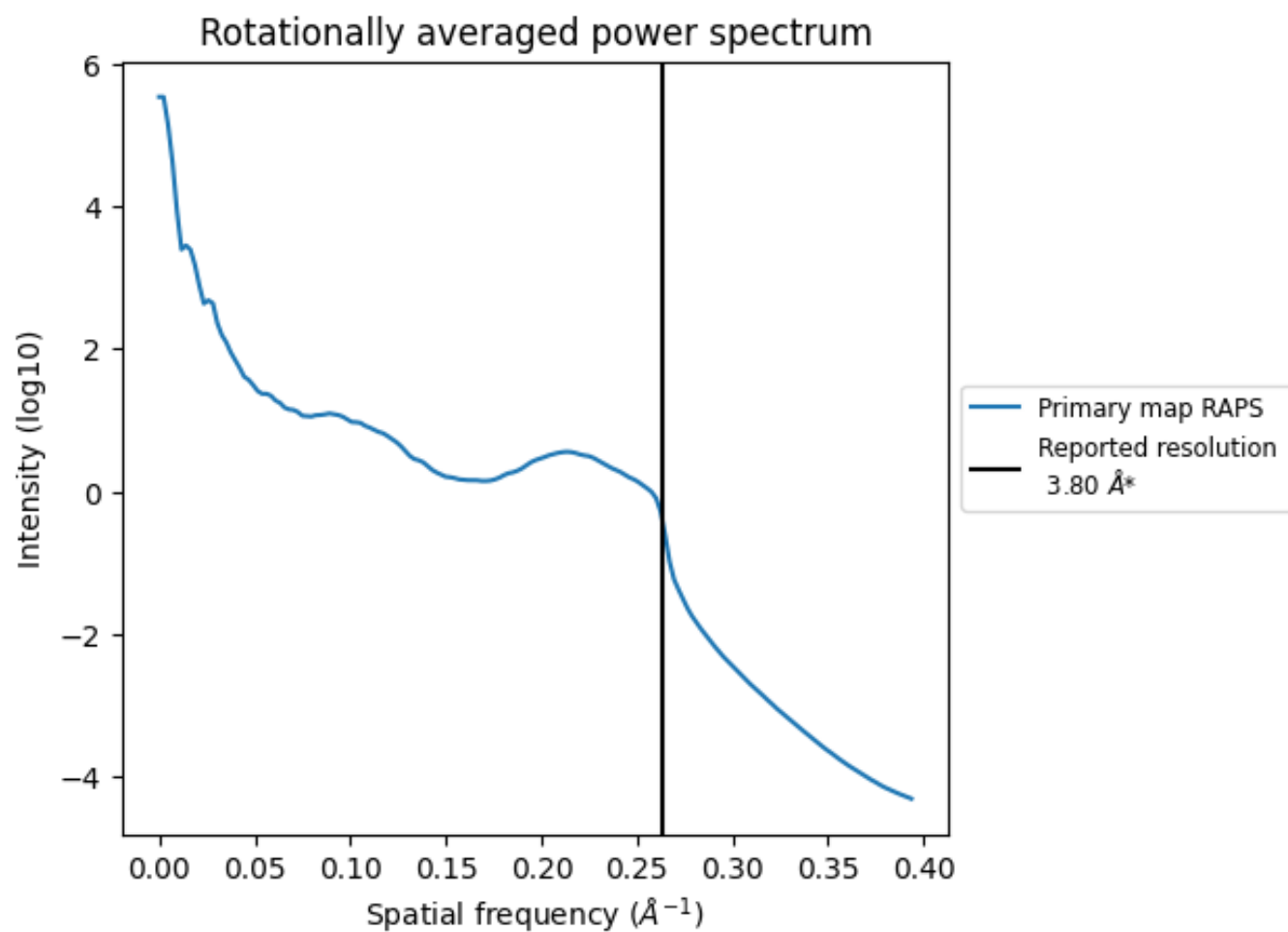
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790 nm³; this corresponds to an approximate mass of 714 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

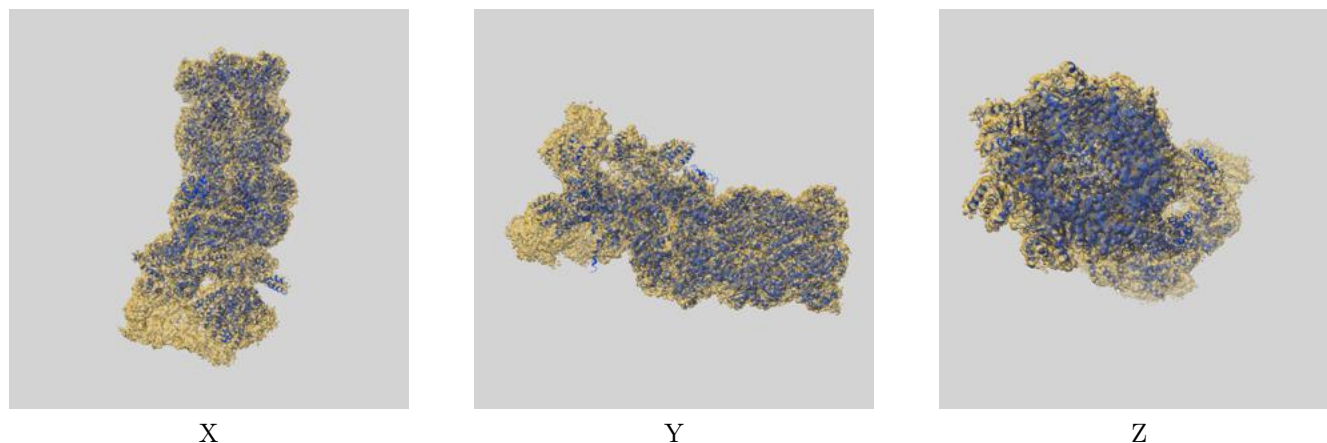
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

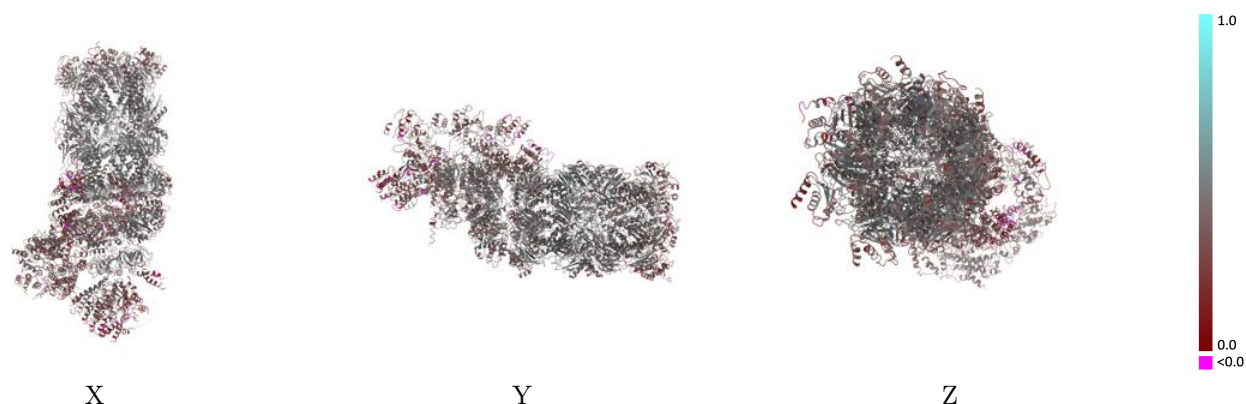
This section contains information regarding the fit between EMDB map EMD-4146 and PDB model 5M32. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



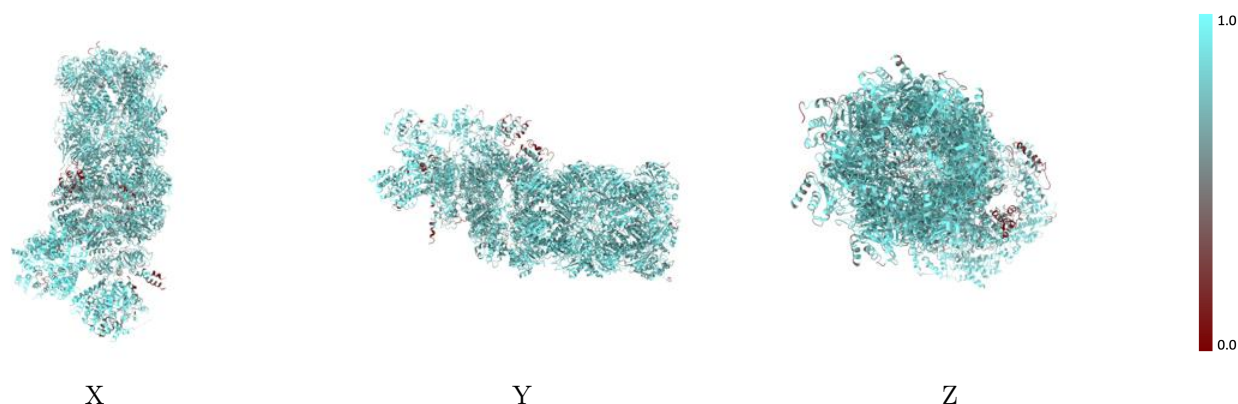
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



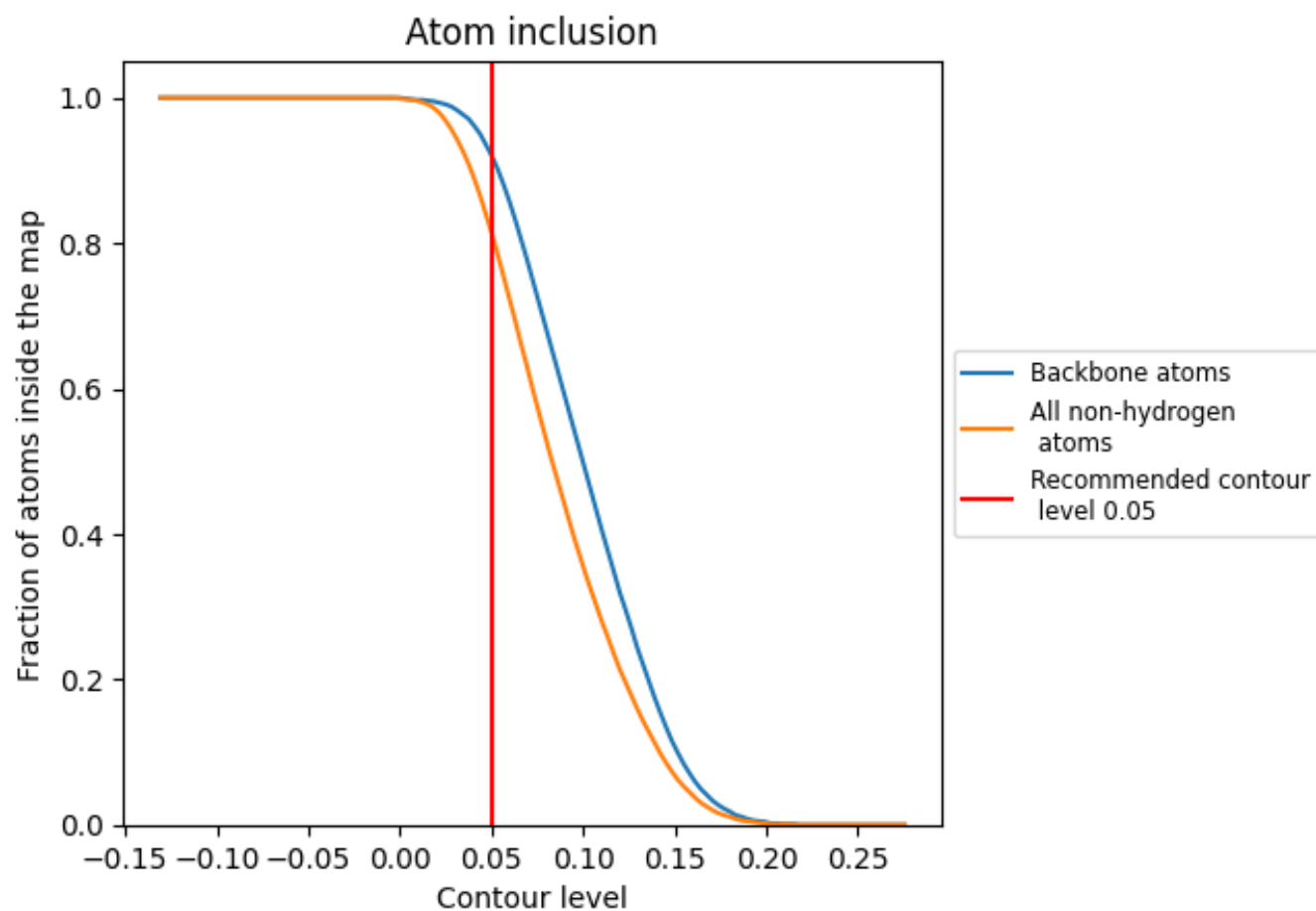
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.4040
A	 0.8360	 0.4360
B	 0.8040	 0.4240
C	 0.8330	 0.4260
D	 0.8190	 0.4310
E	 0.8490	 0.4320
F	 0.8400	 0.4380
G	 0.8200	 0.4210
H	 0.8550	 0.4440
I	 0.8560	 0.4560
J	 0.8730	 0.4530
K	 0.8860	 0.4500
L	 0.8640	 0.4550
M	 0.8650	 0.4590
N	 0.8590	 0.4520
O	 0.8180	 0.3950
P	 0.7780	 0.3820
Q	 0.7960	 0.3800
R	 0.7810	 0.3900
S	 0.8350	 0.4070
T	 0.7960	 0.3880
U	 0.7980	 0.3840
V	 0.8490	 0.4340
W	 0.8460	 0.4430
X	 0.8640	 0.4460
Y	 0.8820	 0.4530
Z	 0.8410	 0.4300
a	 0.8640	 0.4650
b	 0.8390	 0.4450
c	 0.7790	 0.4160
d	 0.7210	 0.3660
e	 0.7750	 0.4090
f	 0.7910	 0.4050
g	 0.7690	 0.4060
h	 0.7600	 0.4060



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Chain	Atom inclusion	Q-score
i	 0.8500	 0.2720
j	 0.8330	 0.2660
k	 0.7490	 0.2950
l	 0.7080	 0.3020
m	 0.8320	 0.3480
n	 0.8300	 0.3410
o	 0.9260	 0.3300
p	 0.7060	 0.2470
q	 0.8220	 0.3410
r	 0.9750	 0.3750
s	 0.8920	 0.3180
t	 0.8650	 0.4950
u	 0.8650	 0.5210