



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:23 AM UTC

PDB ID : 6F1T / pdb_00006f1t
EMDB ID : EMD-4168
Title : Cryo-EM structure of two dynein tail domains bound to dynactin and BICDR1
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-23
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

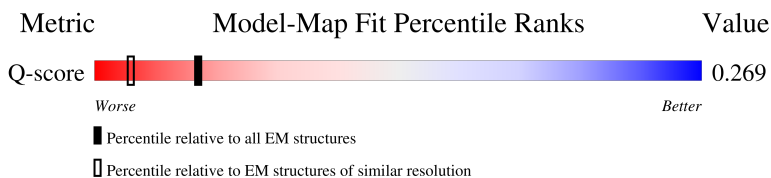
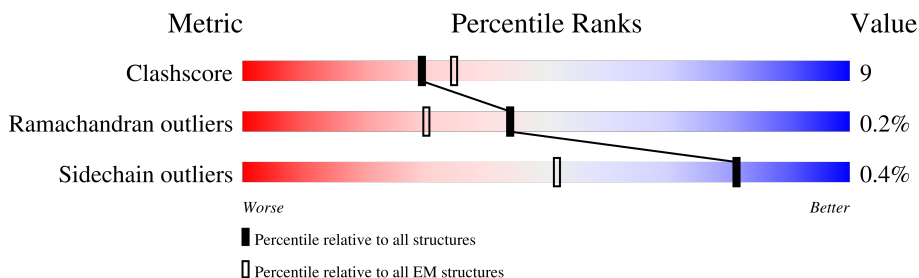
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



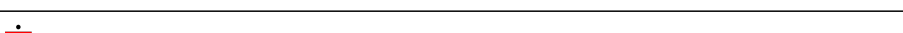
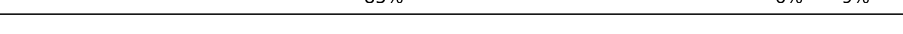
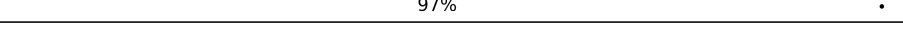
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	376	82% 17% .
1	B	376	76% 22% ..
1	C	376	81% 17% ..
1	D	376	74% 24% .

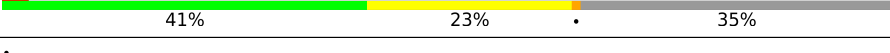
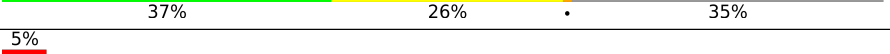
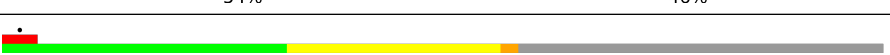
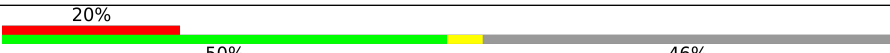
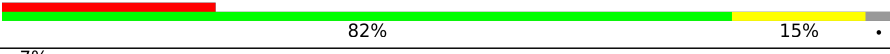
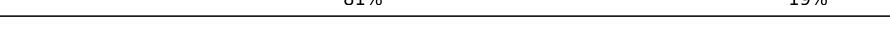
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Mol	Chain	Length	Quality of chain
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	390	
4	K	286	
5	L	272	
6	M	589	
7	N	618	
8	O	65	
8	P	65	
9	Q	87	
9	R	87	
10	U	190	
11	V	182	
12	X	389	
13	Y	263	
14	Z	52	
15	a	66	
16	b	89	
17	c	50	
18	d	26	
19	e	1053	
19	f	1053	

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Mol	Chain	Length	Quality of chain
19	m	1053	
19	n	1053	
20	g	612	
20	h	612	
20	o	612	
20	p	612	
21	i	492	
21	j	492	
21	q	492	
21	r	492	
22	k	96	
22	l	96	
22	s	96	
22	t	96	
23	x	392	
24	z	53	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 92795 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	C	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	G	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	I	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

- Molecule 3 is a protein called Actin related protein 10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	369	Total	C	N	O	S	0	0
			2883	1859	486	522	16		

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	269	Total	C	N	O	S	0	0
			2122	1323	370	418	11		

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	587	Total	C	N	O	0	0
			2935	1761	587	587		

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	616	Total	C	N	O	0	0
			3080	1848	616	616		

- Molecule 8 is a protein called Dynactin Subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	65	Total	C	N	O	0	0
			323	193	65	65		
8	P	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 9 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	87	Total	C	N	O	0	0
			435	261	87	87		
9	R	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	172	Total	C	N	O	0	1
			843	500	171	172		

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	165	Total	C	N	O	0	0
			812	482	165	165		

- Molecule 12 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICDR-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	285	Total	C	N	O	S	0	0
			1715	1028	340	346	1		

- Molecule 13 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	263	Total	C	N	O	0	0
			1315	789	263	263		

- Molecule 14 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Z	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	52	Total	C	N	O	0	0
			405	255	64	86		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 16 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	75	Total	C	N	O	0	0
			585	365	99	121		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 17 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	37	Total	C	N	O	S	0	0
			256	159	42	54	1		

- Molecule 18 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	d	24	Total	C	N	O		0	0
			188	118	29	41			

- Molecule 19 is a protein called Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	926	Total	C	N	O	S	0	0
			5034	3049	982	1000	3		
19	f	929	Total	C	N	O	S	0	0
			6939	4365	1267	1288	19		
19	m	926	Total	C	N	O	S	0	0
			6260	3888	1182	1176	14		
19	n	928	Total	C	N	O	S	0	0
			5730	3518	1099	1104	9		

- Molecule 20 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	g	397	Total	C	N	O		0	0
			1961	1167	397	397			
20	h	400	Total	C	N	O	S	0	0
			3010	1892	532	571	15		
20	o	397	Total	C	N	O	S	0	0
			3126	1969	546	596	15		
20	p	401	Total	C	N	O		0	0
			2116	1273	416	427			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409
o	484	SER	THR	conflict	UNP Q13409
o	499	GLY	ASP	conflict	UNP Q13409
p	484	SER	THR	conflict	UNP Q13409
p	499	GLY	ASP	conflict	UNP Q13409

- Molecule 21 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	268	Total	C	N	O		0	0
			1327	791	268	268			
21	j	288	Total	C	N	O	S	0	0
			2284	1463	379	431	11		
21	q	268	Total	C	N	O		0	0
			1327	791	268	268			
21	r	268	Total	C	N	O		0	0
			1327	791	268	268			

- Molecule 22 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	93	Total	C	N	O		0	0
			462	276	93	93			
22	l	93	Total	C	N	O		0	0
			462	276	93	93			
22	s	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
22	t	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

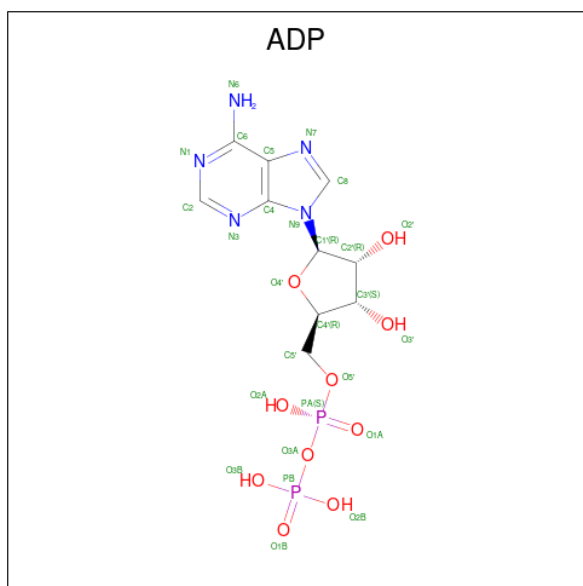
- Molecule 23 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	288	Total	C	N	O	S	0	0
			1695	1018	336	340	1		

- Molecule 24 is a protein called Dynactin Subunit 1.

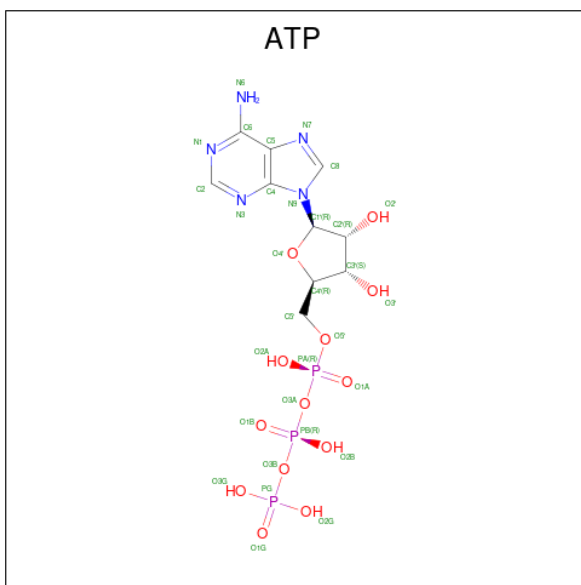
Mol	Chain	Residues	Atoms				AltConf	Trace
24	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 25 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

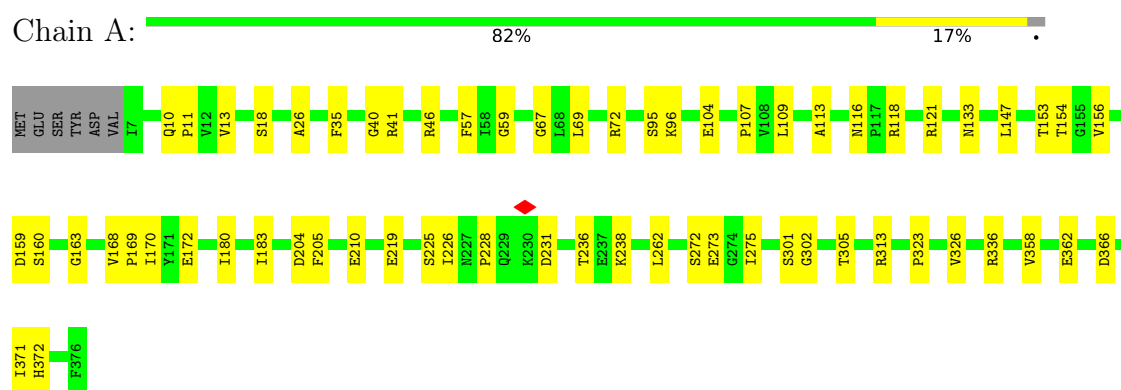


Mol	Chain	Residues	Atoms					AltConf
26	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

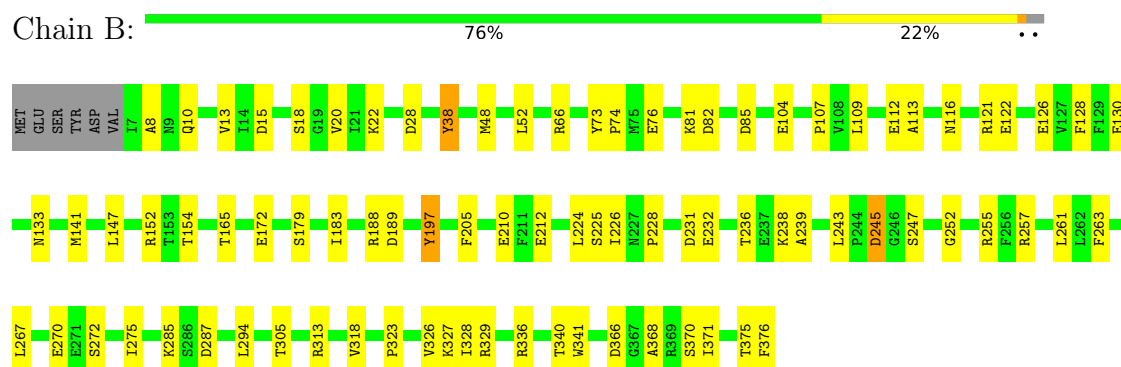
3 Residue-property plots

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.

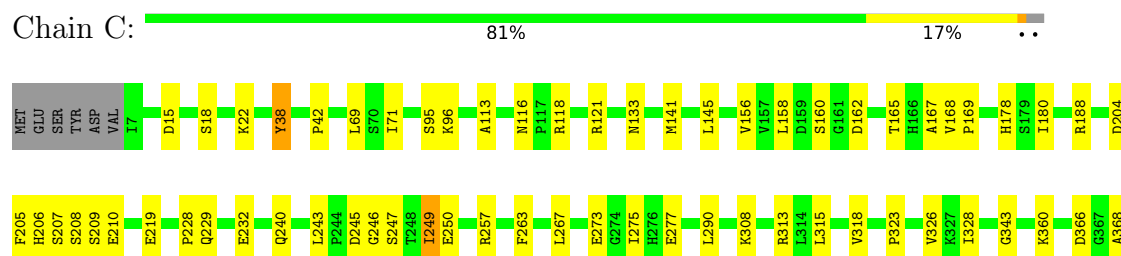
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A



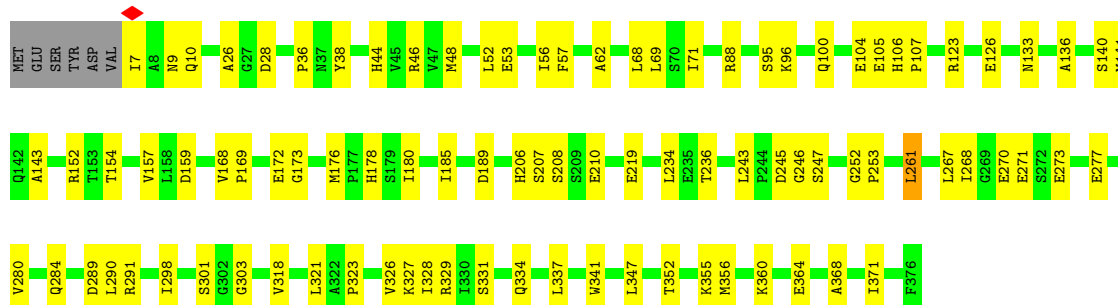
- Molecule 1: ARP1 actin related protein 1 homolog A





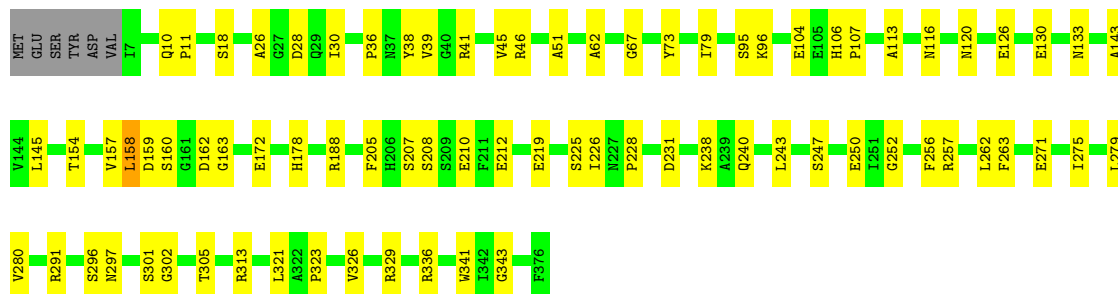
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain D: 74% 24%



- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E: 78% 20%



- Molecule 1: ARP1 actin related protein 1 homolog A

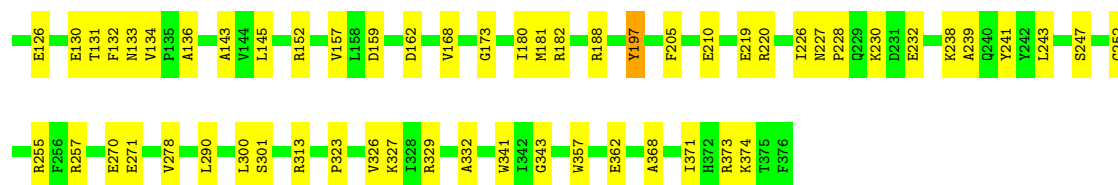
Chain F: 72% 27%



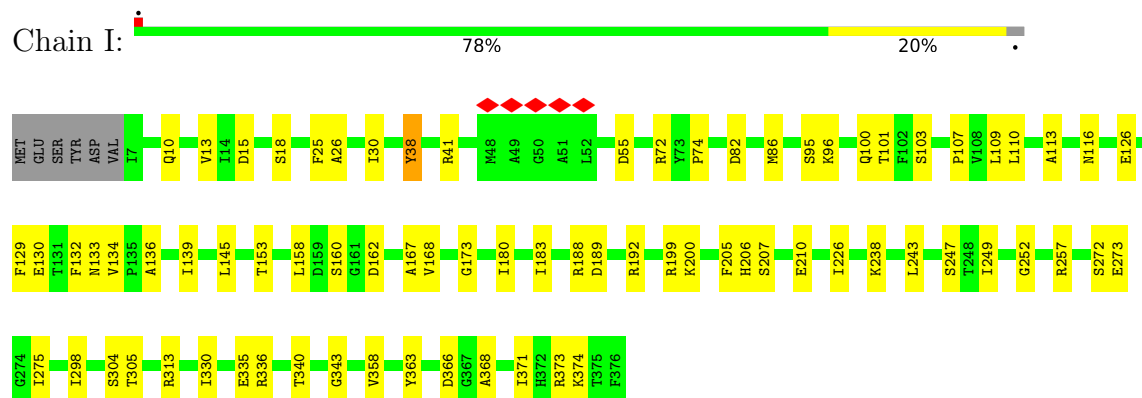
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G: 76% 22%

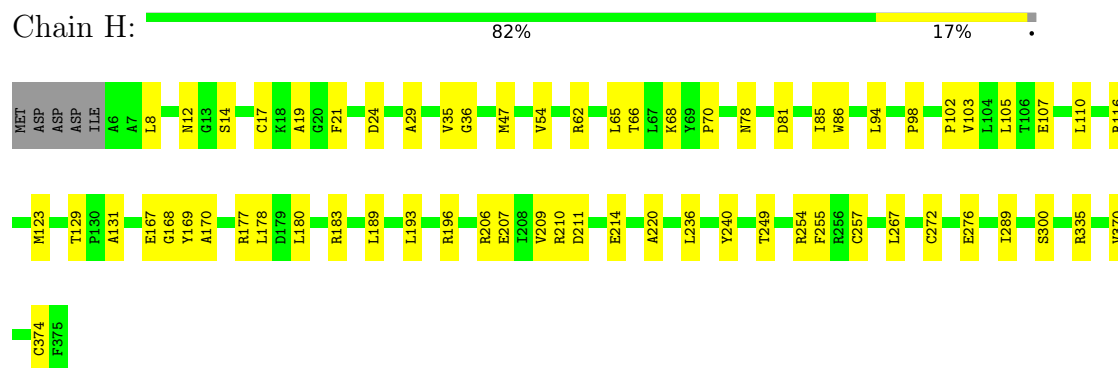




- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 2: Actin, cytoplasmic 1

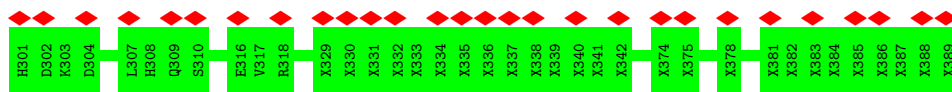


- Molecule 3: Actin related protein 10 homolog



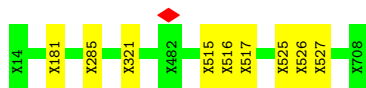
- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1





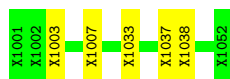
• Molecule 13: Dynactin Subunit 4

Chain Y: 97%



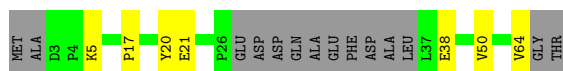
• Molecule 14: Dynactin Subunit 1

Chain Z: 90%



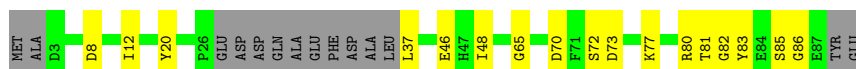
• Molecule 15: Dynactin subunit 2

Chain a: 68%



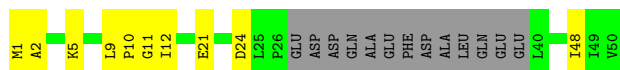
• Molecule 16: Dynactin subunit 2

Chain b: 65%



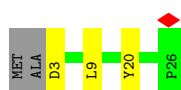
• Molecule 17: Dynactin subunit 2

Chain c: 54%



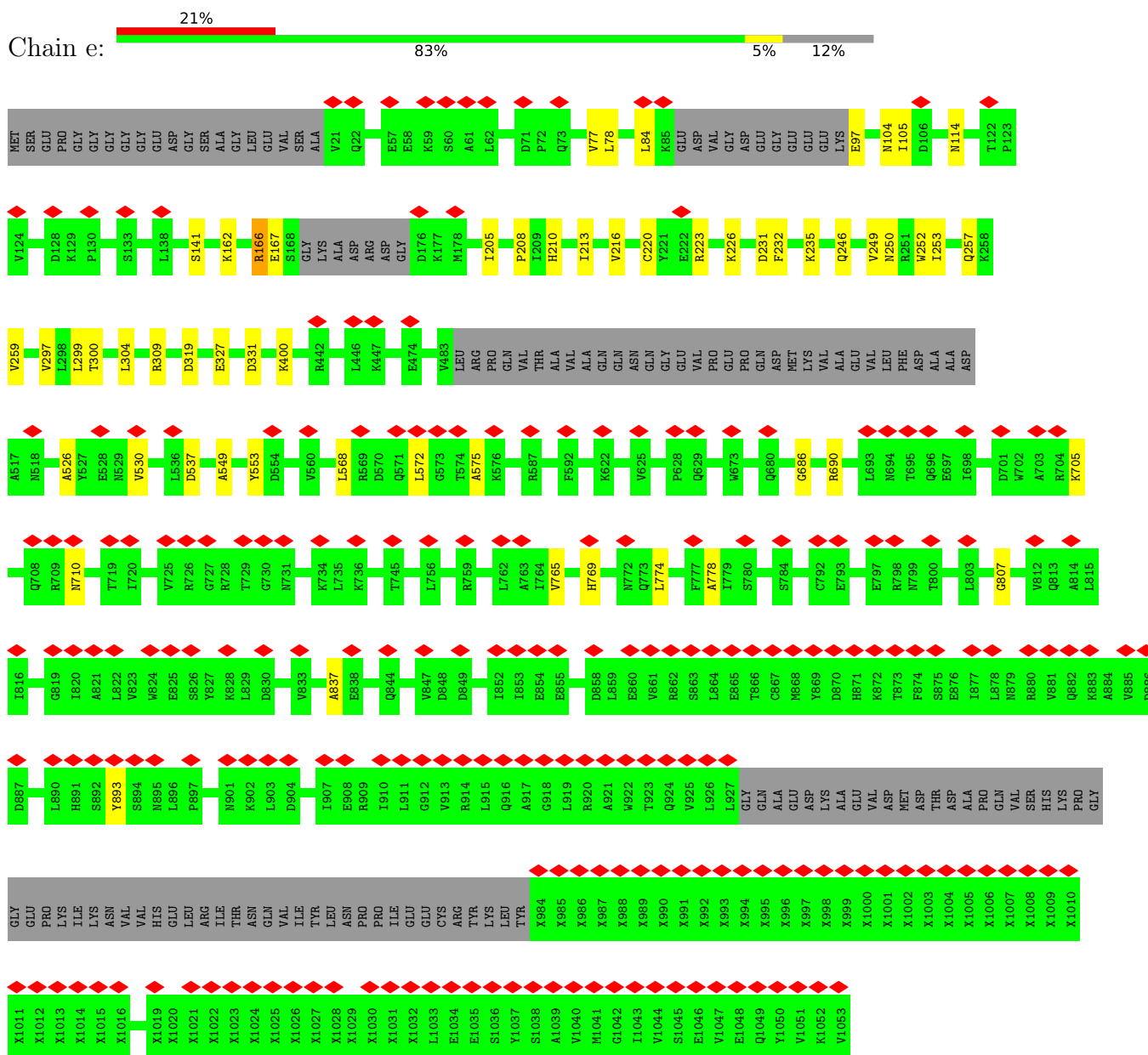
• Molecule 18: Dynactin subunit 2

Chain d: 81%

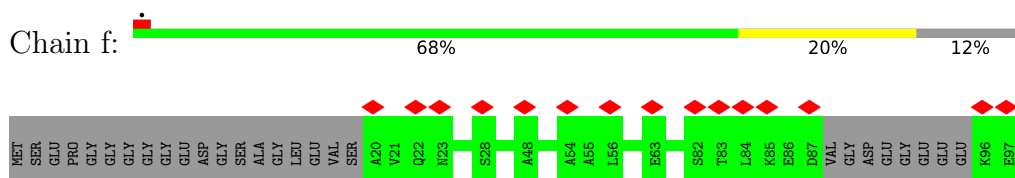


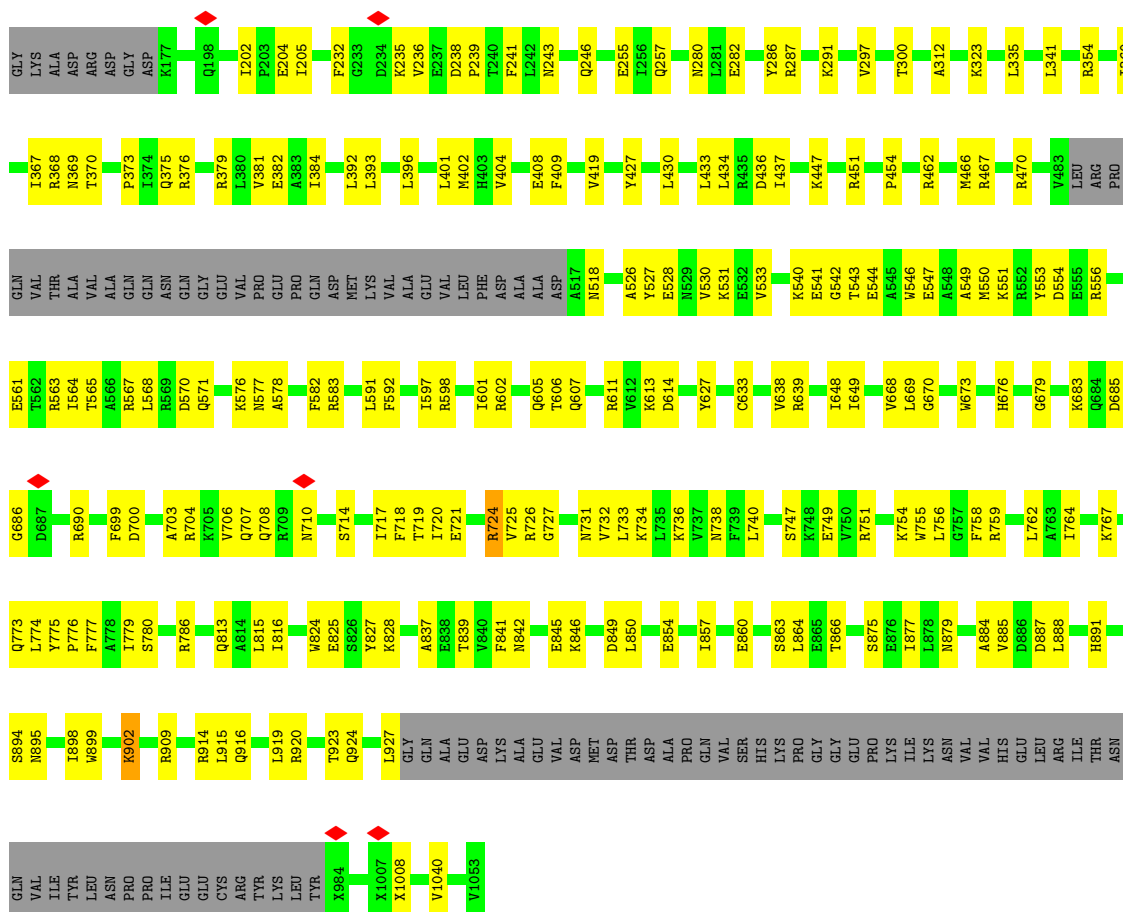
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1

1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

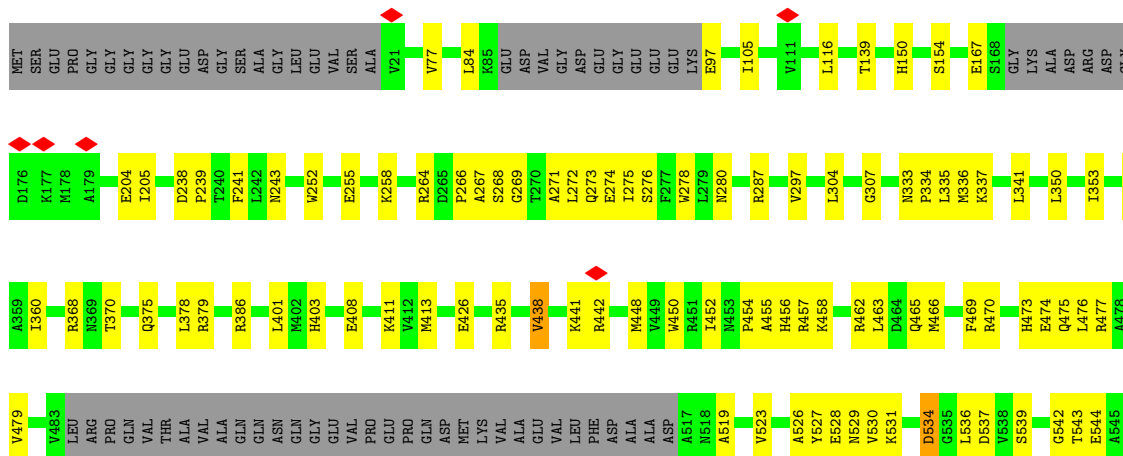


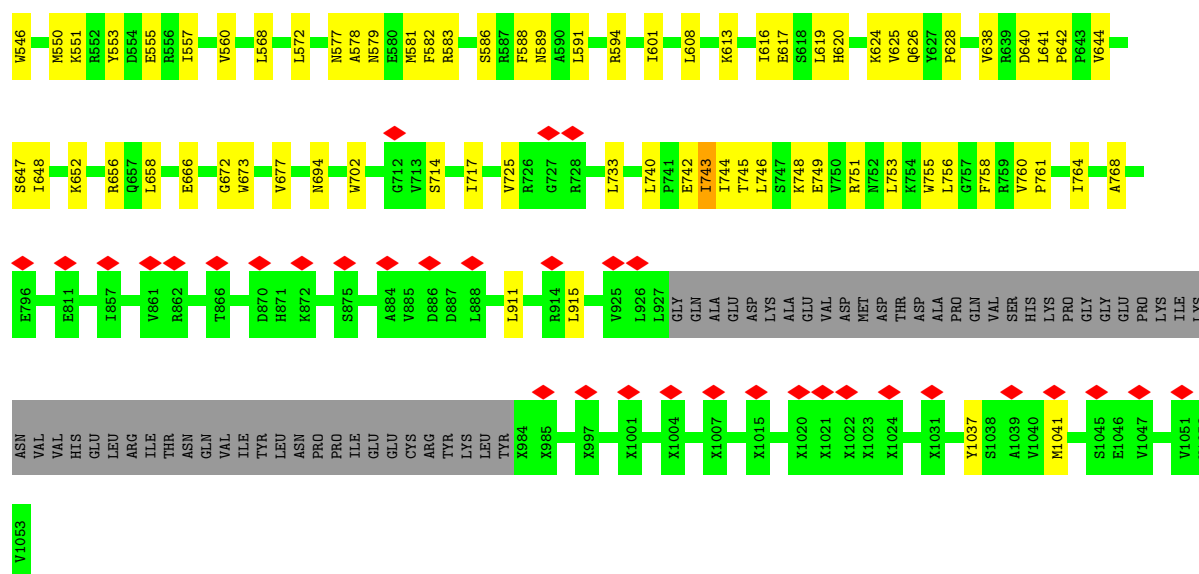
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1



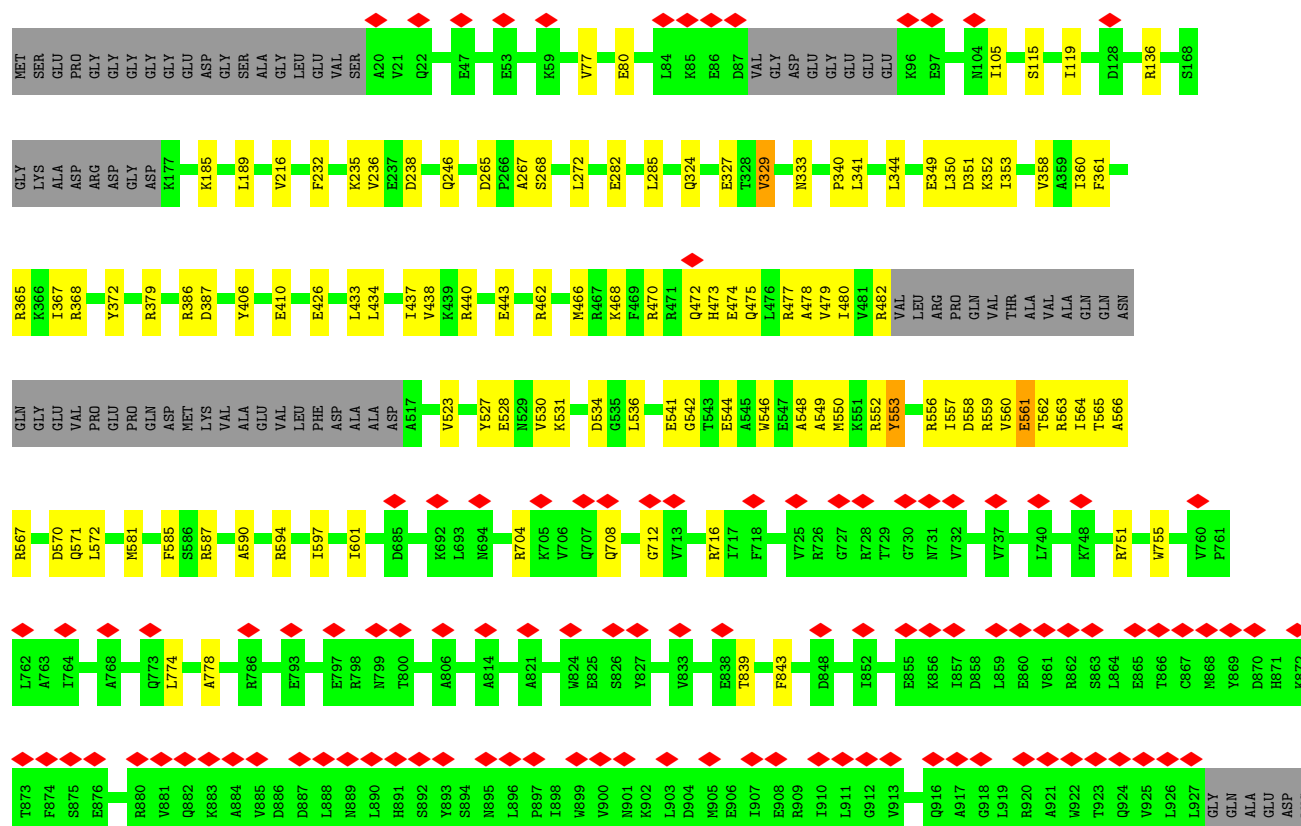
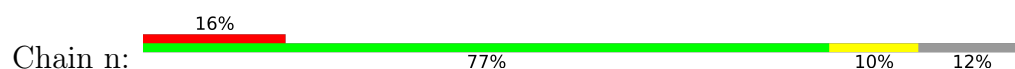


- Molecule 19: Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1, Dynein Heavy Chain, Cytoplasmic dynein 1 heavy chain 1, Cytoplasmic dynein 1 heavy chain 1

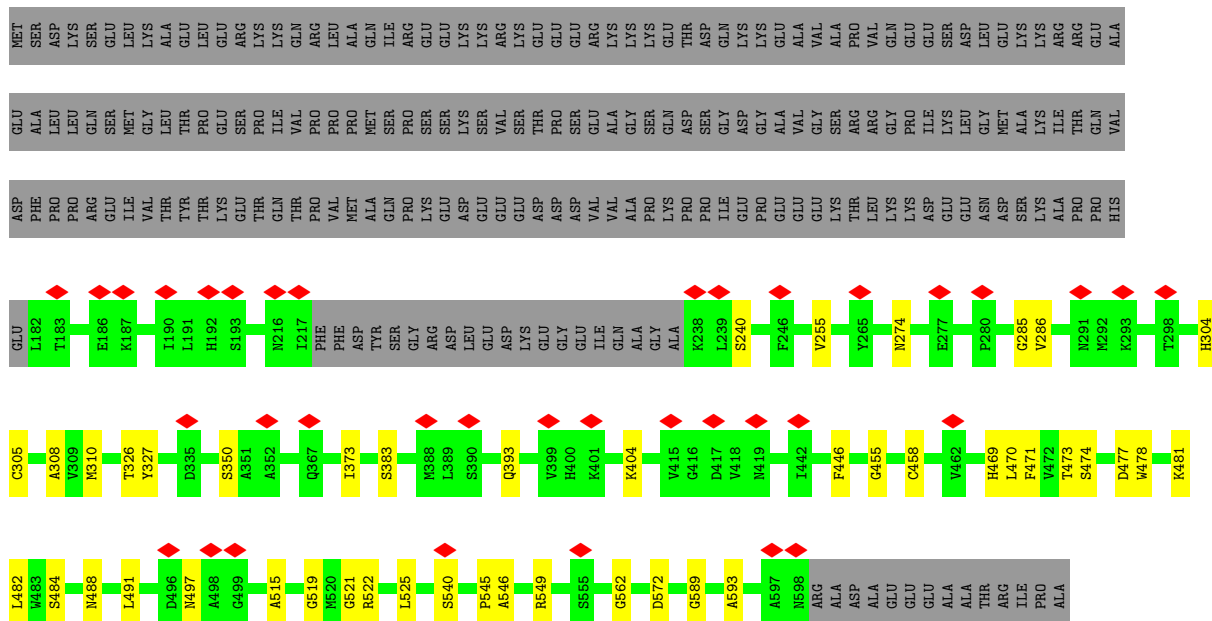




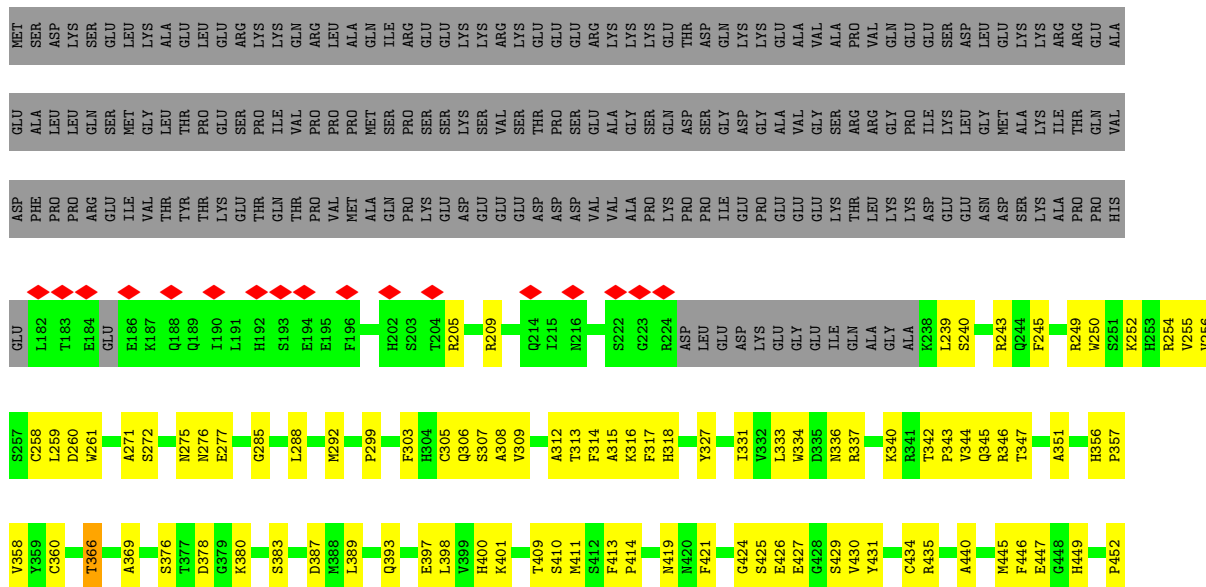
- Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

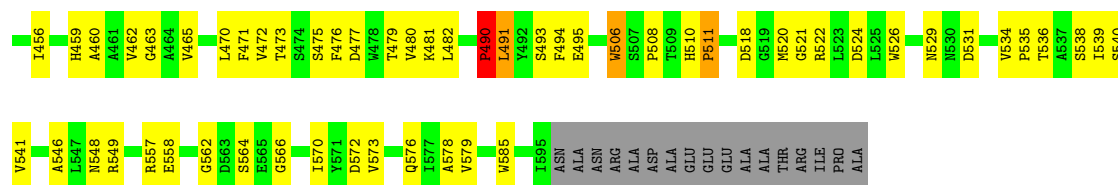


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

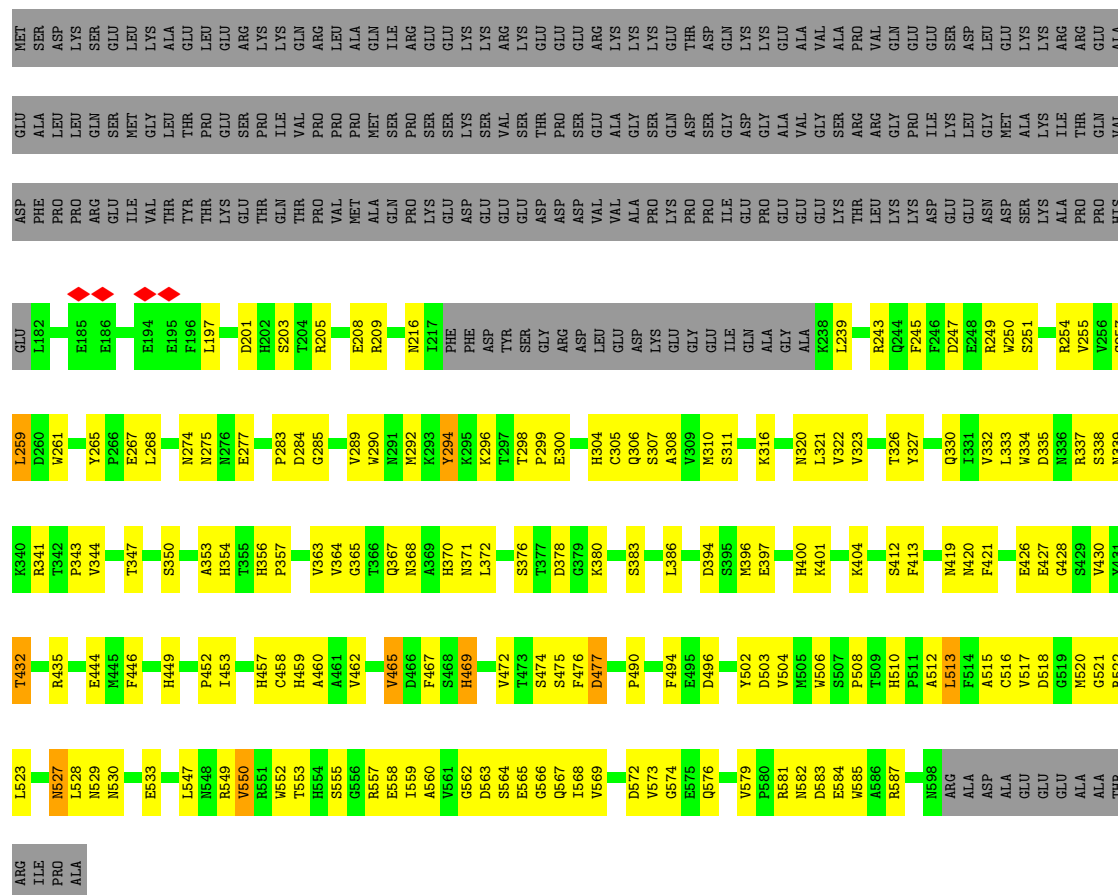


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

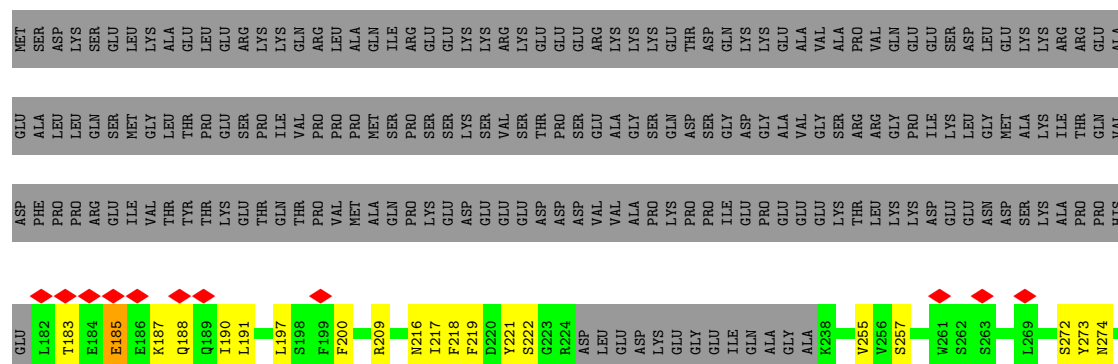


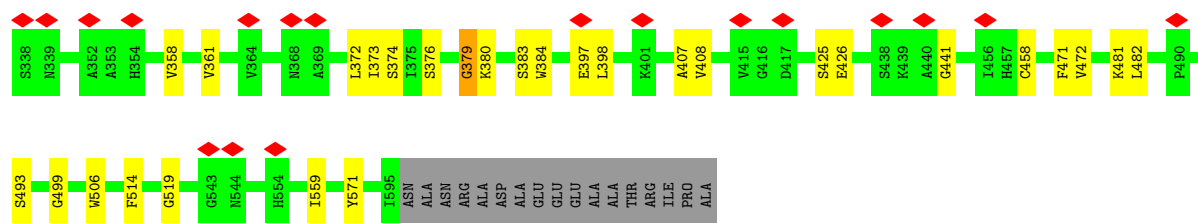


• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

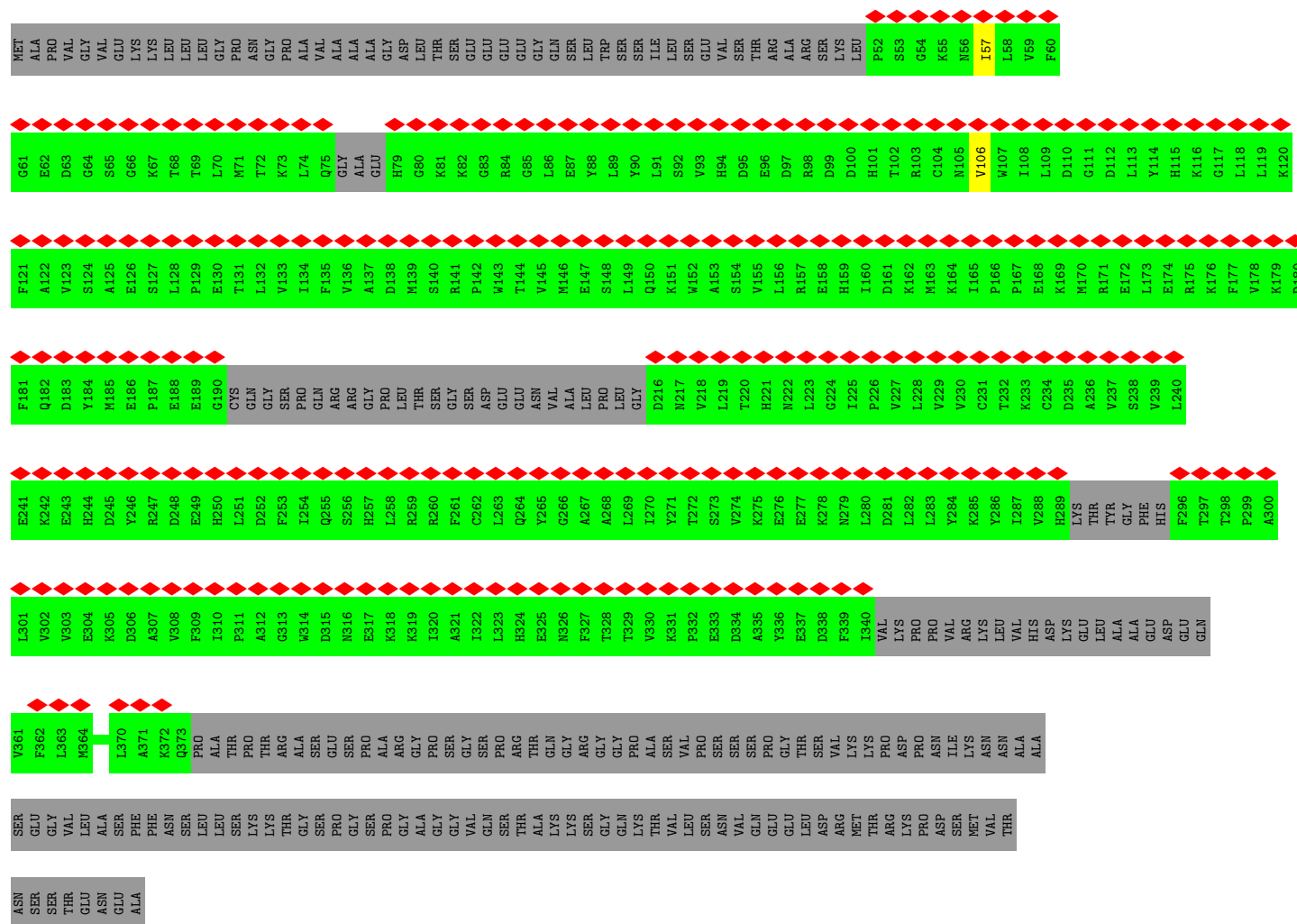


• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

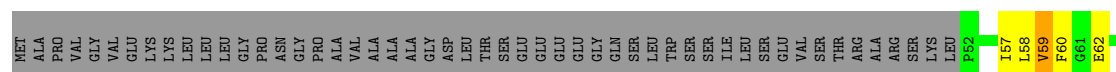
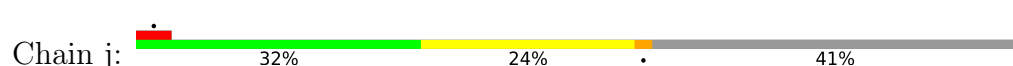


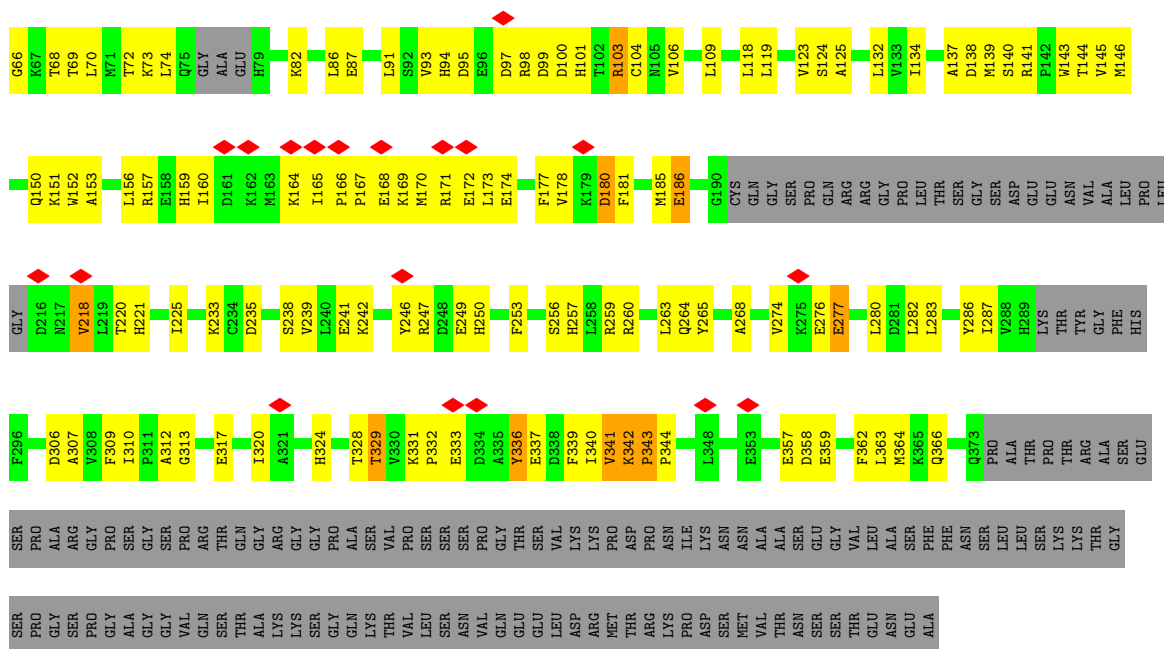


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

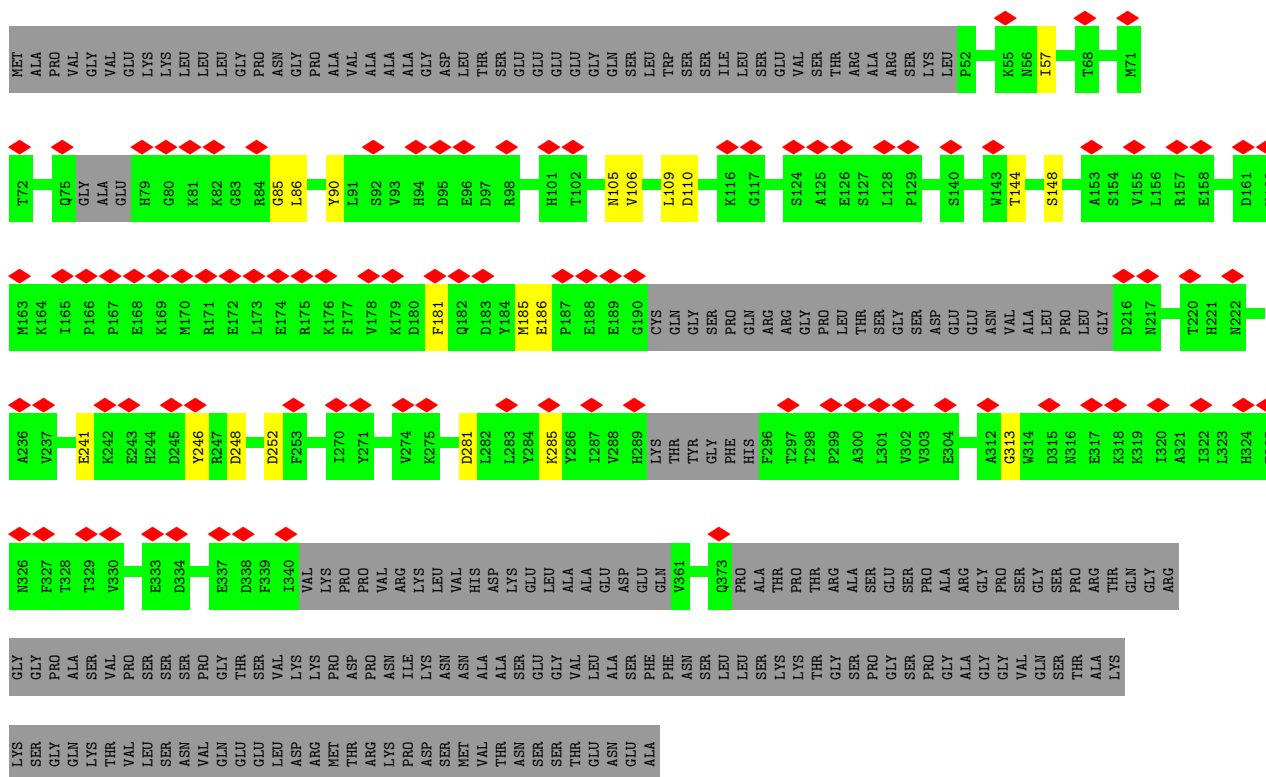


• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2



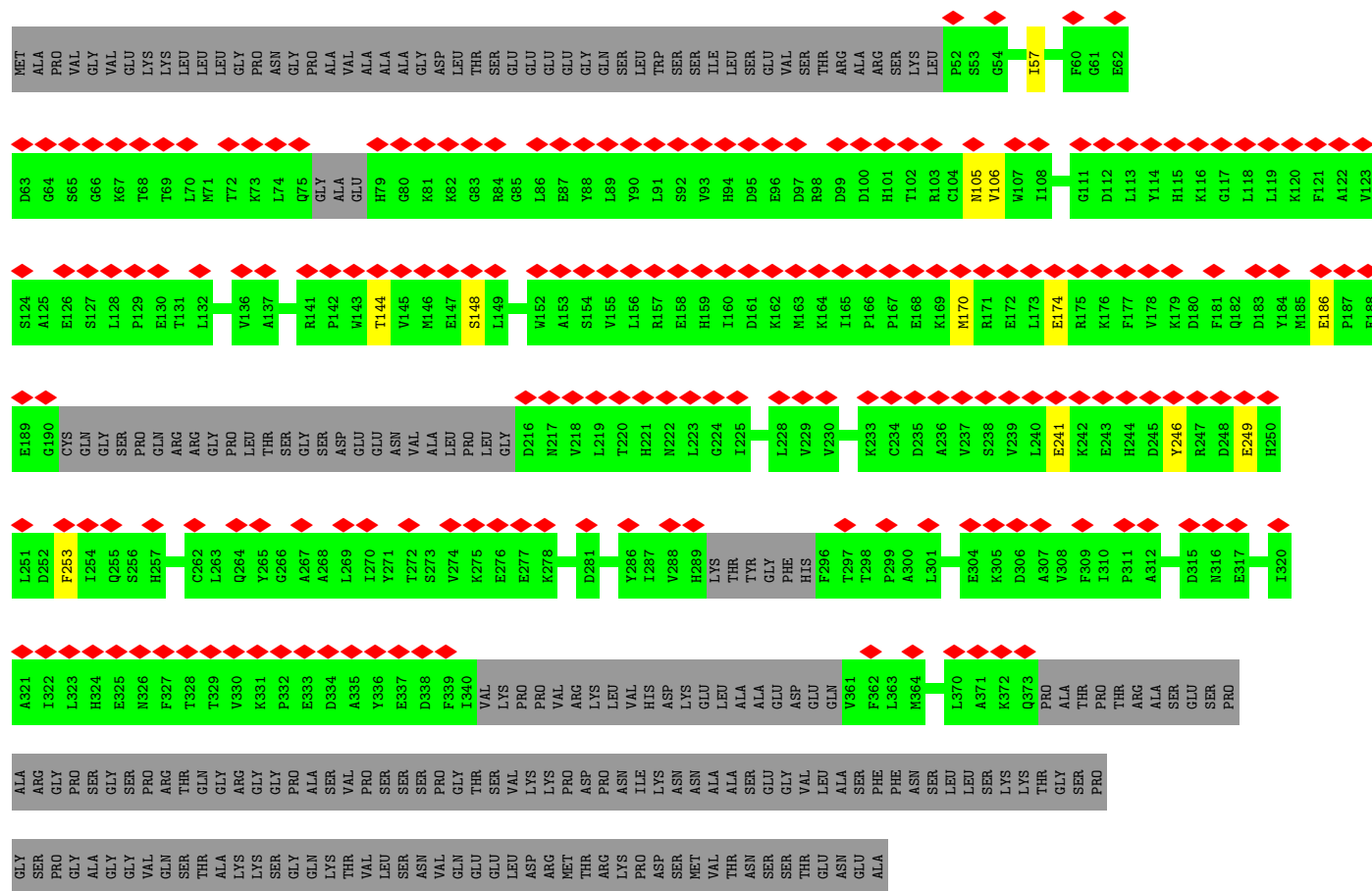


- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

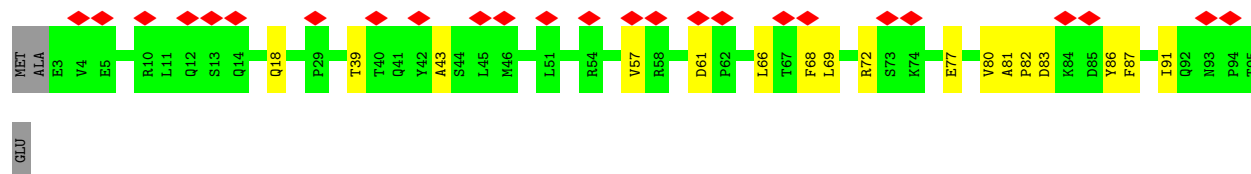
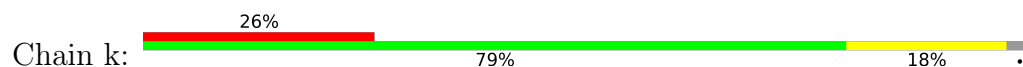


- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

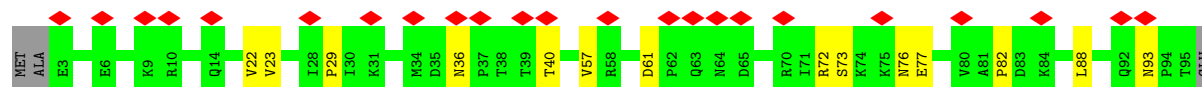
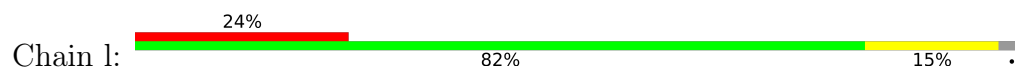




- Molecule 22: Dynein light chain roadblock-type 1

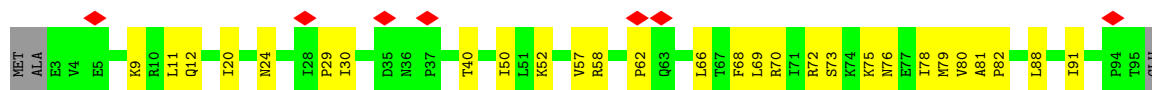


- Molecule 22: Dynein light chain roadblock-type 1

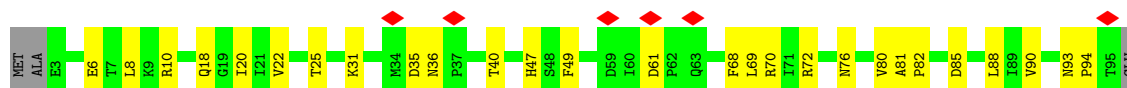


- Molecule 22: Dynein light chain roadblock-type 1

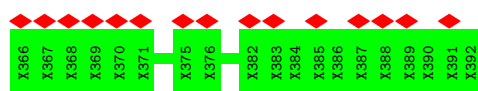
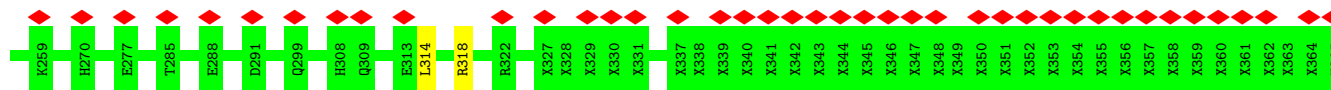
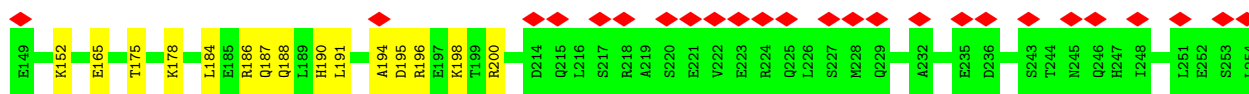
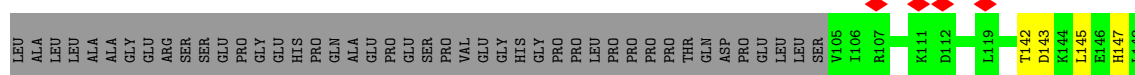
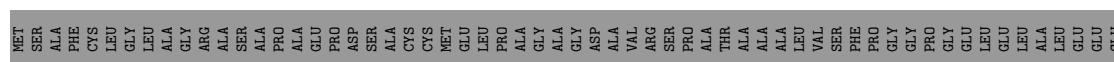




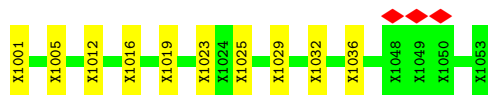
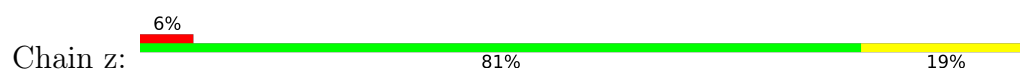
- Molecule 22: Dynein light chain roadblock-type 1



- Molecule 23: BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1



- Molecule 24: Dynactin Subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205611	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.046	Depositor
Map size (Å)	804.0, 804.0, 804.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/3025	0.73	0/4085
1	B	0.82	0/3025	0.89	1/4085 (0.0%)
1	C	0.68	0/3025	0.81	2/4085 (0.0%)
1	D	0.83	0/3025	0.90	0/4085
1	E	0.69	0/3025	0.77	0/4085
1	F	0.86	0/3025	0.97	2/4085 (0.0%)
1	G	0.57	0/3025	0.76	0/4085
1	I	0.26	0/3025	0.68	1/4085 (0.0%)
2	H	0.47	0/2948	0.72	0/3991
3	J	0.28	0/2943	0.73	2/3992 (0.1%)
4	K	0.63	0/2316	0.91	5/3135 (0.2%)
5	L	0.62	0/2156	0.88	2/2906 (0.1%)
10	U	0.43	0/841	0.92	0/1168
11	V	0.35	0/811	0.85	0/1126
12	X	0.40	0/1402	0.79	0/1914
15	a	0.29	0/413	0.71	0/563
16	b	0.38	0/595	0.75	0/803
17	c	0.53	0/260	0.84	0/356
18	d	0.68	0/193	0.84	0/265
19	e	0.33	0/4807	0.85	5/6656 (0.1%)
19	f	0.52	0/6791	0.96	4/9196 (0.0%)
19	m	0.59	0/6087	1.01	14/8287 (0.2%)
19	n	0.41	0/5527	0.92	5/7571 (0.1%)
20	g	0.38	0/1959	0.97	2/2725 (0.1%)
20	h	0.63	0/3087	1.02	8/4213 (0.2%)
20	o	0.73	0/3209	1.19	8/4369 (0.2%)
20	p	0.32	0/2121	0.96	3/2933 (0.1%)
21	i	0.27	0/1322	0.74	0/1835
21	j	0.60	2/2333 (0.1%)	1.36	19/3157 (0.6%)
21	q	0.31	0/1322	0.90	0/1835
21	r	0.30	0/1322	0.89	1/1835 (0.1%)
22	k	0.33	0/461	1.11	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	l	0.35	0/461	0.87	0/642
22	s	0.22	0/752	0.53	0/1017
22	t	0.21	0/752	0.54	0/1017
23	x	0.41	0/1367	0.83	0/1870
All	All	0.55	2/82758 (0.0%)	0.90	84/112699 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
14	Z	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	343	PRO	CA-C	6.09	1.57	1.52
21	j	342	LYS	CA-C	5.74	1.60	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	j	342	LYS	CA-C-N	-13.40	106.58	120.38
21	j	342	LYS	C-N-CA	-13.40	106.58	120.38
20	p	188	GLN	N-CA-C	9.05	121.15	111.28
21	j	343	PRO	CA-C-N	-8.22	109.56	119.84
21	j	343	PRO	C-N-CA	-8.22	109.56	119.84
19	m	672	GLY	N-CA-C	-7.72	94.88	113.18
20	p	183	THR	N-CA-C	7.57	119.17	111.07
19	n	553	TYR	CA-CB-CG	-7.47	100.46	113.90
19	m	640	ASP	N-CA-C	7.34	119.50	110.91
4	K	182	THR	N-CA-C	-7.22	93.07	108.66
20	o	294	TYR	CA-CB-CG	-7.06	101.20	113.90
20	o	490	PRO	N-CA-C	-7.04	97.98	112.47
19	m	740	LEU	N-CA-C	7.00	125.29	109.81
21	j	144	THR	CA-C-N	6.78	129.65	120.77
21	j	144	THR	C-N-CA	6.78	129.65	120.77
21	j	186	GLU	N-CA-C	6.76	124.75	109.81
20	o	527	ASN	N-CA-C	-6.59	100.70	110.46
20	o	513	LEU	CA-CB-CG	6.55	139.24	116.30
1	F	336	ARG	CB-CG-CD	-6.54	96.26	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	TYR	CA-CB-CG	6.46	125.52	113.90
19	m	167	GLU	N-CA-C	-6.42	97.13	110.80
19	n	480	ILE	CA-C-N	6.20	129.28	120.53
19	n	480	ILE	C-N-CA	6.20	129.28	120.53
21	j	277	GLU	CA-CB-CG	-6.14	101.83	114.10
19	f	891	HIS	N-CA-C	-6.05	96.98	108.17
1	C	38	TYR	CA-CB-CG	6.01	124.71	113.90
19	m	694	ASN	CA-C-N	5.92	142.44	122.20
19	m	694	ASN	C-N-CA	5.92	142.44	122.20
21	j	343	PRO	N-CA-C	5.91	117.91	110.70
20	g	477	ASP	CA-C-N	5.90	132.81	121.54
20	g	477	ASP	C-N-CA	5.90	132.81	121.54
21	j	277	GLU	N-CA-C	5.89	118.38	111.02
19	m	601	ILE	CG1-CB-CG2	-5.89	93.04	110.70
1	C	246	GLY	N-CA-C	-5.81	106.97	115.63
4	K	183	PRO	N-CA-C	5.80	117.78	110.70
20	h	490	PRO	CA-C-N	5.80	132.62	121.54
20	h	490	PRO	C-N-CA	5.80	132.62	121.54
21	r	186	GLU	N-CA-C	5.78	122.58	109.81
21	j	225	ILE	N-CA-C	-5.72	96.52	108.88
19	m	717	ILE	N-CA-C	-5.63	107.63	113.10
19	m	536	LEU	CA-C-N	5.55	132.14	121.54
19	m	536	LEU	C-N-CA	5.55	132.14	121.54
19	m	625	VAL	N-CA-C	-5.54	101.67	109.21
20	o	259	LEU	CA-CB-CG	5.50	135.57	116.30
19	n	536	LEU	CA-C-N	5.50	132.04	121.54
19	n	536	LEU	C-N-CA	5.50	132.04	121.54
19	f	902	LYS	CA-CB-CG	-5.49	103.12	114.10
19	m	528	GLU	CA-CB-CG	-5.47	103.15	114.10
20	o	432	THR	N-CA-C	-5.40	101.09	109.72
21	j	180	ASP	CA-C-N	5.38	128.89	120.82
21	j	180	ASP	C-N-CA	5.38	128.89	120.82
19	e	167	GLU	N-CA-C	-5.37	99.37	110.80
20	p	379	GLY	N-CA-C	-5.33	105.70	114.76
5	L	123	ASP	CA-C-N	5.32	131.70	121.54
5	L	123	ASP	C-N-CA	5.32	131.70	121.54
1	I	38	TYR	CA-CB-CG	5.32	123.47	113.90
1	F	227	ASN	N-CA-C	-5.30	97.67	108.12
21	j	336	TYR	N-CA-C	-5.28	105.64	111.71
20	h	557	ARG	CA-C-N	5.20	133.27	122.41
20	h	557	ARG	C-N-CA	5.20	133.27	122.41
20	o	477	ASP	CA-C-N	5.19	134.05	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	o	477	ASP	C-N-CA	5.19	134.05	124.82
19	f	724	ARG	CA-C-N	5.18	129.88	121.95
19	f	724	ARG	C-N-CA	5.18	129.88	121.95
20	h	463	GLY	N-CA-C	-5.15	100.97	113.18
19	e	400	LYS	CA-C-N	5.14	131.36	121.54
19	e	400	LYS	C-N-CA	5.14	131.36	121.54
21	j	97	ASP	CA-C-N	5.14	131.36	122.32
21	j	97	ASP	C-N-CA	5.14	131.36	122.32
21	j	306	ASP	N-CA-C	-5.11	107.01	114.12
4	K	148	ILE	CA-C-N	5.11	131.30	121.54
4	K	148	ILE	C-N-CA	5.11	131.30	121.54
3	J	126	MET	CA-CB-CG	-5.10	103.91	114.10
20	h	506	TRP	CA-CB-CG	5.09	123.28	113.60
19	e	166	ARG	CA-C-N	5.08	131.25	121.54
19	e	166	ARG	C-N-CA	5.08	131.25	121.54
4	K	83	GLY	N-CA-C	5.08	125.21	113.18
3	J	243	PRO	N-CA-C	5.06	116.88	110.70
21	j	342	LYS	CA-C-O	-5.06	113.22	120.16
20	h	366	THR	CA-C-N	5.03	128.36	120.82
20	h	366	THR	C-N-CA	5.03	128.36	120.82
19	m	534	ASP	CA-C-N	5.02	131.25	121.41
19	m	534	ASP	C-N-CA	5.02	131.25	121.41
21	j	329	THR	N-CA-C	-5.02	100.12	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Z	1038	UNK	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	2956	0	2947	38	0
1	B	2956	0	2950	56	0
1	C	2956	0	2950	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2956	0	2950	60	0
1	E	2956	0	2950	52	0
1	F	2956	0	2948	72	0
1	G	2956	0	2947	61	0
1	I	2956	0	2950	50	0
2	H	2885	0	2856	39	0
3	J	2883	0	2972	46	0
4	K	2264	0	2186	80	0
5	L	2122	0	2113	60	0
6	M	2935	0	599	7	0
7	N	3080	0	633	11	0
8	O	323	0	73	7	0
8	P	323	0	74	8	0
9	Q	435	0	93	11	0
9	R	435	0	93	2	0
10	U	843	0	376	5	0
11	V	812	0	344	4	0
12	X	1715	0	1026	14	0
13	Y	1315	0	344	5	0
14	Z	260	0	55	2	0
15	a	405	0	378	5	0
16	b	585	0	565	15	0
17	c	256	0	210	8	0
18	d	188	0	172	4	0
19	e	5034	0	2812	32	0
19	f	6939	0	6419	144	0
19	m	6260	0	5110	109	0
19	n	5730	0	4114	89	0
20	g	1961	0	883	22	0
20	h	3010	0	2751	103	0
20	o	3126	0	2973	144	0
20	p	2116	0	1120	40	0
21	i	1327	0	574	1	0
21	j	2284	0	2207	102	0
21	q	1327	0	574	10	0
21	r	1327	0	574	6	0
22	k	462	0	192	9	0
22	l	462	0	192	7	0
22	s	742	0	768	30	0
22	t	742	0	768	27	0
23	x	1695	0	968	15	0
24	z	265	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	27	0	11	2	0
25	B	27	0	12	0	0
25	C	27	0	12	2	0
25	D	27	0	12	2	0
25	E	27	0	12	2	0
25	F	27	0	11	3	0
25	G	27	0	12	3	0
25	I	27	0	12	0	0
25	J	27	0	11	1	0
26	H	31	0	12	1	0
All	All	92795	0	71926	1515	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 9.

All (1515) 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)
19:n:557:ILE:O	19:n:561:GLU:HG3	1.33	1.25
19:n:556:ARG:O	19:n:560:VAL:HG23	1.30	1.24
19:n:556:ARG:O	19:n:560:VAL:CG2	1.93	1.16
19:m:530:VAL:O	19:m:534:ASP:HB2	1.57	1.05
19:n:559:ARG:HA	19:n:562:THR:OG1	1.55	1.04
19:m:542:GLY:O	19:m:546:TRP:HB3	1.58	1.03
21:j:253:PHE:CE1	21:j:257:HIS:CE1	2.51	0.98
20:o:249:ARG:NH1	22:t:6:GLU:OE2	1.98	0.96
4:K:46:LEU:O	4:K:50:ALA:HB3	1.69	0.92
19:n:542:GLY:O	19:n:546:TRP:HB3	1.72	0.89
19:n:557:ILE:O	19:n:561:GLU:CG	2.20	0.89
21:j:253:PHE:HE2	21:j:339:PHE:CE1	1.90	0.89
8:O:64:UNK:HA	8:O:76:UNK:O	1.71	0.89
1:G:36:PRO:HB2	1:G:38:TYR:CE1	2.07	0.89
20:o:249:ARG:CZ	22:t:6:GLU:OE2	2.22	0.88
4:K:43:ASP:O	4:K:47:ARG:HB2	1.73	0.88
20:o:208:GLU:O	20:o:294:TYR:OH	1.92	0.88
20:h:522:ARG:NH1	20:h:524:ASP:OD2	2.07	0.87
1:D:206:HIS:N	1:D:210:GLU:OE2	2.08	0.86
20:o:337:ARG:NH1	20:p:221:TYR:O	2.09	0.86
5:L:264:GLU:O	5:L:268:ARG:HB2	1.76	0.85
20:o:243:ARG:HH12	20:o:292:MET:HA	1.43	0.84
19:n:557:ILE:C	19:n:561:GLU:HG3	2.02	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:33:UNK:HA	8:O:77:UNK:O	1.80	0.81
19:f:239:PRO:O	19:f:243:ASN:HB2	1.82	0.80
19:f:543:THR:O	19:f:547:GLU:HB3	1.82	0.79
20:o:205:ARG:HH11	20:p:218:PHE:HB3	1.48	0.79
20:o:298:THR:CB	22:t:10:ARG:HH11	1.96	0.79
2:H:107:GLU:OE2	2:H:116:ARG:NE	2.16	0.77
20:h:526:TRP:HB3	20:h:536:THR:H	1.50	0.77
1:D:152:ARG:HH22	1:D:329:ARG:HH12	1.34	0.75
20:o:208:GLU:CD	20:o:296:LYS:NZ	2.45	0.75
1:D:38:TYR:OH	1:D:62:ALA:O	2.03	0.75
19:m:462:ARG:HE	19:m:537:ASP:HB2	1.51	0.74
20:p:187:LYS:HD2	22:s:30:ILE:CG2	2.17	0.74
20:p:187:LYS:HD2	22:s:30:ILE:HG23	1.69	0.74
20:h:430:VAL:HB	20:h:446:PHE:CE1	2.22	0.74
20:h:305:CYS:SG	20:h:306:GLN:N	2.60	0.74
20:o:555:SER:OG	20:o:558:GLU:OE2	2.05	0.72
1:C:228:PRO:O	1:C:232:GLU:HB2	1.89	0.72
20:o:337:ARG:NH2	20:p:222:SER:O	2.22	0.72
21:j:165:ILE:HG13	21:j:166:PRO:HD3	1.71	0.72
1:F:228:PRO:O	1:F:232:GLU:HB2	1.89	0.72
20:o:247:ASP:OD2	20:o:250:TRP:N	2.22	0.72
21:j:138:ASP:OD2	21:j:140:SER:OG	2.06	0.72
20:o:432:THR:OG1	20:o:444:GLU:OE2	2.07	0.72
20:h:331:ILE:H	20:h:347:THR:HB	1.55	0.71
20:o:465:VAL:HG12	20:o:582:ASN:HA	1.72	0.71
8:P:33:UNK:HA	8:P:77:UNK:O	1.90	0.71
19:f:894:SER:OG	21:j:357:GLU:OE2	2.05	0.71
1:G:118:ARG:NH2	16:b:73:ASP:OD2	2.24	0.71
2:H:62:ARG:NE	3:J:294:ASP:OD2	2.23	0.71
1:I:366:ASP:OD2	1:I:373:ARG:NH2	2.23	0.70
20:o:323:VAL:HG21	20:o:372:LEU:HD21	1.73	0.70
1:B:112:GLU:OE2	1:B:116:ASN:ND2	2.18	0.70
19:n:406:TYR:O	19:n:410:GLU:HB2	1.90	0.70
3:J:88:ARG:HH12	3:J:369:GLY:HA2	1.56	0.70
5:L:61:LEU:HA	5:L:65:ASN:HD21	1.55	0.70
19:m:401:LEU:HD11	19:m:413:MET:HE2	1.74	0.70
19:n:232:PHE:HB3	19:n:235:LYS:HB3	1.72	0.69
20:o:316:LYS:H	20:o:363:VAL:HG21	1.56	0.69
20:o:549:ARG:HB2	20:o:562:GLY:HA3	1.74	0.69
19:f:718:PHE:HA	19:f:824:TRP:HB2	1.74	0.69
1:I:72:ARG:NH2	1:I:82:ASP:OD2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:240:SER:HB2	20:h:572:ASP:HB3	1.75	0.69
19:m:641:LEU:HD21	20:o:426:GLU:OE2	1.91	0.69
20:o:208:GLU:OE1	20:o:296:LYS:NZ	2.25	0.69
21:j:253:PHE:CE2	21:j:339:PHE:CE1	2.80	0.68
21:j:98:ARG:NH1	21:j:100:ASP:OD1	2.27	0.68
21:j:139:MET:H	21:j:233:LYS:HB3	1.59	0.68
1:E:329:ARG:HG2	15:a:21:GLU:HG2	1.76	0.68
1:F:351:ASP:OD2	19:f:257:GLN:NE2	2.26	0.68
19:f:202:ILE:HG21	19:f:280:ASN:HB3	1.75	0.68
20:h:426:GLU:HG3	20:h:427:GLU:HG2	1.75	0.68
1:G:368:ALA:HA	1:G:371:ILE:HD12	1.76	0.68
1:B:239:ALA:HB3	1:B:255:ARG:HH12	1.59	0.68
4:K:16:ILE:HG21	5:L:31:LEU:HD11	1.75	0.68
20:h:462:VAL:HB	20:h:465:VAL:HB	1.75	0.67
20:p:408:VAL:HA	20:p:425:SER:HA	1.76	0.67
1:B:152:ARG:HH22	1:B:329:ARG:HH12	1.42	0.67
21:j:164:LYS:NZ	21:j:167:PRO:O	2.28	0.67
19:m:586:SER:HA	19:m:589:ASN:HD21	1.59	0.67
19:f:885:VAL:HA	19:f:888:LEU:HD12	1.77	0.67
22:k:82:PRO:HA	22:k:87:PHE:HA	1.76	0.67
4:K:121:ARG:O	4:K:125:ASP:HB2	1.94	0.67
20:o:335:ASP:OD2	20:o:338:SER:N	2.28	0.67
1:G:228:PRO:HD3	1:G:313:ARG:HH12	1.60	0.66
4:K:204:VAL:HG21	5:L:232:TYR:HB3	1.76	0.66
20:o:197:LEU:HB3	20:o:339:ASN:ND2	2.11	0.66
20:p:187:LYS:HB3	22:s:30:ILE:HG21	1.76	0.66
19:m:642:PRO:HG2	19:m:749:GLU:HG3	1.77	0.66
20:p:398:LEU:HA	20:p:441:GLY:HA2	1.77	0.66
1:B:243:LEU:HD12	1:B:247:SER:HB2	1.76	0.66
1:A:104:GLU:HG2	1:A:133:ASN:H	1.60	0.66
20:h:449:HIS:HB2	20:h:477:ASP:OD2	1.95	0.66
19:m:334:PRO:HG2	19:m:370:THR:HG22	1.76	0.66
1:D:104:GLU:HG2	1:D:133:ASN:HB2	1.77	0.66
1:E:208:SER:N	1:F:271:GLU:OE2	2.27	0.66
1:E:228:PRO:HD3	1:E:313:ARG:HH12	1.59	0.66
1:E:243:LEU:HD12	1:E:247:SER:HB2	1.77	0.66
20:h:429:SER:H	20:h:447:GLU:HG2	1.61	0.65
1:B:82:ASP:OD2	1:B:85:ASP:N	2.17	0.65
19:f:382:GLU:HG3	19:f:454:PRO:HB3	1.78	0.65
20:h:258:CYS:HA	20:h:549:ARG:HG3	1.78	0.65
22:s:75:LYS:NZ	22:t:61:ASP:OD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:258:CYS:SG	20:o:259:LEU:N	2.66	0.65
1:C:208:SER:N	1:D:271:GLU:OE2	2.22	0.65
21:j:253:PHE:CD1	21:j:257:HIS:CE1	2.84	0.65
19:m:335:LEU:HB2	19:m:370:THR:HG21	1.79	0.65
20:o:208:GLU:CD	20:o:296:LYS:HZ2	2.03	0.65
1:C:368:ALA:HA	1:C:371:ILE:HD12	1.79	0.65
19:f:282:GLU:O	19:f:286:TYR:HB2	1.97	0.65
3:J:102:ARG:HE	3:J:120:LEU:HD13	1.62	0.65
19:n:556:ARG:O	19:n:560:VAL:CB	2.45	0.65
1:B:104:GLU:OE2	1:B:133:ASN:HB2	1.97	0.65
4:K:169:TRP:HB3	4:K:198:TYR:HD1	1.62	0.64
20:h:351:ALA:O	20:h:380:LYS:NZ	2.30	0.64
20:h:462:VAL:HA	20:h:511:PRO:HG3	1.79	0.64
21:j:185:MET:HG2	21:j:312:ALA:HB1	1.79	0.64
21:j:256:SER:O	21:j:260:ARG:HB2	1.96	0.64
21:j:337:GLU:O	21:j:341:VAL:CB	2.45	0.64
1:G:48:MET:HE1	1:I:153:THR:HA	1.79	0.64
21:j:169:LYS:O	21:j:173:LEU:HB3	1.98	0.64
22:l:23:VAL:HA	22:l:29:PRO:HA	1.79	0.64
22:s:50:ILE:HD13	22:s:69:LEU:HD22	1.80	0.64
19:f:409:PHE:HZ	19:f:467:ARG:HA	1.63	0.64
4:K:47:ARG:O	4:K:51:ALA:HB2	1.98	0.64
20:o:367:GLN:HA	20:o:370:HIS:HD2	1.62	0.63
19:e:213:ILE:HD13	19:e:300:THR:HG22	1.80	0.63
19:e:530:VAL:HA	19:e:549:ALA:HB1	1.80	0.63
19:f:668:VAL:HG12	19:f:669:LEU:HD12	1.81	0.63
22:t:22:VAL:HG13	22:t:88:LEU:HA	1.80	0.63
1:D:368:ALA:HA	1:D:371:ILE:HD12	1.80	0.63
3:J:92:ILE:HD11	3:J:358:GLY:HA3	1.80	0.63
20:o:267:GLU:HB3	20:o:292:MET:H	1.63	0.63
12:X:191:LEU:HB2	23:x:191:LEU:HD13	1.78	0.63
2:H:272:CYS:HB3	2:H:276:GLU:HG3	1.81	0.63
4:K:223:GLN:O	4:K:227:GLU:HB2	1.99	0.63
1:I:15:ASP:OD2	1:I:340:THR:OG1	2.09	0.63
4:K:158:ILE:HB	4:K:175:SER:HB3	1.80	0.63
21:q:186:GLU:HA	21:q:313:GLY:HA2	1.81	0.63
19:e:807:GLY:HA3	19:e:893:TYR:HA	1.79	0.63
20:o:400:HIS:H	20:o:404:LYS:HA	1.63	0.63
21:j:253:PHE:HE2	21:j:339:PHE:HE1	1.44	0.63
1:A:160:SER:H	1:A:302:GLY:HA3	1.62	0.63
12:X:112:ASP:O	12:X:116:ALA:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:205:ILE:O	19:f:291:LYS:NZ	2.32	0.63
19:f:526:ALA:HB2	19:f:556:ARG:HG2	1.79	0.63
22:t:69:LEU:HB3	22:t:80:VAL:HB	1.81	0.63
1:F:207:SER:OG	1:G:271:GLU:OE2	2.09	0.62
20:h:252:LYS:O	20:h:276:ASN:ND2	2.31	0.62
20:h:471:PHE:HA	20:h:506:TRP:HH2	1.64	0.62
1:F:112:GLU:HG2	1:F:116:ASN:HD22	1.63	0.62
5:L:51:ARG:NH1	5:L:57:LYS:O	2.32	0.62
5:L:148:TRP:NE1	5:L:150:SER:OG	2.32	0.62
1:F:238:LYS:HG2	1:F:252:GLY:HA2	1.82	0.62
20:o:584:GLU:HA	20:o:587:ARG:HD2	1.79	0.62
8:P:37:UNK:HA	8:P:73:UNK:O	1.99	0.62
19:n:559:ARG:HA	19:n:562:THR:HG1	1.61	0.62
19:f:401:LEU:HA	19:f:404:VAL:HG12	1.82	0.62
20:g:286:VAL:HA	20:g:304:HIS:HA	1.82	0.62
20:o:517:VAL:HG13	20:o:550:VAL:HG22	1.82	0.62
20:o:503:ASP:HB3	20:o:550:VAL:HG23	1.80	0.62
20:p:185:GLU:CD	20:p:185:GLU:H	2.08	0.62
1:D:140:SER:OG	1:D:141:MET:N	2.33	0.61
19:f:638:VAL:HG21	20:h:255:VAL:HG11	1.81	0.61
19:f:895:ASN:HB3	19:f:898:ILE:HD12	1.80	0.61
22:s:69:LEU:HB3	22:s:80:VAL:HB	1.82	0.61
1:D:133:ASN:HD21	19:f:368:ARG:HH21	1.49	0.61
1:B:165:THR:HG23	1:B:183:ILE:HG13	1.83	0.61
1:G:243:LEU:HD12	1:G:247:SER:HB2	1.82	0.61
15:a:17:PRO:HG2	15:a:20:TYR:HE1	1.66	0.61
19:n:572:LEU:HD12	19:n:581:MET:HA	1.81	0.61
1:B:245:ASP:OD2	1:B:247:SER:OG	2.13	0.61
20:h:243:ARG:NH1	20:h:292:MET:SD	2.74	0.61
24:z:1001:UNK:O	24:z:1005:UNK:CB	2.49	0.61
1:G:36:PRO:HB2	1:G:38:TYR:HE1	1.60	0.61
20:o:527:ASN:ND2	20:o:530:ASN:OD1	2.33	0.61
20:o:496:ASP:OD1	20:o:496:ASP:N	2.34	0.61
1:A:225:SER:HB2	1:A:231:ASP:OD2	2.01	0.60
21:j:57:ILE:HD12	21:j:106:VAL:HG22	1.84	0.60
1:D:7:ILE:HD11	1:D:105:GLU:HG2	1.82	0.60
19:n:562:THR:HG22	19:n:563:ARG:HH21	1.67	0.60
1:B:368:ALA:HA	1:B:371:ILE:HD12	1.83	0.60
21:j:253:PHE:HZ	21:j:336:TYR:CE1	2.20	0.60
19:m:588:PHE:HB3	19:m:591:LEU:HB2	1.83	0.60
19:n:563:ARG:HA	19:n:563:ARG:NE	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLY:HA3	25:D:800:ADP:H5'2	1.83	0.60
1:F:10:GLN:O	1:F:106:HIS:ND1	2.34	0.60
20:g:515:ALA:HA	20:g:525:LEU:HA	1.83	0.59
21:j:277:GLU:HB3	21:j:309:PHE:HZ	1.66	0.59
1:D:96:LYS:O	1:D:100:GLN:NE2	2.35	0.59
1:B:225:SER:HB2	1:B:231:ASP:OD2	2.02	0.59
19:n:77:VAL:HA	19:n:105:ILE:HA	1.85	0.59
19:n:475:GLN:NE2	19:n:590:ALA:O	2.36	0.59
1:B:366:ASP:HB2	1:B:370:SER:HB3	1.84	0.59
4:K:40:LEU:HD23	4:K:46:LEU:HB3	1.84	0.59
20:g:522:ARG:HA	20:g:540:SER:HA	1.83	0.59
19:m:205:ILE:HG21	19:m:255:GLU:HB3	1.84	0.59
20:p:361:VAL:HA	20:p:374:SER:HA	1.84	0.59
1:D:337:LEU:HD12	17:c:11:GLY:HA3	1.84	0.59
19:m:551:LYS:HG3	19:m:555:GLU:OE2	2.02	0.59
20:o:208:GLU:CD	20:o:296:LYS:HZ1	2.11	0.59
1:F:104:GLU:HG2	1:F:133:ASN:HB2	1.83	0.59
20:o:475:SER:OG	20:o:476:PHE:N	2.32	0.59
8:P:25:UNK:HA	8:P:36:UNK:HA	1.84	0.59
19:n:474:GLU:O	19:n:478:ALA:HB3	2.02	0.59
12:X:187:GLN:OE1	23:x:188:GLN:NE2	2.33	0.59
19:n:541:GLU:HA	19:n:544:GLU:HB3	1.85	0.59
1:E:226:ILE:O	1:E:313:ARG:NH1	2.36	0.59
1:G:48:MET:HB3	1:I:173:GLY:HA2	1.83	0.59
21:j:336:TYR:O	21:j:340:ILE:CB	2.51	0.59
1:G:226:ILE:O	1:G:313:ARG:NH1	2.36	0.58
20:h:342:THR:HG23	20:h:346:ARG:HH21	1.66	0.58
21:j:95:ASP:N	21:j:98:ARG:O	2.35	0.58
20:o:320:ASN:HD22	20:o:337:ARG:HG2	1.68	0.58
1:B:113:ALA:HB3	1:B:116:ASN:HD21	1.68	0.58
3:J:166:LEU:HG	3:J:270:LEU:HD12	1.85	0.58
21:j:186:GLU:HA	21:j:313:GLY:HA3	1.86	0.58
21:j:220:THR:HA	21:j:264:GLN:HA	1.85	0.58
20:p:187:LYS:HB3	22:s:30:ILE:HD13	1.84	0.58
21:q:86:LEU:H	21:q:109:LEU:HA	1.68	0.58
5:L:212:ASN:OD1	5:L:215:ARG:NH2	2.36	0.58
19:m:470:ARG:O	19:m:474:GLU:HB3	2.03	0.58
23:x:143:ASP:O	23:x:147:HIS:ND1	2.35	0.58
1:B:28:ASP:HB2	1:B:341:TRP:HH2	1.68	0.58
4:K:174:ARG:HH12	4:K:193:LYS:HE3	1.68	0.58
21:i:57:ILE:O	21:i:106:VAL:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:84:LEU:O	19:m:97:GLU:N	2.37	0.58
20:o:380:LYS:HA	20:o:397:GLU:HA	1.83	0.58
1:G:357:TRP:O	1:G:374:LYS:NZ	2.36	0.58
5:L:166:HIS:NE2	5:L:198:GLU:OE2	2.37	0.58
19:f:530:VAL:HA	19:f:533:VAL:HG22	1.84	0.58
21:j:137:ALA:HB1	21:j:145:VAL:HG22	1.85	0.58
20:o:205:ARG:NH1	20:p:218:PHE:HB3	2.18	0.58
20:o:563:ASP:OD2	20:o:569:VAL:N	2.36	0.58
1:E:305:THR:O	1:E:336:ARG:NH1	2.37	0.58
1:C:158:LEU:HD23	1:C:167:ALA:HB2	1.84	0.58
1:F:206:HIS:N	1:F:210:GLU:OE1	2.35	0.58
19:e:686:GLY:O	19:e:690:ARG:N	2.36	0.58
19:f:613:LYS:NZ	19:f:685:ASP:OD2	2.30	0.58
20:o:289:VAL:HG23	20:o:300:GLU:HB3	1.85	0.58
20:o:521:GLY:HA2	20:o:547:LEU:HG	1.86	0.58
19:m:77:VAL:HA	19:m:105:ILE:HA	1.86	0.58
19:m:638:VAL:HG21	20:o:255:VAL:HG21	1.86	0.58
19:n:581:MET:O	19:n:585:PHE:CB	2.51	0.58
22:s:11:LEU:HD22	22:s:20:ILE:HD12	1.86	0.58
22:t:81:ALA:HB3	22:t:88:LEU:HB2	1.85	0.58
1:A:305:THR:O	1:A:336:ARG:NH1	2.37	0.58
1:D:234:LEU:HD12	1:D:236:THR:HG22	1.86	0.58
19:f:239:PRO:O	19:f:243:ASN:CB	2.51	0.57
19:f:639:ARG:NH2	20:h:548:ASN:OD1	2.26	0.57
19:f:751:ARG:O	19:f:755:TRP:CB	2.52	0.57
12:X:184:LEU:HA	23:x:184:LEU:HD13	1.85	0.57
19:m:413:MET:HE1	19:m:463:LEU:HD22	1.86	0.57
19:n:468:LYS:O	19:n:472:GLN:NE2	2.36	0.57
1:D:154:THR:HG22	1:D:172:GLU:H	1.68	0.57
4:K:210:LYS:NZ	5:L:182:SER:O	2.38	0.57
1:F:352:THR:O	1:F:356:MET:HB2	2.04	0.57
20:h:345:GLN:HE21	20:h:389:LEU:HB3	1.69	0.57
1:B:126:GLU:O	1:B:130:GLU:HB2	2.04	0.57
1:E:18:SER:O	1:E:188:ARG:NH2	2.38	0.57
19:e:232:PHE:HB3	19:e:235:LYS:HB2	1.86	0.57
20:h:522:ARG:HA	20:h:540:SER:HA	1.86	0.57
19:f:649:ILE:HD13	20:h:452:PRO:HG3	1.86	0.57
1:A:226:ILE:O	1:A:313:ARG:NH1	2.37	0.57
4:K:86:ARG:NH2	4:K:107:ASP:OD2	2.30	0.57
1:E:154:THR:HG22	1:E:172:GLU:H	1.70	0.57
3:J:150:PRO:HG2	3:J:157:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:499:UNK:O	7:N:503:UNK:N	2.38	0.57
2:H:78:ASN:ND2	2:H:81:ASP:OD2	2.38	0.57
2:H:211:ASP:OD2	2:H:240:TYR:OH	2.13	0.57
4:K:117:LEU:HB2	4:K:145:ALA:HB1	1.87	0.57
20:o:354:HIS:NE2	20:o:380:LYS:O	2.36	0.57
1:A:236:THR:HG23	1:A:238:LYS:H	1.69	0.56
20:h:529:ASN:HB3	20:h:585:TRP:HB2	1.87	0.56
19:n:557:ILE:HG22	19:n:561:GLU:HG2	1.86	0.56
20:o:557:ARG:HE	20:o:574:GLY:HA2	1.69	0.56
1:C:71:ILE:HD12	1:C:209:SER:HA	1.86	0.56
21:j:170:MET:O	21:j:174:GLU:HB3	2.05	0.56
19:n:570:ASP:HA	20:o:368:ASN:HD22	1.69	0.56
1:I:243:LEU:HD12	1:I:247:SER:HB2	1.86	0.56
4:K:255:PHE:O	4:K:259:ARG:N	2.38	0.56
5:L:67:ASP:OD2	5:L:87:ALA:N	2.37	0.56
9:Q:55:UNK:O	9:Q:59:UNK:CB	2.54	0.56
19:f:576:LYS:O	19:f:611:ARG:NE	2.39	0.56
1:B:154:THR:HG22	1:B:172:GLU:H	1.70	0.56
3:J:13:LYS:O	3:J:365:GLN:NE2	2.38	0.56
3:J:17:VAL:HG21	3:J:359:ALA:HA	1.87	0.56
20:o:249:ARG:CZ	22:t:6:GLU:CD	2.77	0.56
1:A:10:GLN:NE2	1:A:26:ALA:O	2.34	0.56
4:K:25:PRO:HG2	4:K:28:GLU:HB2	1.88	0.56
16:b:85:SER:OG	16:b:86:GLY:N	2.39	0.56
7:N:482:UNK:O	7:N:486:UNK:N	2.39	0.56
16:b:65:GLY:HA3	16:b:85:SER:HB3	1.88	0.56
19:m:725:VAL:HA	19:m:733:LEU:HA	1.86	0.56
20:o:563:ASP:OD2	20:o:567:GLN:HG2	2.06	0.56
20:p:187:LYS:CG	22:s:30:ILE:HD13	2.36	0.56
20:g:470:LEU:HA	20:g:484:SER:HA	1.88	0.56
20:h:546:ALA:HB3	20:h:564:SER:HB3	1.88	0.56
22:k:72:ARG:HA	22:k:77:GLU:HA	1.88	0.56
22:l:76:ASN:HA	22:l:93:ASN:HA	1.88	0.56
1:E:104:GLU:HG2	1:E:133:ASN:HB2	1.88	0.56
1:F:28:ASP:HB2	1:F:341:TRP:HH2	1.71	0.56
1:I:305:THR:O	1:I:336:ARG:NH1	2.39	0.56
4:K:138:ASN:ND2	4:K:162:GLN:OE1	2.39	0.56
20:h:275:ASN:ND2	20:h:277:GLU:OE2	2.39	0.56
2:H:102:PRO:HB3	2:H:131:ALA:HB3	1.88	0.56
19:m:458:LYS:HE2	19:m:539:SER:HB3	1.87	0.56
19:n:559:ARG:NH2	20:o:420:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:284:ASP:OD2	20:o:308:ALA:N	2.39	0.56
1:D:329:ARG:HG2	17:c:21:GLU:HG2	1.88	0.56
8:O:24:UNK:N	8:O:37:UNK:O	2.39	0.56
12:X:197:GLU:HA	12:X:200:ARG:HD2	1.88	0.56
1:F:162:ASP:OD1	25:F:800:ADP:O3'	2.22	0.55
10:U:14:GLY:O	10:U:15:ALA:N	2.39	0.55
19:f:466:MET:HG2	19:f:546:TRP:HZ2	1.70	0.55
21:j:282:LEU:O	21:j:286:TYR:CB	2.54	0.55
5:L:76:SER:O	5:L:78:LYS:NZ	2.36	0.55
8:O:25:UNK:HA	8:O:36:UNK:HA	1.88	0.55
19:f:583:ARG:HH12	20:h:534:VAL:HG13	1.71	0.55
20:h:260:ASP:OD2	20:h:313:THR:OG1	2.16	0.55
20:h:431:TYR:HE1	20:h:445:MET:HG2	1.71	0.55
19:n:473:HIS:CE1	19:n:477:ARG:HE	2.25	0.55
23:x:314:LEU:O	23:x:318:ARG:CB	2.54	0.55
1:E:262:LEU:HB3	1:E:275:ILE:HD12	1.88	0.55
3:J:348:ALA:HB2	3:J:356:LEU:HD13	1.88	0.55
19:f:335:LEU:HB2	19:f:370:THR:HG21	1.88	0.55
19:f:707:GLN:HG3	19:f:764:ILE:HD11	1.87	0.55
21:j:221:HIS:HD2	21:j:264:GLN:HB3	1.72	0.55
19:n:546:TRP:O	19:n:550:MET:CB	2.53	0.55
20:o:383:SER:HB3	20:o:394:ASP:H	1.71	0.55
20:o:515:ALA:HB1	20:o:523:LEU:HD11	1.89	0.55
1:A:323:PRO:HG2	1:A:326:VAL:HG21	1.88	0.55
20:h:249:ARG:O	20:h:252:LYS:NZ	2.39	0.55
21:j:170:MET:HA	21:j:173:LEU:HB3	1.88	0.55
20:o:203:SER:HB2	22:t:88:LEU:HD21	1.89	0.55
1:I:183:ILE:HD13	1:I:272:SER:HB3	1.89	0.55
12:X:172:GLU:OE2	19:f:762:LEU:HD13	2.07	0.55
19:f:341:LEU:HA	19:f:360:ILE:HD11	1.88	0.55
20:h:481:LYS:HE2	20:h:493:SER:HB2	1.88	0.55
21:j:282:LEU:O	21:j:286:TYR:HB3	2.07	0.55
22:s:29:PRO:HD2	22:s:40:THR:HG23	1.88	0.55
1:G:36:PRO:CB	1:G:38:TYR:HE1	2.20	0.55
1:G:112:GLU:HG2	1:G:116:ASN:HD22	1.71	0.55
12:X:142:THR:HA	12:X:145:LEU:HD12	1.89	0.55
19:m:755:TRP:CG	20:o:427:GLU:HG3	2.42	0.55
20:o:572:ASP:OD1	20:o:573:VAL:N	2.37	0.55
22:s:57:VAL:HG21	22:s:66:LEU:HD21	1.89	0.55
1:C:243:LEU:HD12	1:C:247:SER:HB2	1.88	0.55
4:K:23:HIS:HB3	5:L:17:PRO:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:543:THR:O	19:f:547:GLU:CB	2.55	0.55
19:f:724:ARG:HD3	19:f:734:LYS:HB2	1.89	0.55
21:j:73:LYS:HE3	21:j:274:VAL:HA	1.88	0.55
21:j:276:GLU:HB3	21:j:277:GLU:HG3	1.89	0.55
6:M:298:UNK:O	6:M:302:UNK:N	2.39	0.55
19:e:84:LEU:O	19:e:97:GLU:N	2.39	0.55
19:f:815:LEU:HD12	19:f:839:THR:HG21	1.87	0.55
19:m:378:LEU:HB3	19:m:452:ILE:HD11	1.89	0.55
1:F:16:ASN:HB3	1:F:75:MET:HE1	1.88	0.54
1:F:56:ILE:HD13	1:F:88:ARG:HD3	1.88	0.54
5:L:132:ILE:HB	5:L:152:HIS:HB2	1.87	0.54
1:D:334:GLN:HB3	17:c:12:ILE:HG23	1.89	0.54
21:j:253:PHE:CE2	21:j:339:PHE:HE1	2.20	0.54
19:n:119:ILE:O	19:n:136:ARG:N	2.39	0.54
20:o:452:PRO:HD2	20:o:476:PHE:HB2	1.90	0.54
22:t:36:ASN:ND2	22:t:40:THR:OG1	2.41	0.54
1:G:10:GLN:O	1:G:106:HIS:ND1	2.38	0.54
20:h:358:VAL:HA	20:h:376:SER:HA	1.89	0.54
20:h:510:HIS:HB2	20:h:578:ALA:HA	1.90	0.54
19:n:557:ILE:C	19:n:561:GLU:CG	2.78	0.54
20:p:407:ALA:O	20:p:426:GLU:N	2.39	0.54
22:s:70:ARG:HB3	22:t:70:ARG:HB2	1.88	0.54
1:A:154:THR:HG22	1:A:172:GLU:H	1.72	0.54
1:B:76:GLU:O	1:B:81:LYS:NZ	2.39	0.54
3:J:227:GLN:HA	3:J:230:LYS:HZ3	1.73	0.54
20:h:260:ASP:OD1	20:h:261:TRP:N	2.41	0.54
19:m:616:ILE:O	19:m:620:HIS:ND1	2.40	0.54
19:n:563:ARG:O	19:n:567:ARG:N	2.32	0.54
19:f:598:ARG:HA	19:f:601:ILE:HB	1.89	0.54
19:f:706:VAL:HA	19:f:710:ASN:HB2	1.88	0.54
19:f:863:SER:O	19:f:866:THR:OG1	2.23	0.54
20:h:452:PRO:HG2	20:h:476:PHE:HD2	1.72	0.54
19:m:358:VAL:HA	19:m:426:GLU:OE2	2.08	0.54
20:o:356:HIS:HB2	20:o:376:SER:HB2	1.89	0.54
19:m:746:LEU:HD13	19:m:768:ALA:HA	1.89	0.54
20:o:304:HIS:H	20:o:341:ARG:HB3	1.72	0.54
1:A:228:PRO:HB3	1:A:313:ARG:HH22	1.73	0.54
1:B:18:SER:O	1:B:188:ARG:NH2	2.41	0.54
1:D:10:GLN:NE2	1:D:26:ALA:O	2.41	0.54
1:I:13:VAL:HG13	1:I:109:LEU:HD23	1.87	0.54
1:I:257:ARG:NH1	3:J:388:CYS:SG	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:24:PHE:HA	3:J:40:PRO:HA	1.89	0.54
16:b:70:ASP:HB2	16:b:80:ARG:HD2	1.90	0.54
19:f:567:ARG:HD3	19:f:570:ASP:OD2	2.07	0.54
20:h:526:TRP:HB3	20:h:535:PRO:HA	1.90	0.54
20:o:321:LEU:HG	20:o:333:LEU:HD11	1.88	0.54
1:E:238:LYS:HA	1:E:252:GLY:HA2	1.90	0.54
1:I:160:SER:HB3	1:I:304:SER:HB2	1.90	0.54
5:L:163:ARG:HB3	5:L:203:VAL:HB	1.89	0.54
19:m:1037:TYR:O	19:m:1041:MET:CB	2.56	0.54
19:n:563:ARG:HE	19:n:563:ARG:CA	2.20	0.54
20:o:401:LYS:O	20:o:404:LYS:NZ	2.41	0.54
21:q:144:THR:O	21:q:148:SER:CB	2.55	0.54
1:F:279:LEU:HD21	1:F:298:ILE:HD13	1.90	0.54
19:m:745:THR:OG1	19:m:746:LEU:N	2.40	0.54
19:n:349:GLU:OE1	19:n:352:LYS:NZ	2.38	0.54
20:o:528:LEU:HD22	20:o:585:TRP:HH2	1.72	0.54
7:N:479:UNK:O	7:N:483:UNK:N	2.41	0.54
11:V:35:VAL:O	11:V:57:VAL:CB	2.56	0.54
14:Z:1033:UNK:O	14:Z:1037:UNK:CB	2.56	0.54
19:f:591:LEU:HD13	19:f:597:ILE:HG12	1.90	0.54
21:j:178:VAL:HA	21:j:181:PHE:HB3	1.89	0.54
19:m:341:LEU:HA	19:m:360:ILE:HD11	1.89	0.54
21:j:277:GLU:OE2	21:j:307:ALA:HB1	2.08	0.53
19:m:652:LYS:HB3	19:m:656:ARG:HH22	1.73	0.53
20:o:245:PHE:N	20:o:568:ILE:O	2.41	0.53
20:o:449:HIS:NE2	20:o:477:ASP:OD2	2.42	0.53
1:D:46:ARG:NH1	1:D:52:LEU:O	2.41	0.53
5:L:253:SER:O	5:L:257:ALA:HB2	2.08	0.53
19:e:765:VAL:O	19:e:769:HIS:CB	2.56	0.53
20:h:240:SER:N	20:h:572:ASP:O	2.39	0.53
24:z:1012:UNK:O	24:z:1016:UNK:CB	2.57	0.53
1:F:95:SER:OG	1:F:96:LYS:N	2.41	0.53
5:L:90:SER:HB2	5:L:93:LEU:HB2	1.90	0.53
19:f:561:GLU:HA	19:f:564:ILE:HB	1.91	0.53
19:m:546:TRP:NE1	19:m:550:MET:SD	2.82	0.53
1:F:243:LEU:HD12	1:F:247:SER:HB2	1.90	0.53
2:H:35:VAL:HG12	2:H:54:VAL:HG22	1.90	0.53
2:H:220:ALA:HB2	2:H:255:PHE:HB2	1.89	0.53
6:M:240:UNK:O	6:M:244:UNK:N	2.41	0.53
4:K:46:LEU:O	4:K:50:ALA:CB	2.50	0.53
20:o:261:TRP:CD1	20:o:553:THR:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:z:1025:UNK:O	24:z:1029:UNK:CB	2.57	0.53
1:E:36:PRO:HB2	1:E:38:TYR:CE2	2.43	0.53
1:E:162:ASP:OD2	1:E:188:ARG:HB2	2.09	0.53
19:f:860:GLU:HB3	19:f:877:ILE:HG23	1.89	0.53
20:g:310:MET:H	20:g:326:THR:HA	1.74	0.53
20:h:481:LYS:HD3	20:h:490:PRO:HD2	1.89	0.53
1:C:323:PRO:HG2	1:C:326:VAL:HG21	1.91	0.53
19:e:572:LEU:HA	19:e:575:ALA:HB3	1.91	0.53
19:m:469:PHE:HB2	19:m:550:MET:HE1	1.90	0.53
20:o:457:HIS:CD2	20:o:506:TRP:H	2.27	0.53
23:x:142:THR:HA	23:x:145:LEU:HD12	1.90	0.53
1:E:79:ILE:HG23	1:E:120:ASN:HD21	1.73	0.53
4:K:218:VAL:HA	4:K:224:THR:HG21	1.91	0.53
4:K:240:GLN:NE2	5:L:244:ARG:O	2.41	0.53
19:f:751:ARG:O	19:f:755:TRP:HB3	2.09	0.53
20:g:255:VAL:O	20:g:274:ASN:N	2.39	0.53
21:j:169:LYS:O	21:j:173:LEU:CB	2.57	0.53
1:E:225:SER:HB2	1:E:231:ASP:OD2	2.09	0.53
1:I:162:ASP:OD2	1:I:188:ARG:HB2	2.08	0.53
3:J:145:GLU:HG2	3:J:165:PRO:HA	1.91	0.53
19:m:150:HIS:O	19:m:154:SER:CB	2.57	0.53
1:D:28:ASP:HB2	1:D:341:TRP:HH2	1.74	0.52
1:I:134:VAL:HG12	1:I:136:ALA:H	1.73	0.52
11:V:101:ALA:HB3	11:V:118:ARG:HA	1.89	0.52
12:X:161:ASN:OD1	19:f:773:GLN:NE2	2.42	0.52
20:h:254:ARG:HG2	20:h:276:ASN:HB2	1.91	0.52
20:h:548:ASN:N	20:h:562:GLY:O	2.42	0.52
21:j:170:MET:HB3	21:j:174:GLU:HB2	1.92	0.52
21:j:235:ASP:OD2	21:j:274:VAL:HB	2.08	0.52
1:B:73:TYR:OH	1:B:212:GLU:OE2	2.26	0.52
8:P:64:UNK:HA	8:P:76:UNK:O	2.10	0.52
19:m:350:LEU:HD23	19:m:353:ILE:HD12	1.91	0.52
1:B:327:LYS:HG3	17:c:48:ILE:HA	1.91	0.52
1:D:243:LEU:HD12	1:D:247:SER:HB2	1.90	0.52
1:F:330:ILE:HB	18:d:20:TYR:HB2	1.91	0.52
1:I:113:ALA:O	1:I:116:ASN:ND2	2.42	0.52
1:I:189:ASP:OD1	1:I:192:ARG:NH1	2.43	0.52
1:A:168:VAL:HG22	1:A:180:ILE:HG23	1.91	0.52
1:I:25:PHE:HZ	1:I:101:THR:HG21	1.75	0.52
21:j:95:ASP:HB2	21:j:100:ASP:H	1.74	0.52
19:m:572:LEU:HD11	19:m:581:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:530:VAL:HB	19:n:553:TYR:HD1	1.74	0.52
1:D:57:PHE:HD2	1:D:69:LEU:HD21	1.75	0.52
1:E:263:PHE:HD2	1:E:313:ARG:HE	1.57	0.52
5:L:166:HIS:ND1	5:L:200:ASP:OD1	2.33	0.52
20:o:258:CYS:HB2	20:o:311:SER:HA	1.92	0.52
1:F:351:ASP:OD1	1:F:354:LYS:NZ	2.39	0.52
3:J:126:MET:HG2	3:J:129:LEU:HD12	1.92	0.52
3:J:262:ILE:HD12	3:J:265:SER:HB3	1.91	0.52
4:K:94:ILE:HA	4:K:111:GLU:H	1.72	0.52
19:f:909:ARG:NH2	19:f:1008:UNK:O	2.42	0.52
20:h:419:ASN:HB2	20:h:435:ARG:HB2	1.92	0.52
22:l:36:ASN:O	22:l:40:THR:CB	2.57	0.52
22:t:36:ASN:O	22:t:40:THR:OG1	2.26	0.52
1:A:183:ILE:HD13	1:A:273:GLU:H	1.74	0.52
3:J:21:GLY:O	3:J:41:SER:OG	2.27	0.52
4:K:95:SER:N	4:K:109:GLN:O	2.36	0.52
4:K:182:THR:OG1	4:K:185:THR:O	2.27	0.52
9:Q:67:UNK:O	9:Q:71:UNK:CB	2.58	0.52
19:n:546:TRP:O	19:n:550:MET:HB3	2.10	0.52
20:o:330:GLN:NE2	20:o:347:THR:O	2.29	0.52
1:A:153:THR:HA	5:L:266:LEU:HD11	1.91	0.52
1:D:123:ARG:NH1	1:D:126:GLU:OE1	2.42	0.52
19:f:404:VAL:HG11	19:f:408:GLU:HB2	1.92	0.52
19:n:80:GLU:HA	19:n:115:SER:HA	1.92	0.52
1:A:358:VAL:HG21	1:A:371:ILE:HG12	1.92	0.52
1:G:329:ARG:NH2	16:b:46:GLU:OE1	2.41	0.52
4:K:61:GLN:OE1	4:K:172:ARG:NH2	2.43	0.52
20:h:425:SER:OG	20:h:426:GLU:N	2.42	0.52
19:m:543:THR:OG1	19:m:544:GLU:N	2.43	0.52
1:F:264:ARG:NH1	16:b:77:LYS:O	2.42	0.52
2:H:47:MET:HE3	3:J:129:LEU:HD22	1.92	0.52
1:I:205:PHE:HD1	1:I:210:GLU:HG2	1.75	0.52
19:f:714:SER:HB2	19:f:767:LYS:HB3	1.92	0.52
19:n:774:LEU:O	19:n:778:ALA:N	2.38	0.52
5:L:135:LYS:NZ	5:L:147:CYS:SG	2.83	0.51
18:d:3:ASP:OD1	18:d:3:ASP:N	2.41	0.51
19:f:749:GLU:OE2	19:f:764:ILE:HG22	2.09	0.51
20:p:187:LYS:CB	22:s:30:ILE:HD13	2.40	0.51
20:p:380:LYS:HA	20:p:397:GLU:HA	1.92	0.51
1:E:45:VAL:HA	16:b:81:THR:HG23	1.92	0.51
5:L:90:SER:O	5:L:94:ARG:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:308:ALA:HB3	20:o:327:TYR:HB2	1.92	0.51
20:o:322:VAL:O	20:o:334:TRP:N	2.42	0.51
24:z:1032:UNK:O	24:z:1036:UNK:CB	2.58	0.51
19:f:369:ASN:OD1	19:f:369:ASN:N	2.41	0.51
20:o:465:VAL:HG11	20:o:585:TRP:CD1	2.45	0.51
11:V:53:ALA:HB1	11:V:84:PRO:HA	1.93	0.51
19:e:210:HIS:HB3	19:e:213:ILE:HD12	1.91	0.51
20:h:303:PHE:HB3	20:h:334:TRP:CE2	2.45	0.51
19:n:530:VAL:HG21	19:n:556:ARG:HG3	1.91	0.51
20:p:197:LEU:HA	20:p:200:PHE:HB2	1.91	0.51
1:B:122:GLU:HG2	1:B:368:ALA:HB1	1.93	0.51
1:C:245:ASP:OD2	1:E:291:ARG:NH1	2.42	0.51
1:G:11:PRO:HB3	1:G:107:PRO:HB2	1.93	0.51
5:L:48:LYS:HB2	5:L:61:LEU:HB2	1.92	0.51
21:j:156:LEU:HD12	21:j:159:HIS:HB3	1.92	0.51
21:j:333:GLU:HA	21:j:336:TYR:HE2	1.76	0.51
19:m:204:GLU:OE2	19:m:287:ARG:NH1	2.43	0.51
19:n:558:ASP:O	19:n:561:GLU:CD	2.40	0.51
19:n:563:ARG:NE	19:n:563:ARG:CA	2.73	0.51
1:B:287:ASP:OD1	4:K:266:ARG:NE	2.44	0.51
1:C:18:SER:O	1:C:188:ARG:NH2	2.43	0.51
4:K:118:LYS:HB3	4:K:121:ARG:HH21	1.75	0.51
4:K:141:CYS:SG	4:K:142:THR:N	2.84	0.51
19:f:427:TYR:HA	19:f:430:LEU:HD12	1.92	0.51
20:h:481:LYS:NZ	20:h:490:PRO:O	2.35	0.51
19:m:438:VAL:O	19:m:442:ARG:N	2.44	0.51
19:n:344:LEU:HD21	19:n:387:ASP:HB3	1.91	0.51
22:s:68:PHE:HB3	22:t:72:ARG:HB3	1.92	0.51
19:e:249:VAL:HG21	19:e:304:LEU:HD11	1.91	0.51
21:j:263:LEU:HD12	21:j:264:GLN:HG3	1.92	0.51
20:o:275:ASN:ND2	20:o:283:PRO:O	2.44	0.51
21:q:57:ILE:O	21:q:106:VAL:HA	2.11	0.51
1:G:232:GLU:O	1:G:257:ARG:NH2	2.43	0.51
19:m:452:ILE:HG22	19:m:454:PRO:HD3	1.91	0.51
22:t:25:THR:OG1	22:t:85:ASP:O	2.28	0.51
1:G:113:ALA:O	1:G:116:ASN:ND2	2.44	0.51
4:K:183:PRO:HA	4:K:218:VAL:HB	1.93	0.51
19:e:78:LEU:N	19:e:104:ASN:O	2.34	0.51
22:k:66:LEU:HA	22:l:73:SER:HA	1.92	0.51
22:s:73:SER:OG	22:s:76:ASN:OD1	2.28	0.51
1:C:121:ARG:HH22	1:C:141:MET:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:GLN:HG2	1:F:250:GLU:OE2	2.11	0.51
2:H:12:ASN:ND2	2:H:17:CYS:SG	2.84	0.51
19:f:518:ASN:HB3	19:f:563:ARG:HH12	1.76	0.51
19:m:577:ASN:ND2	20:o:533:GLU:OE2	2.43	0.51
1:F:158:LEU:HD23	1:F:167:ALA:HB2	1.92	0.50
1:G:159:ASP:HB3	1:G:301:SER:HB3	1.92	0.50
3:J:242:PRO:HG2	3:J:264:ASP:OD2	2.11	0.50
20:o:510:HIS:CE1	20:o:512:ALA:HB3	2.46	0.50
20:p:506:TRP:HA	20:p:514:PHE:HA	1.93	0.50
22:t:20:ILE:HA	22:t:90:VAL:HG23	1.93	0.50
23:x:196:ARG:HB3	23:x:200:ARG:HH12	1.76	0.50
1:C:95:SER:OG	1:C:96:LYS:N	2.42	0.50
7:N:1:UNK:HA	8:P:41:UNK:HA	1.92	0.50
19:f:375:GLN:OE1	19:f:379:ARG:NH1	2.44	0.50
19:m:620:HIS:O	19:m:624:LYS:HB2	2.11	0.50
20:o:298:THR:CA	22:t:10:ARG:HH11	2.23	0.50
1:B:228:PRO:HD3	1:B:313:ARG:HH12	1.77	0.50
1:C:243:LEU:HD21	1:C:249:ILE:HD12	1.93	0.50
1:E:162:ASP:OD1	25:E:800:ADP:O3'	2.29	0.50
1:E:240:GLN:HG2	1:E:250:GLU:HG2	1.93	0.50
1:F:38:TYR:HA	1:F:74:PRO:HD3	1.93	0.50
3:J:253:GLU:OE2	10:U:132:ASN:HA	2.11	0.50
19:m:470:ARG:O	19:m:474:GLU:CB	2.58	0.50
20:o:510:HIS:HB3	20:o:513:LEU:HG	1.94	0.50
22:t:25:THR:O	22:t:47:HIS:NE2	2.38	0.50
19:f:726:ARG:N	19:f:732:VAL:O	2.44	0.50
21:j:218:VAL:HG11	21:j:263:LEU:HD13	1.93	0.50
22:l:57:VAL:O	22:l:61:ASP:N	2.37	0.50
19:m:626:GLN:HB3	19:m:628:PRO:HD2	1.93	0.50
19:n:267:ALA:O	19:n:386:ARG:NH2	2.44	0.50
19:n:470:ARG:O	19:n:474:GLU:HB2	2.11	0.50
19:f:205:ILE:HG21	19:f:255:GLU:HB3	1.92	0.50
19:f:568:LEU:HD11	19:f:597:ILE:HG13	1.93	0.50
19:f:727:GLY:HA2	19:f:731:ASN:HD22	1.77	0.50
23:x:186:ARG:O	23:x:190:HIS:ND1	2.35	0.50
1:B:263:PHE:HD2	1:B:313:ARG:HE	1.59	0.50
12:X:112:ASP:O	12:X:116:ALA:CB	2.59	0.50
19:f:854:GLU:HA	19:f:857:ILE:HD12	1.94	0.50
21:j:170:MET:O	21:j:174:GLU:CB	2.60	0.50
21:j:238:SER:HA	21:j:241:GLU:HG2	1.92	0.50
22:k:69:LEU:N	22:k:80:VAL:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:333:ASN:O	19:m:337:LYS:N	2.44	0.50
1:C:232:GLU:O	1:C:257:ARG:NH2	2.43	0.50
1:F:273:GLU:HB3	1:F:277:GLU:HB2	1.94	0.50
4:K:251:SER:O	5:L:225:ARG:NH2	2.44	0.50
19:n:563:ARG:HE	19:n:563:ARG:N	2.10	0.50
20:o:378:ASP:OD2	20:o:380:LYS:HG3	2.11	0.50
21:q:241:GLU:HA	21:q:246:TYR:H	1.77	0.50
1:F:223:TYR:HE1	1:F:255:ARG:HG3	1.76	0.50
1:I:243:LEU:HD21	1:I:249:ILE:HD12	1.94	0.50
19:f:717:ILE:HG21	19:f:774:LEU:HD13	1.94	0.50
20:h:239:LEU:HD12	20:h:539:ILE:HB	1.94	0.50
19:n:523:VAL:O	19:n:527:TYR:HB2	2.12	0.50
1:F:68:LEU:HD11	2:H:169:TYR:HD2	1.77	0.50
1:G:362:GLU:OE2	1:G:373:ARG:NH2	2.45	0.50
5:L:119:VAL:HG22	5:L:132:ILE:HG12	1.93	0.50
8:P:26:UNK:O	8:P:35:UNK:N	2.45	0.50
20:o:261:TRP:CD2	20:o:553:THR:HG23	2.47	0.50
20:o:275:ASN:HB2	20:o:285:GLY:H	1.77	0.50
20:o:305:CYS:SG	20:o:306:GLN:N	2.85	0.50
2:H:214:GLU:OE2	26:H:401:ATP:H2'	2.12	0.49
19:n:235:LYS:HA	19:n:238:ASP:OD2	2.12	0.49
20:p:472:VAL:HA	20:p:482:LEU:HA	1.93	0.49
1:A:118:ARG:HG3	1:A:372:HIS:CE1	2.47	0.49
1:D:169:PRO:HB2	1:D:176:MET:HE3	1.95	0.49
9:Q:32:UNK:O	9:Q:36:UNK:CB	2.60	0.49
19:f:884:ALA:HA	19:f:887:ASP:OD2	2.13	0.49
1:E:11:PRO:HB3	1:E:107:PRO:HB2	1.94	0.49
3:J:76:TYR:CZ	3:J:84:PRO:HB3	2.47	0.49
19:f:719:THR:O	19:f:738:ASN:ND2	2.45	0.49
19:m:743:ILE:HD12	19:m:744:ILE:HG13	1.94	0.49
1:E:10:GLN:NE2	1:E:26:ALA:O	2.38	0.49
1:E:46:ARG:NH1	16:b:83:TYR:O	2.38	0.49
1:I:238:LYS:HG2	1:I:252:GLY:HA2	1.94	0.49
4:K:117:LEU:HD23	4:K:181:ILE:HD12	1.93	0.49
19:e:327:GLU:O	19:e:331:ASP:HB2	2.12	0.49
20:o:563:ASP:OD2	20:o:569:VAL:HG23	2.12	0.49
1:A:219:GLU:OE2	25:A:800:ADP:H2'	2.12	0.49
1:D:36:PRO:HB2	1:D:38:TYR:CE2	2.47	0.49
1:E:51:ALA:HB2	1:G:173:GLY:HA3	1.94	0.49
1:G:126:GLU:O	1:G:130:GLU:HB2	2.12	0.49
1:G:238:LYS:HG2	1:G:252:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:217:VAL:HG13	3:J:267:VAL:HG11	1.94	0.49
5:L:70:SER:HA	5:L:81:PRO:HD2	1.94	0.49
7:N:162:UNK:O	7:N:166:UNK:N	2.45	0.49
20:h:558:GLU:HG2	20:h:572:ASP:HB2	1.93	0.49
19:f:754:LYS:HD3	20:h:426:GLU:OE2	2.13	0.49
19:f:775:TYR:CZ	19:f:779:ILE:HD11	2.48	0.49
19:f:777:PHE:O	19:f:780:SER:OG	2.30	0.49
20:h:531:ASP:OD2	20:h:536:THR:OG1	2.30	0.49
1:A:262:LEU:HB3	1:A:275:ILE:HD12	1.94	0.49
1:C:156:VAL:HG22	1:C:169:PRO:HB3	1.95	0.49
1:I:158:LEU:HD23	1:I:167:ALA:HB2	1.95	0.49
20:o:459:HIS:ND1	20:o:460:ALA:O	2.39	0.49
20:p:373:ILE:HA	20:p:383:SER:HA	1.93	0.49
1:C:162:ASP:OD1	25:C:800:ADP:O3'	2.30	0.49
1:G:10:GLN:NE2	1:G:26:ALA:O	2.46	0.49
3:J:103:GLU:HG2	3:J:384:ILE:HD12	1.93	0.49
19:f:542:GLY:O	19:f:546:TRP:HB2	2.13	0.49
20:p:255:VAL:O	20:p:274:ASN:N	2.40	0.49
1:I:200:LYS:NZ	3:J:388:CYS:SG	2.71	0.49
19:f:845:GLU:O	19:f:849:ASP:HB2	2.13	0.49
20:h:459:HIS:HE1	20:h:470:LEU:HB2	1.77	0.49
19:m:530:VAL:O	19:m:534:ASP:CB	2.46	0.49
1:E:10:GLN:O	1:E:106:HIS:ND1	2.41	0.49
1:G:113:ALA:HB3	1:G:116:ASN:HD21	1.78	0.49
3:J:43:ILE:HD11	3:J:48:MET:HG2	1.95	0.49
4:K:143:VAL:HG13	4:K:154:ILE:HG23	1.94	0.49
19:f:611:ARG:HA	19:f:614:ASP:OD2	2.12	0.49
20:g:240:SER:N	20:g:572:ASP:O	2.40	0.49
20:p:190:ILE:HG13	20:p:191:LEU:N	2.27	0.49
20:p:372:LEU:O	20:p:384:TRP:N	2.39	0.49
1:B:267:LEU:O	1:C:178:HIS:NE2	2.46	0.48
1:F:44:HIS:HD2	1:F:68:LEU:HD12	1.77	0.48
6:M:503:UNK:O	6:M:507:UNK:N	2.46	0.48
19:e:77:VAL:HA	19:e:105:ILE:HA	1.95	0.48
19:f:246:GLN:HG3	19:f:312:ALA:HB2	1.95	0.48
19:f:541:GLU:HB3	19:f:544:GLU:HB3	1.94	0.48
20:g:285:GLY:O	20:g:305:CYS:N	2.46	0.48
20:h:327:TYR:HA	20:h:357:PRO:HB3	1.95	0.48
21:j:333:GLU:OE1	21:j:336:TYR:OH	2.31	0.48
1:F:64:GLU:OE1	19:e:226:LYS:NZ	2.43	0.48
19:f:373:PRO:HB2	19:f:376:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:350:LEU:HD23	19:n:353:ILE:HD12	1.95	0.48
19:n:474:GLU:O	19:n:478:ALA:CB	2.61	0.48
22:s:24:ASN:HD22	22:s:30:ILE:HB	1.77	0.48
1:F:214:VAL:HA	1:F:217:ILE:HD12	1.94	0.48
2:H:196:ARG:NH1	2:H:249:THR:O	2.46	0.48
2:H:207:GLU:HA	2:H:210:ARG:HG2	1.96	0.48
4:K:254:THR:HG22	5:L:177:LEU:HD22	1.96	0.48
7:N:310:UNK:O	7:N:314:UNK:N	2.46	0.48
9:Q:7:UNK:O	9:Q:11:UNK:CB	2.61	0.48
20:g:549:ARG:O	20:g:562:GLY:N	2.34	0.48
19:m:644:VAL:HG21	19:m:702:TRP:CE2	2.48	0.48
19:n:462:ARG:NH2	19:n:534:ASP:OD1	2.47	0.48
8:P:27:UNK:HA	8:P:34:UNK:HA	1.95	0.48
20:h:434:CYS:HB2	20:h:440:ALA:HA	1.96	0.48
19:m:474:GLU:HG2	19:m:477:ARG:HH21	1.78	0.48
19:n:282:GLU:HG2	19:n:329:VAL:HG13	1.94	0.48
1:B:287:ASP:OD2	4:K:266:ARG:HG3	2.13	0.48
1:F:225:SER:OG	1:F:226:ILE:N	2.45	0.48
4:K:47:ARG:O	4:K:51:ALA:CB	2.62	0.48
19:m:438:VAL:HA	19:m:441:LYS:HB3	1.95	0.48
19:m:475:GLN:OE1	19:m:594:ARG:NH2	2.46	0.48
19:m:617:GLU:HA	19:m:620:HIS:HD1	1.78	0.48
4:K:77:THR:HB	4:K:144:TYR:CE2	2.49	0.48
4:K:272:ASN:O	4:K:276:SER:OG	2.27	0.48
8:O:35:UNK:HA	8:O:75:UNK:O	2.13	0.48
20:h:313:THR:OG1	20:h:314:PHE:N	2.43	0.48
21:j:60:PHE:HB3	21:j:152:TRP:CE2	2.48	0.48
19:m:264:ARG:HD2	19:m:274:GLU:HG2	1.95	0.48
19:m:911:LEU:O	19:m:915:LEU:CB	2.61	0.48
20:p:358:VAL:HA	20:p:376:SER:HA	1.96	0.48
1:B:179:SER:OG	1:B:285:LYS:O	2.23	0.48
3:J:141:CYS:HB3	3:J:309:THR:HB	1.96	0.48
4:K:117:LEU:HD21	4:K:152:GLN:HB3	1.95	0.48
9:Q:79:UNK:O	9:Q:83:UNK:CB	2.61	0.48
20:g:482:LEU:O	20:g:491:LEU:N	2.47	0.48
21:j:66:GLY:O	21:j:70:LEU:N	2.46	0.48
19:n:751:ARG:O	19:n:755:TRP:CB	2.61	0.48
24:z:1019:UNK:O	24:z:1023:UNK:CB	2.61	0.48
1:C:133:ASN:HB3	1:C:360:LYS:HZ2	1.78	0.48
1:I:145:LEU:O	1:I:343:GLY:HA3	2.14	0.48
7:N:276:UNK:O	7:N:280:UNK:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:232:PHE:HB3	19:f:235:LYS:HB2	1.95	0.48
19:m:579:ASN:HA	19:m:582:PHE:HD2	1.79	0.48
19:n:272:LEU:HD13	19:n:341:LEU:HD22	1.94	0.48
19:n:365:ARG:HG3	19:n:433:LEU:HD11	1.94	0.48
19:n:563:ARG:HA	19:n:563:ARG:HE	1.76	0.48
1:B:238:LYS:HG2	1:B:252:GLY:HA2	1.95	0.48
1:D:261:LEU:HD21	1:D:268:ILE:HB	1.95	0.48
1:F:76:GLU:HG2	1:F:188:ARG:HH12	1.79	0.48
2:H:66:THR:OG1	2:H:68:LYS:NZ	2.47	0.48
2:H:178:LEU:HG	2:H:180:LEU:H	1.78	0.48
1:I:368:ALA:HA	1:I:371:ILE:HD12	1.95	0.48
5:L:73:SER:O	5:L:77:ASN:N	2.43	0.48
12:X:175:THR:OG1	19:f:759:ARG:NH1	2.36	0.48
19:f:776:PRO:HA	19:f:779:ILE:HD12	1.96	0.48
19:f:899:TRP:HA	19:f:902:LYS:HD2	1.94	0.48
21:j:124:SER:OG	21:j:125:ALA:N	2.46	0.48
20:o:386:LEU:HD23	20:o:386:LEU:HA	1.74	0.48
1:D:323:PRO:HG2	1:D:326:VAL:HG21	1.95	0.48
1:F:154:THR:HG22	1:F:172:GLU:H	1.78	0.48
1:G:13:VAL:O	1:G:341:TRP:NE1	2.42	0.48
1:G:104:GLU:HG2	1:G:133:ASN:H	1.78	0.48
20:o:216:ASN:HA	20:p:209:ARG:HD2	1.95	0.48
22:s:78:ILE:HG12	22:s:91:ILE:HA	1.95	0.48
1:A:183:ILE:HD13	1:A:272:SER:HB3	1.96	0.47
1:D:347:LEU:HD11	1:D:356:MET:HE1	1.94	0.47
1:G:56:ILE:HG21	1:G:88:ARG:HD3	1.95	0.47
1:I:10:GLN:NE2	1:I:26:ALA:O	2.46	0.47
19:f:837:ALA:O	19:f:841:PHE:HB2	2.14	0.47
21:j:177:PHE:O	21:j:181:PHE:HB3	2.14	0.47
1:A:46:ARG:HH12	15:a:64:VAL:HG13	1.79	0.47
1:E:95:SER:OG	1:E:96:LYS:N	2.46	0.47
1:G:56:ILE:HG22	1:G:58:ILE:HD11	1.96	0.47
2:H:206:ARG:HA	2:H:209:VAL:HG12	1.96	0.47
4:K:43:ASP:O	4:K:47:ARG:CB	2.55	0.47
19:e:246:GLN:OE1	19:e:309:ARG:NH1	2.46	0.47
19:f:433:LEU:HA	19:f:436:ASP:OD2	2.14	0.47
20:h:573:VAL:HB	20:h:576:GLN:HB2	1.96	0.47
1:A:35:PHE:HB2	1:A:59:GLY:HA2	1.96	0.47
1:C:113:ALA:O	1:C:116:ASN:ND2	2.47	0.47
1:G:42:PRO:HA	1:G:69:LEU:HA	1.96	0.47
1:I:126:GLU:O	1:I:130:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:SER:HB2	1:I:305:THR:HG23	1.95	0.47
3:J:324:ARG:NH2	3:J:341:PHE:O	2.45	0.47
19:e:257:GLN:NE2	19:e:319:ASP:O	2.45	0.47
19:e:774:LEU:O	19:e:778:ALA:N	2.46	0.47
19:f:367:ILE:HD12	19:f:433:LEU:HD22	1.95	0.47
19:n:324:GLN:HA	19:n:327:GLU:HG2	1.96	0.47
19:n:527:TYR:HA	19:n:553:TYR:CE1	2.50	0.47
21:q:248:ASP:O	21:q:252:ASP:CB	2.62	0.47
21:r:57:ILE:O	21:r:106:VAL:HA	2.13	0.47
1:C:15:ASP:OD2	1:C:22:LYS:HE2	2.13	0.47
1:E:38:TYR:HE1	1:E:62:ALA:HB1	1.79	0.47
1:G:15:ASP:HB3	1:G:22:LYS:HB2	1.97	0.47
19:f:434:LEU:HA	19:f:437:ILE:HD12	1.96	0.47
20:h:452:PRO:HG2	20:h:476:PHE:CD2	2.49	0.47
20:h:524:ASP:HA	20:h:538:SER:HB2	1.96	0.47
21:j:74:LEU:HD23	21:j:280:LEU:HD11	1.97	0.47
21:j:336:TYR:HA	21:j:339:PHE:CE1	2.50	0.47
19:m:761:PRO:HG2	19:m:764:ILE:HD12	1.96	0.47
19:n:839:THR:O	19:n:843:PHE:CB	2.62	0.47
21:r:249:GLU:O	21:r:253:PHE:CB	2.63	0.47
1:F:75:MET:O	1:F:188:ARG:NH2	2.47	0.47
1:F:83:TRP:CE2	1:F:123:ARG:HG2	2.50	0.47
1:G:36:PRO:CB	1:G:38:TYR:CE1	2.88	0.47
1:G:51:ALA:HB2	1:I:173:GLY:HA3	1.96	0.47
1:G:300:LEU:HD12	1:G:332:ALA:HB2	1.96	0.47
1:I:199:ARG:HD2	3:J:96:LEU:HD13	1.97	0.47
5:L:25:LEU:HD13	5:L:43:VAL:HG11	1.95	0.47
20:g:308:ALA:O	20:g:327:TYR:N	2.41	0.47
20:g:373:ILE:HA	20:g:383:SER:HA	1.96	0.47
21:j:168:GLU:HG2	21:j:171:ARG:HH11	1.78	0.47
19:m:375:GLN:HE21	19:m:379:ARG:HH22	1.63	0.47
19:m:408:GLU:HA	19:m:411:LYS:HE2	1.95	0.47
1:B:189:ASP:OD2	1:B:261:LEU:HD21	2.15	0.47
1:F:67:GLY:HA3	2:H:289:ILE:HG23	1.96	0.47
1:F:236:THR:OG1	1:F:237:GLU:N	2.48	0.47
1:G:28:ASP:HB2	1:G:341:TRP:HH2	1.78	0.47
2:H:70:PRO:HG3	2:H:85:ILE:HD12	1.96	0.47
19:e:705:LYS:O	19:e:710:ASN:N	2.45	0.47
21:j:146:MET:HG3	21:j:339:PHE:HZ	1.80	0.47
21:j:331:LYS:HG2	21:j:333:GLU:OE2	2.15	0.47
19:n:267:ALA:HB2	19:n:379:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:OG	1:A:96:LYS:N	2.47	0.47
1:A:121:ARG:HD2	1:A:372:HIS:CE1	2.50	0.47
1:F:113:ALA:HB3	1:F:116:ASN:HD21	1.80	0.47
2:H:193:LEU:HD12	2:H:209:VAL:HG23	1.95	0.47
3:J:76:TYR:HA	3:J:80:LEU:HD12	1.95	0.47
5:L:108:ARG:HD3	5:L:117:SER:HB3	1.96	0.47
10:U:61:LEU:O	10:U:96:SER:N	2.46	0.47
20:h:256:VAL:HG23	20:h:566:GLY:HA2	1.97	0.47
20:h:470:LEU:HB3	20:h:482:LEU:HD11	1.95	0.47
19:m:553:TYR:CE2	19:m:557:ILE:HD11	2.49	0.47
19:n:367:ILE:HB	19:n:372:TYR:HB2	1.96	0.47
20:o:337:ARG:HD3	20:p:221:TYR:O	2.15	0.47
20:o:474:SER:OG	20:o:502:TYR:O	2.29	0.47
20:o:503:ASP:OD1	20:o:504:VAL:N	2.43	0.47
1:B:15:ASP:OD2	1:B:340:THR:OG1	2.31	0.47
1:E:296:SER:OG	1:E:297:ASN:N	2.48	0.47
1:G:18:SER:N	25:G:800:ADP:O3B	2.44	0.47
3:J:119:LEU:HD13	3:J:372:SER:HA	1.97	0.47
9:R:57:UNK:O	9:R:61:UNK:CB	2.63	0.47
21:j:363:LEU:O	21:j:366:GLN:NE2	2.48	0.47
19:n:704:ARG:O	19:n:708:GLN:CB	2.63	0.47
20:o:201:ASP:OD2	20:o:339:ASN:ND2	2.47	0.47
20:p:481:LYS:HA	20:p:493:SER:HA	1.97	0.47
1:C:204:ASP:OD1	1:C:204:ASP:N	2.47	0.47
6:M:620:UNK:O	6:M:624:UNK:CB	2.63	0.47
20:h:272:SER:HB3	20:h:312:ALA:HB3	1.96	0.47
20:h:409:THR:N	20:h:424:GLY:O	2.48	0.47
19:m:526:ALA:HA	19:m:529:ASN:HD22	1.80	0.47
19:n:265:ASP:HB3	19:n:268:SER:HB2	1.96	0.47
20:o:208:GLU:O	20:o:294:TYR:CZ	2.67	0.47
21:q:90:TYR:HA	21:q:105:ASN:HA	1.95	0.47
22:s:75:LYS:HZ3	22:t:61:ASP:CG	2.18	0.47
1:A:113:ALA:O	1:A:116:ASN:ND2	2.47	0.47
1:E:113:ALA:O	1:E:116:ASN:ND2	2.48	0.47
1:F:10:GLN:NE2	1:F:26:ALA:O	2.36	0.47
19:n:564:ILE:HA	19:n:567:ARG:HB2	1.97	0.47
20:o:518:ASP:OD2	20:o:520:MET:HB2	2.15	0.47
1:A:11:PRO:HB3	1:A:107:PRO:HB2	1.96	0.46
1:C:267:LEU:O	1:D:178:HIS:NE2	2.44	0.46
1:C:318:VAL:HG12	1:C:328:ILE:HD13	1.97	0.46
1:G:131:THR:OG1	1:G:132:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:245:ASN:HA	3:J:263:ARG:HH21	1.79	0.46
7:N:433:UNK:O	7:N:437:UNK:N	2.49	0.46
19:f:381:VAL:HA	19:f:384:ILE:HD12	1.96	0.46
19:f:676:HIS:HB3	19:f:679:GLY:H	1.80	0.46
1:B:232:GLU:OE2	1:B:257:ARG:NH2	2.48	0.46
1:D:143:ALA:HA	1:D:157:VAL:HG11	1.97	0.46
1:D:168:VAL:HG22	1:D:180:ILE:HG12	1.97	0.46
2:H:189:LEU:HD13	2:H:257:CYS:HB2	1.97	0.46
4:K:185:THR:HG22	4:K:187:GLN:HG3	1.98	0.46
7:N:602:UNK:O	7:N:606:UNK:N	2.48	0.46
13:Y:516:UNK:HA	13:Y:526:UNK:HA	1.97	0.46
20:o:249:ARG:NH1	22:t:6:GLU:CD	2.70	0.46
20:o:412:SER:OG	20:o:458:CYS:SG	2.74	0.46
20:p:458:CYS:HA	20:p:471:PHE:HA	1.96	0.46
1:C:219:GLU:OE2	25:C:800:ADP:H2'	2.15	0.46
1:D:68:LEU:HD12	1:F:171:TYR:HD2	1.81	0.46
1:E:30:ILE:HD11	15:a:5:LYS:HB3	1.97	0.46
1:F:206:HIS:NE2	1:G:270:GLU:OE2	2.49	0.46
20:h:366:THR:H	20:h:369:ALA:HB3	1.80	0.46
21:j:68:THR:O	21:j:72:THR:OG1	2.27	0.46
21:j:249:GLU:HG2	21:j:328:THR:HA	1.96	0.46
19:n:482:ARG:NE	19:n:587:ARG:O	2.48	0.46
19:n:528:GLU:HA	19:n:531:LYS:HG2	1.97	0.46
20:o:364:VAL:O	20:o:371:ASN:N	2.38	0.46
20:o:419:ASN:O	20:o:435:ARG:N	2.48	0.46
5:L:264:GLU:O	5:L:268:ARG:CB	2.57	0.46
19:f:547:GLU:HG2	19:f:551:LYS:HE2	1.97	0.46
1:E:219:GLU:OE2	25:E:800:ADP:H2'	2.15	0.46
2:H:14:SER:HB3	2:H:183:ARG:HH22	1.81	0.46
3:J:209:ASP:HB3	3:J:213:ARG:HH21	1.81	0.46
12:X:198:LYS:NZ	23:x:195:ASP:OD1	2.43	0.46
19:n:285:LEU:HD12	19:n:329:VAL:HG21	1.98	0.46
1:B:113:ALA:O	1:B:116:ASN:ND2	2.48	0.46
1:D:208:SER:N	1:E:271:GLU:OE2	2.26	0.46
1:F:103:SER:HB2	1:F:132:PHE:HB3	1.98	0.46
4:K:72:ASP:HB3	4:K:91:ARG:HH11	1.81	0.46
19:f:724:ARG:HB2	19:f:734:LYS:H	1.81	0.46
21:j:168:GLU:HG2	21:j:171:ARG:HE	1.80	0.46
21:j:256:SER:O	21:j:260:ARG:CB	2.62	0.46
19:m:756:LEU:HB3	19:m:758:PHE:HD1	1.80	0.46
22:s:68:PHE:HA	22:s:82:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:VAL:HG11	1:D:321:LEU:HB3	1.97	0.46
1:E:28:ASP:HB2	1:E:341:TRP:HH2	1.80	0.46
1:E:126:GLU:O	1:E:130:GLU:HB2	2.15	0.46
1:F:361:LYS:HE2	1:F:361:LYS:HB2	1.77	0.46
4:K:13:LYS:HB3	4:K:40:LEU:HD11	1.96	0.46
19:f:733:LEU:H	21:j:362:PHE:HE1	1.64	0.46
19:f:751:ARG:O	19:f:755:TRP:HB2	2.16	0.46
19:f:825:GLU:HG3	19:f:828:LYS:H	1.79	0.46
21:j:221:HIS:N	21:j:264:GLN:O	2.48	0.46
21:j:358:ASP:N	21:j:358:ASP:OD1	2.47	0.46
19:n:475:GLN:HE22	19:n:594:ARG:N	2.14	0.46
20:o:335:ASP:O	20:o:338:SER:OG	2.26	0.46
22:t:68:PHE:HA	22:t:82:PRO:HD2	1.97	0.46
1:G:239:ALA:HB3	1:G:255:ARG:HH12	1.80	0.46
4:K:60:ASP:OD1	4:K:61:GLN:N	2.49	0.46
4:K:121:ARG:HE	4:K:121:ARG:HB3	1.57	0.46
5:L:60:LEU:O	5:L:65:ASN:ND2	2.49	0.46
19:e:208:PRO:O	19:e:252:TRP:NE1	2.46	0.46
20:h:288:LEU:HD22	20:h:299:PRO:HB2	1.98	0.46
20:o:337:ARG:HA	20:o:337:ARG:HD2	1.83	0.46
21:q:85:GLY:HA2	21:q:110:ASP:H	1.81	0.46
1:B:318:VAL:HG12	1:B:328:ILE:HD13	1.98	0.46
1:I:363:TYR:HE1	1:I:371:ILE:HD11	1.81	0.46
4:K:81:ASP:HA	4:K:87:PHE:HA	1.97	0.46
5:L:139:ASP:HB2	5:L:142:LYS:HB2	1.98	0.46
19:e:568:LEU:O	19:e:572:LEU:CB	2.64	0.46
1:D:352:THR:HA	1:D:355:LYS:HE2	1.98	0.46
20:o:547:LEU:HD22	20:o:563:ASP:HA	1.98	0.46
5:L:16:LEU:HD11	5:L:24:ASN:HB3	1.97	0.45
5:L:74:PRO:HD3	5:L:120:TYR:HE1	1.81	0.45
10:U:29:ILE:HA	10:U:50:ILE:H	1.81	0.45
17:c:1:MET:N	19:m:307:GLY:O	2.49	0.45
19:e:297:VAL:O	19:e:300:THR:OG1	2.24	0.45
19:f:648:ILE:HD12	19:f:699:PHE:HE1	1.81	0.45
19:f:786:ARG:HE	20:h:306:GLN:NE2	2.13	0.45
21:j:363:LEU:HA	21:j:366:GLN:HE21	1.80	0.45
22:k:83:ASP:N	22:k:86:TYR:O	2.47	0.45
1:D:207:SER:N	1:D:210:GLU:OE2	2.37	0.45
5:L:136:LYS:O	5:L:148:TRP:N	2.45	0.45
14:Z:1003:UNK:O	14:Z:1007:UNK:CB	2.64	0.45
19:f:540:LYS:HG3	19:f:541:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:n:216:VAL:HG21	19:n:232:PHE:HE1	1.80	0.45
19:n:361:PHE:HB2	19:n:426:GLU:OE2	2.17	0.45
1:G:36:PRO:HB2	1:G:38:TYR:CD1	2.50	0.45
1:I:158:LEU:HD11	1:I:275:ILE:HG23	1.99	0.45
4:K:99:ASP:HB3	4:K:102:ARG:HB3	1.97	0.45
19:e:213:ILE:HG23	19:e:299:LEU:HD22	1.97	0.45
21:j:59:VAL:HG12	21:j:134:ILE:HB	1.98	0.45
21:j:177:PHE:HA	21:j:180:ASP:OD2	2.16	0.45
20:o:307:SER:HB3	20:o:326:THR:HB	1.98	0.45
1:B:8:ALA:HB3	1:B:107:PRO:HD3	1.97	0.45
1:B:121:ARG:NH1	1:B:375:THR:OG1	2.49	0.45
8:O:24:UNK:O	8:O:37:UNK:N	2.49	0.45
19:f:864:LEU:O	19:f:914:ARG:NH1	2.49	0.45
20:h:521:GLY:O	20:h:541:VAL:N	2.39	0.45
21:j:69:THR:HG22	21:j:73:LYS:HE2	1.98	0.45
19:m:266:PRO:HA	19:m:274:GLU:OE2	2.16	0.45
19:m:748:LYS:HD2	19:m:751:ARG:HH21	1.81	0.45
20:o:251:SER:HB3	20:o:566:GLY:HA2	1.97	0.45
20:o:529:ASN:OD1	20:o:529:ASN:N	2.48	0.45
20:p:187:LYS:HG2	22:s:30:ILE:HD13	1.97	0.45
20:p:273:TYR:O	20:p:286:VAL:N	2.49	0.45
21:q:281:ASP:O	21:q:285:LYS:CB	2.65	0.45
23:x:175:THR:HA	23:x:178:LYS:HD2	1.99	0.45
3:J:127:ALA:HB1	3:J:306:ILE:HG21	1.99	0.45
4:K:121:ARG:O	4:K:125:ASP:CB	2.60	0.45
5:L:194:THR:O	5:L:195:ARG:NH2	2.45	0.45
19:f:756:LEU:HD23	19:f:758:PHE:HE1	1.80	0.45
19:f:815:LEU:HA	19:f:815:LEU:HD23	1.79	0.45
20:h:481:LYS:NZ	20:h:491:LEU:O	2.47	0.45
21:j:150:GLN:NE2	21:j:265:TYR:OH	2.50	0.45
19:m:466:MET:HE3	19:m:534:ASP:OD2	2.17	0.45
20:o:268:LEU:HD11	20:p:218:PHE:HZ	1.82	0.45
1:B:141:MET:HG2	1:B:376:PHE:HE1	1.80	0.45
1:B:257:ARG:HH12	1:C:118:ARG:HH12	1.65	0.45
1:G:327:LYS:HE2	1:G:329:ARG:HD2	1.98	0.45
3:J:273:GLN:HE22	3:J:326:LEU:HD21	1.81	0.45
8:P:24:UNK:O	8:P:37:UNK:N	2.50	0.45
19:f:550:MET:O	19:f:554:ASP:HB2	2.16	0.45
20:g:519:GLY:HA2	20:g:546:ALA:HA	1.98	0.45
22:k:39:THR:O	22:k:43:ALA:CB	2.64	0.45
19:m:268:SER:OG	19:m:269:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:m:268:SER:HA	19:m:386:ARG:HH12	1.81	0.45
20:o:275:ASN:HD22	20:o:284:ASP:HA	1.82	0.45
20:o:428:GLY:HA2	20:o:453:ILE:HD11	1.98	0.45
20:o:582:ASN:OD1	20:o:583:ASP:N	2.48	0.45
1:C:145:LEU:O	1:C:343:GLY:HA3	2.16	0.45
4:K:121:ARG:HB2	4:K:145:ALA:HB2	1.98	0.45
6:M:201:UNK:O	6:M:205:UNK:N	2.49	0.45
13:Y:515:UNK:O	13:Y:527:UNK:N	2.49	0.45
19:e:250:ASN:HA	19:e:253:ILE:HD12	1.98	0.45
19:f:759:ARG:HA	19:f:759:ARG:HD3	1.76	0.45
19:f:894:SER:OG	19:f:895:ASN:OD1	2.35	0.45
20:h:258:CYS:O	20:h:272:SER:OG	2.33	0.45
20:h:400:HIS:CG	20:h:401:LYS:H	2.34	0.45
21:j:359:GLU:HB3	21:j:364:MET:HE3	1.98	0.45
19:m:272:LEU:HB2	19:m:341:LEU:HD11	1.98	0.45
19:n:368:ARG:HG3	19:n:437:ILE:HG12	1.98	0.45
20:p:379:GLY:O	20:p:398:LEU:N	2.49	0.45
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.85	0.45
1:B:147:LEU:HA	1:B:147:LEU:HD23	1.81	0.45
1:B:323:PRO:HG2	1:B:326:VAL:HG21	1.97	0.45
1:C:160:SER:HA	1:C:165:THR:HG22	1.98	0.45
1:C:240:GLN:HG2	1:C:250:GLU:HG2	1.99	0.45
1:E:159:ASP:HB3	1:E:301:SER:HB3	1.99	0.45
1:F:45:VAL:O	2:H:170:ALA:N	2.43	0.45
1:I:95:SER:OG	1:I:96:LYS:N	2.50	0.45
1:I:110:LEU:HD23	1:I:139:ILE:HG12	1.99	0.45
4:K:97:LYS:O	4:K:106:SER:N	2.45	0.45
9:Q:33:UNK:O	9:Q:37:UNK:CB	2.64	0.45
20:h:383:SER:O	20:h:393:GLN:N	2.50	0.45
20:h:414:PRO:HD3	20:h:421:PHE:HA	1.97	0.45
19:m:475:GLN:O	19:m:479:VAL:HG23	2.17	0.45
19:m:714:SER:HA	19:m:742:GLU:HG2	1.99	0.45
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.76	0.45
1:C:308:LYS:HE2	15:a:38:GLU:HB2	1.99	0.45
1:E:205:PHE:HD1	1:E:210:GLU:HG2	1.81	0.45
4:K:154:ILE:O	4:K:179:PHE:N	2.49	0.45
4:K:196:VAL:HB	4:K:206:LEU:HB3	1.99	0.45
5:L:134:ILE:HB	5:L:150:SER:HB2	1.98	0.45
20:g:478:TRP:O	20:g:497:ASN:N	2.34	0.45
19:n:282:GLU:OE2	19:n:333:ASN:HA	2.17	0.45
19:n:434:LEU:HA	19:n:437:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:564:SER:OG	20:o:565:GLU:N	2.50	0.45
1:B:74:PRO:HB3	1:B:85:ASP:HB2	1.98	0.45
1:B:130:GLU:O	19:m:368:ARG:NH2	2.40	0.45
1:D:56:ILE:HD13	1:D:88:ARG:HD3	2.00	0.45
1:E:45:VAL:HG13	16:b:82:GLY:H	1.82	0.45
2:H:8:LEU:HB2	2:H:103:VAL:HG12	1.99	0.45
5:L:35:LEU:HA	5:L:38:ASP:OD2	2.16	0.45
5:L:67:ASP:CG	5:L:87:ALA:H	2.23	0.45
19:f:577:ASN:OD1	19:f:578:ALA:N	2.49	0.45
22:k:68:PHE:HA	22:k:81:ALA:HA	1.98	0.45
19:m:278:TRP:HB2	19:m:336:MET:HG2	1.99	0.45
20:o:254:ARG:HG3	20:o:275:ASN:HA	1.98	0.45
20:o:350:SER:HB3	20:o:353:ALA:HB2	1.99	0.45
1:A:13:VAL:HA	1:A:109:LEU:HB3	1.99	0.44
1:B:48:MET:HB3	1:D:173:GLY:HA2	1.97	0.44
1:C:273:GLU:HB3	1:C:277:GLU:HB2	1.99	0.44
3:J:43:ILE:H	3:J:51:PRO:HB2	1.81	0.44
19:f:915:LEU:HD21	19:f:1040:VAL:HG11	1.98	0.44
20:h:205:ARG:O	20:h:209:ARG:CB	2.65	0.44
20:h:307:SER:OG	20:h:308:ALA:N	2.50	0.44
21:j:283:LEU:O	21:j:287:ILE:HB	2.17	0.44
21:q:181:PHE:O	21:q:185:MET:N	2.50	0.44
1:A:18:SER:OG	1:A:163:GLY:N	2.50	0.44
1:I:74:PRO:HB2	1:I:86:MET:HG2	1.98	0.44
3:J:82:VAL:HG11	3:J:87:ARG:HD2	1.98	0.44
4:K:102:ARG:NE	4:K:104:GLU:OE1	2.50	0.44
4:K:136:TYR:CZ	5:L:244:ARG:HD2	2.52	0.44
20:h:475:SER:OG	20:h:476:PHE:N	2.48	0.44
21:j:58:LEU:HD11	21:j:123:VAL:HG22	1.97	0.44
21:j:259:ARG:HH11	21:j:310:ILE:HD12	1.83	0.44
19:m:474:GLU:HA	19:m:477:ARG:HE	1.82	0.44
4:K:224:THR:HA	4:K:227:GLU:HB3	1.99	0.44
19:m:648:ILE:HD11	19:m:756:LEU:HD21	1.99	0.44
20:o:304:HIS:HD2	20:o:341:ARG:HB2	1.82	0.44
1:D:53:GLU:OE1	19:f:323:LYS:NZ	2.44	0.44
1:D:298:ILE:O	1:D:331:SER:N	2.49	0.44
1:I:226:ILE:O	1:I:313:ARG:NH1	2.51	0.44
4:K:128:LEU:HD12	4:K:131:TYR:HB3	1.98	0.44
5:L:61:LEU:HD22	5:L:71:TYR:CG	2.53	0.44
20:h:285:GLY:HA3	20:h:309:VAL:H	1.82	0.44
20:h:333:LEU:HD12	20:h:333:LEU:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:j:82:LYS:HA	21:j:87:GLU:OE2	2.17	0.44
21:j:153:ALA:O	21:j:157:ARG:HG2	2.17	0.44
19:m:276:SER:O	19:m:280:ASN:ND2	2.50	0.44
19:n:564:ILE:HG13	19:n:565:THR:N	2.31	0.44
19:n:712:GLY:O	19:n:716:ARG:N	2.51	0.44
1:A:159:ASP:HB3	1:A:301:SER:HB3	1.98	0.44
1:D:360:LYS:HE2	1:D:364:GLU:OE2	2.18	0.44
1:E:39:VAL:HG11	1:E:41:ARG:HH21	1.81	0.44
1:E:208:SER:H	1:F:271:GLU:CD	2.25	0.44
1:G:220:ARG:HD3	1:G:241:TYR:HE1	1.82	0.44
19:f:568:LEU:HA	19:f:571:GLN:HG2	1.99	0.44
20:h:518:ASP:OD2	20:h:520:MET:HB2	2.17	0.44
21:j:143:TRP:CH2	21:j:343:PRO:HB2	2.52	0.44
20:o:513:LEU:HD21	20:o:576:GLN:HB3	2.00	0.44
1:B:20:VAL:O	1:B:22:LYS:NZ	2.48	0.44
1:C:121:ARG:NH1	1:C:375:THR:OG1	2.50	0.44
1:F:254:SER:HA	1:F:257:ARG:HB2	2.00	0.44
9:Q:56:UNK:O	9:Q:60:UNK:CB	2.66	0.44
19:f:549:ALA:O	19:f:553:TYR:CB	2.66	0.44
19:f:920:ARG:O	19:f:923:THR:OG1	2.29	0.44
20:h:535:PRO:HB2	20:h:538:SER:HB3	2.00	0.44
1:B:263:PHE:HE1	1:B:275:ILE:HB	1.83	0.44
1:C:315:LEU:HD23	1:C:315:LEU:HA	1.86	0.44
1:D:9:ASN:O	1:D:106:HIS:ND1	2.37	0.44
1:F:131:THR:OG1	1:F:132:PHE:N	2.51	0.44
1:F:253:PRO:HG2	1:F:257:ARG:HH12	1.82	0.44
4:K:30:ASN:OD1	4:K:103:LYS:NZ	2.50	0.44
4:K:154:ILE:HD13	4:K:154:ILE:HA	1.85	0.44
5:L:19:GLN:HG3	5:L:176:TRP:CZ3	2.53	0.44
21:j:91:LEU:HA	21:j:91:LEU:HD23	1.67	0.44
21:j:141:ARG:HA	21:j:143:TRP:CZ3	2.53	0.44
21:j:324:HIS:HD2	21:j:331:LYS:H	1.66	0.44
19:m:616:ILE:HG22	19:m:620:HIS:CE1	2.52	0.44
19:n:565:THR:OG1	19:n:566:ALA:N	2.50	0.44
20:o:354:HIS:HB3	20:o:376:SER:HB3	1.99	0.44
20:o:365:GLY:HA3	20:o:370:HIS:HA	1.99	0.44
1:F:241:TYR:HD2	1:F:249:ILE:HD11	1.82	0.44
1:G:83:TRP:CD1	1:G:123:ARG:HE	2.35	0.44
4:K:109:GLN:HA	4:K:110:PRO:HD3	1.91	0.44
4:K:136:TYR:OH	4:K:173:TRP:NE1	2.51	0.44
5:L:60:LEU:O	5:L:120:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:392:LEU:HD23	19:f:392:LEU:HA	1.86	0.44
21:j:139:MET:HB2	21:j:233:LYS:O	2.18	0.44
19:n:358:VAL:HA	19:n:426:GLU:OE2	2.18	0.44
22:t:8:LEU:HD12	22:t:31:LYS:HE2	1.99	0.44
1:E:73:TYR:OH	1:E:212:GLU:OE2	2.27	0.44
1:F:147:LEU:HD23	1:F:147:LEU:HA	1.80	0.44
1:F:303:GLY:N	25:F:800:ADP:O2A	2.37	0.44
4:K:241:THR:O	4:K:244:SER:OG	2.29	0.44
19:f:720:ILE:HG22	19:f:721:GLU:OE2	2.18	0.44
20:h:340:LYS:HD3	20:h:344:VAL:HG12	1.99	0.44
20:h:343:PRO:HG2	20:h:346:ARG:HE	1.83	0.44
20:h:510:HIS:HD2	20:h:579:VAL:H	1.66	0.44
19:m:641:LEU:HD23	19:m:641:LEU:HA	1.76	0.44
19:n:597:ILE:O	19:n:601:ILE:CB	2.66	0.44
20:o:553:THR:HG22	20:o:555:SER:H	1.82	0.44
22:s:72:ARG:HE	22:t:68:PHE:HB3	1.83	0.44
4:K:79:HIS:CD2	4:K:155:ILE:HG21	2.53	0.43
19:f:528:GLU:O	19:f:531:LYS:HG2	2.17	0.43
20:h:245:PHE:CD2	20:h:570:ILE:HD11	2.54	0.43
20:h:572:ASP:OD1	20:h:573:VAL:N	2.50	0.43
1:A:41:ARG:HH12	1:A:72:ARG:HD3	1.84	0.43
1:B:10:GLN:OE1	19:n:246:GLN:NE2	2.47	0.43
1:B:197:TYR:HD1	1:B:197:TYR:HA	1.67	0.43
1:B:226:ILE:O	1:B:313:ARG:NH1	2.50	0.43
1:C:42:PRO:HA	1:C:69:LEU:HA	2.00	0.43
1:F:199:ARG:HH22	1:G:182:ARG:HB3	1.83	0.43
1:I:200:LYS:NZ	3:J:387:TRP:O	2.51	0.43
7:N:478:UNK:O	7:N:482:UNK:N	2.51	0.43
19:f:850:LEU:HD23	19:f:850:LEU:HA	1.79	0.43
20:g:455:GLY:O	20:g:474:SER:N	2.51	0.43
1:A:204:ASP:OD1	1:A:204:ASP:N	2.51	0.43
1:I:207:SER:HB3	1:I:210:GLU:HB2	1.99	0.43
13:Y:517:UNK:N	13:Y:525:UNK:O	2.51	0.43
19:f:592:PHE:O	19:f:598:ARG:NH2	2.52	0.43
20:h:360:CYS:HB2	20:h:410:SER:HA	1.99	0.43
19:m:619:LEU:HA	19:m:619:LEU:HD23	1.75	0.43
22:t:18:GLN:NE2	22:t:93:ASN:OD1	2.51	0.43
1:A:57:PHE:HD2	1:A:69:LEU:HD11	1.83	0.43
1:G:152:ARG:HH21	16:b:48:ILE:HD11	1.83	0.43
9:Q:64:UNK:O	9:Q:68:UNK:CB	2.66	0.43
19:f:700:ASP:O	19:f:704:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:786:ARG:HH11	20:h:306:GLN:HE21	1.66	0.43
21:j:143:TRP:HA	21:j:339:PHE:CE2	2.54	0.43
1:F:126:GLU:O	1:F:130:GLU:HB2	2.19	0.43
2:H:300:SER:HA	2:H:335:ARG:HB2	2.01	0.43
1:I:168:VAL:HG22	1:I:180:ILE:HG12	1.99	0.43
5:L:159:LYS:HD2	5:L:164:THR:HG23	1.99	0.43
19:f:393:LEU:HA	19:f:396:LEU:HB3	2.00	0.43
21:j:282:LEU:O	21:j:286:TYR:HB2	2.18	0.43
19:n:232:PHE:HB2	19:n:236:VAL:HG23	2.01	0.43
20:o:413:PHE:CE2	20:o:421:PHE:HB3	2.54	0.43
21:r:144:THR:O	21:r:148:SER:CB	2.66	0.43
1:B:128:PHE:O	1:B:133:ASN:N	2.52	0.43
1:C:168:VAL:HG22	1:C:180:ILE:HG12	2.00	0.43
1:C:206:HIS:NE2	1:D:270:GLU:OE2	2.52	0.43
1:D:44:HIS:CG	1:F:176:MET:HG2	2.54	0.43
1:E:67:GLY:HA3	1:G:290:LEU:HG	1.99	0.43
2:H:12:ASN:CG	2:H:86:TRP:HE1	2.26	0.43
19:f:565:THR:HA	19:f:568:LEU:HD12	2.01	0.43
19:f:724:ARG:HH12	19:f:726:ARG:HD3	1.83	0.43
20:h:254:ARG:O	20:h:566:GLY:N	2.51	0.43
21:j:119:LEU:O	21:j:123:VAL:N	2.52	0.43
22:k:18:GLN:N	22:k:91:ILE:O	2.52	0.43
20:o:453:ILE:HD13	20:o:475:SER:HB2	2.00	0.43
20:o:472:VAL:HB	20:o:506:TRP:CZ2	2.54	0.43
1:F:75:MET:HE3	1:F:75:MET:HB2	1.89	0.43
1:F:354:LYS:HG2	1:F:357:TRP:CH2	2.54	0.43
1:G:197:TYR:HD1	1:G:197:TYR:HA	1.71	0.43
6:M:162:UNK:O	6:M:166:UNK:CB	2.67	0.43
19:f:864:LEU:HD23	19:f:864:LEU:HA	1.81	0.43
20:h:315:ALA:HB3	20:h:318:HIS:HB2	1.99	0.43
20:o:460:ALA:HB1	20:o:508:PRO:HA	2.00	0.43
22:s:52:LYS:HB3	22:t:49:PHE:CE1	2.54	0.43
1:G:181:MET:HB2	1:G:278:VAL:HG13	2.01	0.43
1:I:96:LYS:HA	1:I:100:GLN:HG2	2.01	0.43
1:I:330:ILE:HB	16:b:20:TYR:HB2	2.00	0.43
9:Q:34:UNK:O	9:Q:38:UNK:CB	2.66	0.43
17:c:2:ALA:HB1	17:c:5:LYS:HD3	2.01	0.43
20:h:256:VAL:O	20:h:548:ASN:ND2	2.52	0.43
19:n:185:LYS:O	19:n:189:LEU:CB	2.67	0.43
19:n:479:VAL:HG11	19:n:590:ALA:HB3	2.00	0.43
20:o:327:TYR:HA	20:o:357:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:494:PHE:HZ	20:o:528:LEU:HD21	1.83	0.43
20:p:185:GLU:CD	20:p:185:GLU:N	2.74	0.43
1:C:366:ASP:HB2	1:C:370:SER:HB3	2.00	0.43
1:D:219:GLU:OE2	25:D:800:ADP:H2'	2.18	0.43
1:E:36:PRO:HB2	1:E:38:TYR:CD2	2.54	0.43
4:K:47:ARG:HE	4:K:48:GLU:HG3	1.84	0.43
21:j:91:LEU:O	21:j:104:CYS:N	2.47	0.43
19:n:340:PRO:HG2	19:n:360:ILE:HG12	2.01	0.43
19:n:556:ARG:O	19:n:560:VAL:HB	2.16	0.43
20:o:277:GLU:H	20:o:277:GLU:HG3	1.52	0.43
20:o:396:MET:HE3	20:o:396:MET:HB2	1.55	0.43
1:G:134:VAL:HG12	1:G:136:ALA:H	1.84	0.43
1:G:168:VAL:HG22	1:G:180:ILE:HG12	2.00	0.43
2:H:98:PRO:HB2	2:H:129:THR:HG22	2.01	0.43
1:I:183:ILE:HD11	1:I:273:GLU:H	1.84	0.43
4:K:159:GLU:OE2	4:K:161:HIS:HB3	2.18	0.43
19:e:526:ALA:HB1	19:e:553:TYR:HA	2.00	0.43
19:f:549:ALA:O	19:f:553:TYR:HB2	2.19	0.43
20:h:480:VAL:O	20:h:494:PHE:N	2.52	0.43
21:j:132:LEU:HD23	21:j:132:LEU:HA	1.90	0.43
19:m:304:LEU:HD23	19:m:304:LEU:HA	1.87	0.43
1:A:67:GLY:HA3	1:C:290:LEU:HG	2.00	0.42
1:E:207:SER:OG	1:F:271:GLU:OE2	2.25	0.42
1:F:362:GLU:OE2	1:F:366:ASP:OD2	2.38	0.42
1:G:227:ASN:HB3	1:G:230:LYS:HB2	2.00	0.42
13:Y:181:UNK:N	13:Y:285:UNK:O	2.52	0.42
19:f:238:ASP:HB2	19:f:241:PHE:HB3	2.01	0.42
19:f:875:SER:O	19:f:879:ASN:ND2	2.52	0.42
20:h:479:THR:HA	20:h:495:GLU:HA	2.00	0.42
1:I:30:ILE:HD13	16:b:8:ASP:HB2	2.00	0.42
1:I:298:ILE:HB	1:I:330:ILE:HA	2.00	0.42
11:V:146:PHE:HA	11:V:153:PHE:HA	2.02	0.42
21:j:253:PHE:CZ	21:j:336:TYR:CE1	3.04	0.42
19:n:548:ALA:O	19:n:552:ARG:HB2	2.17	0.42
20:o:245:PHE:HD1	20:o:245:PHE:HA	1.65	0.42
20:o:469:HIS:CD2	20:o:469:HIS:H	2.35	0.42
1:B:305:THR:O	1:B:336:ARG:NH1	2.52	0.42
1:C:228:PRO:O	1:C:232:GLU:CB	2.63	0.42
1:D:159:ASP:HB3	1:D:301:SER:HB3	2.01	0.42
1:D:273:GLU:HB3	1:D:277:GLU:HB2	2.01	0.42
1:E:280:VAL:HG11	1:E:321:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:LEU:HD23	1:F:198:LEU:HA	1.83	0.42
1:G:145:LEU:O	1:G:343:GLY:HA3	2.19	0.42
3:J:210:ILE:O	3:J:214:THR:OG1	2.32	0.42
4:K:225:ALA:O	4:K:229:ILE:HG12	2.20	0.42
9:Q:66:UNK:O	9:Q:70:UNK:CB	2.67	0.42
19:f:561:GLU:O	19:f:565:THR:OG1	2.25	0.42
20:h:259:LEU:HD23	20:h:271:ALA:HA	2.01	0.42
20:h:459:HIS:CE1	20:h:470:LEU:HB2	2.54	0.42
21:j:86:LEU:H	21:j:109:LEU:HA	1.83	0.42
19:n:349:GLU:HG2	19:n:351:ASP:H	1.84	0.42
20:o:335:ASP:HB3	20:o:344:VAL:HG11	2.01	0.42
20:p:187:LYS:HD2	22:s:30:ILE:HG12	2.00	0.42
1:F:96:LYS:HA	1:F:100:GLN:HG2	2.01	0.42
1:F:197:TYR:HD1	1:F:197:TYR:HA	1.66	0.42
1:I:129:PHE:O	1:I:133:ASN:ND2	2.52	0.42
4:K:13:LYS:HZ2	5:L:31:LEU:HA	1.84	0.42
4:K:159:GLU:OE2	4:K:172:ARG:HG3	2.19	0.42
20:g:589:GLY:O	20:g:593:ALA:HB2	2.20	0.42
19:m:465:GLN:HB2	19:m:546:TRP:HH2	1.83	0.42
19:m:473:HIS:NE2	19:m:523:VAL:HG12	2.35	0.42
19:m:476:LEU:HD23	19:m:476:LEU:HA	1.89	0.42
19:m:581:MET:HE2	19:m:608:LEU:HG	2.02	0.42
20:p:559:ILE:N	20:p:571:TYR:O	2.45	0.42
22:s:9:LYS:HA	22:s:12:GLN:HG2	2.00	0.42
1:I:18:SER:O	1:I:188:ARG:NH2	2.53	0.42
1:I:206:HIS:CE1	3:J:165:PRO:HG3	2.55	0.42
4:K:13:LYS:HD3	4:K:16:ILE:HD12	2.02	0.42
5:L:72:ARG:NH2	5:L:97:GLU:OE2	2.52	0.42
5:L:112:PHE:O	5:L:136:LYS:NZ	2.46	0.42
9:Q:80:UNK:O	9:Q:84:UNK:CB	2.68	0.42
19:e:253:ILE:HG21	19:e:319:ASP:OD2	2.19	0.42
19:f:924:GLN:HA	19:f:927:LEU:HG	2.01	0.42
20:g:383:SER:O	20:g:393:GLN:N	2.51	0.42
20:h:419:ASN:HB2	20:h:435:ARG:HD3	2.01	0.42
21:j:247:ARG:HG3	21:j:249:GLU:H	1.85	0.42
20:o:294:TYR:CE2	20:o:296:LYS:HB3	2.55	0.42
20:o:465:VAL:HG11	20:o:585:TRP:HD1	1.84	0.42
21:r:241:GLU:HA	21:r:246:TYR:H	1.83	0.42
23:x:191:LEU:HA	23:x:191:LEU:HD23	1.83	0.42
1:B:66:ARG:HD2	1:D:289:ASP:OD2	2.19	0.42
1:D:252:GLY:HA3	1:D:253:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:724:ARG:HB3	19:f:725:VAL:H	1.58	0.42
20:h:336:ASN:OD1	20:h:337:ARG:N	2.53	0.42
20:h:470:LEU:HD23	20:h:482:LEU:HD11	2.01	0.42
19:m:519:ALA:O	19:m:523:VAL:HG23	2.19	0.42
1:E:143:ALA:HA	1:E:157:VAL:HG11	2.00	0.42
1:F:260:GLU:OE2	1:F:313:ARG:NH1	2.52	0.42
2:H:236:LEU:O	2:H:254:ARG:NH1	2.48	0.42
1:I:103:SER:HB2	1:I:132:PHE:HB3	2.01	0.42
4:K:33:PHE:HA	4:K:36:VAL:HG12	2.02	0.42
5:L:136:LYS:HB3	5:L:148:TRP:HB3	2.01	0.42
12:X:188:GLN:NE2	23:x:187:GLN:OE1	2.35	0.42
19:f:602:ARG:HA	19:f:605:GLN:CD	2.44	0.42
19:f:736:LYS:HZ3	19:f:740:LEU:HD11	1.84	0.42
19:f:916:GLN:HA	19:f:919:LEU:HD12	2.02	0.42
21:j:317:GLU:HA	21:j:320:ILE:HD11	2.00	0.42
22:s:52:LYS:HE3	22:t:49:PHE:HE1	1.84	0.42
1:A:205:PHE:HD1	1:A:210:GLU:OE2	2.02	0.42
1:F:338:TYR:CE2	18:d:9:LEU:HD13	2.55	0.42
3:J:326:LEU:HD22	3:J:329:LYS:HD2	2.00	0.42
12:X:148:LEU:O	23:x:152:LYS:NZ	2.49	0.42
20:h:356:HIS:HB2	20:h:378:ASP:HB2	2.02	0.42
21:j:57:ILE:HB	21:j:106:VAL:HA	2.01	0.42
19:m:448:MET:HB2	19:m:450:TRP:CE2	2.55	0.42
20:o:579:VAL:O	20:o:581:ARG:N	2.47	0.42
22:s:81:ALA:HB3	22:s:88:LEU:HB3	2.01	0.42
22:t:76:ASN:HA	22:t:94:PRO:HD3	2.01	0.42
1:A:156:VAL:HA	1:A:169:PRO:HA	2.01	0.42
1:C:263:PHE:HE1	1:C:275:ILE:HB	1.85	0.42
4:K:97:LYS:HB3	4:K:106:SER:HB2	2.02	0.42
4:K:192:LEU:HD21	4:K:236:GLU:HG2	2.01	0.42
4:K:208:SER:OG	4:K:209:HIS:N	2.53	0.42
19:f:232:PHE:HB2	19:f:236:VAL:HG23	2.02	0.42
19:f:567:ARG:HA	19:f:570:ASP:HB2	2.02	0.42
20:h:250:TRP:HB2	20:h:288:LEU:HD11	2.01	0.42
20:p:499:GLY:HA3	20:p:519:GLY:H	1.84	0.42
1:B:205:PHE:HB3	1:B:210:GLU:HG2	2.02	0.42
1:E:257:ARG:NH2	1:F:118:ARG:HH22	2.17	0.42
1:F:20:VAL:HA	1:F:36:PRO:HA	2.02	0.42
1:F:223:TYR:CE1	1:F:255:ARG:HG3	2.55	0.42
1:G:219:GLU:OE2	25:G:800:ADP:H2'	2.20	0.42
2:H:19:ALA:HB3	2:H:29:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:110:LEU:HB2	2:H:177:ARG:HD2	2.02	0.42
1:I:107:PRO:HB3	1:I:136:ALA:HB3	2.02	0.42
1:I:358:VAL:HG22	1:I:374:LYS:HD2	2.02	0.42
5:L:12:LEU:HA	5:L:12:LEU:HD12	1.86	0.42
5:L:142:LYS:HA	5:L:142:LYS:HD2	1.84	0.42
19:f:606:THR:OG1	19:f:607:GLN:N	2.51	0.42
19:f:686:GLY:O	19:f:690:ARG:HG2	2.20	0.42
19:f:703:ALA:O	19:f:707:GLN:HB2	2.20	0.42
19:m:116:LEU:HA	19:m:139:THR:HA	2.00	0.42
19:n:546:TRP:HA	19:n:549:ALA:HB3	2.02	0.42
20:o:197:LEU:HB3	20:o:339:ASN:HD22	1.85	0.42
20:o:261:TRP:CZ2	20:o:560:ALA:HB2	2.55	0.42
20:o:320:ASN:OD1	20:o:320:ASN:N	2.50	0.42
20:o:401:LYS:HD2	20:o:401:LYS:HA	1.83	0.42
1:A:147:LEU:HD12	1:A:170:ILE:HB	2.02	0.41
1:C:229:GLN:HA	1:C:232:GLU:HB3	2.01	0.41
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.84	0.41
2:H:370:VAL:O	2:H:374:CYS:N	2.53	0.41
12:X:149:GLU:HB3	19:f:827:TYR:CD1	2.55	0.41
19:e:220:CYS:SG	19:e:223:ARG:NH1	2.92	0.41
19:f:627:TYR:O	19:f:633:CYS:HB2	2.20	0.41
20:g:458:CYS:HA	20:g:471:PHE:HA	2.01	0.41
20:g:473:THR:N	20:g:481:LYS:O	2.44	0.41
20:h:316:LYS:HG3	20:h:317:PHE:CD2	2.55	0.41
21:j:174:GLU:HA	21:j:177:PHE:HB3	2.02	0.41
19:m:255:GLU:HA	19:m:258:LYS:HD2	2.02	0.41
19:m:469:PHE:HZ	19:m:527:TYR:HA	1.85	0.41
19:n:564:ILE:CG1	19:n:565:THR:N	2.83	0.41
1:A:362:GLU:O	1:A:366:ASP:HB2	2.20	0.41
1:G:162:ASP:OD2	1:G:188:ARG:HB2	2.20	0.41
1:G:162:ASP:OD1	25:G:800:ADP:O3'	2.39	0.41
5:L:60:LEU:HD23	5:L:60:LEU:HA	1.86	0.41
19:e:837:ALA:HB1	20:g:350:SER:HA	2.02	0.41
19:f:409:PHE:CD1	19:f:470:ARG:HD3	2.55	0.41
20:h:477:ASP:OD1	20:h:477:ASP:N	2.52	0.41
21:j:93:VAL:HG12	21:j:94:HIS:H	1.85	0.41
21:j:169:LYS:HA	21:j:172:GLU:OE2	2.20	0.41
19:m:435:ARG:HG3	23:x:165:GLU:OE2	2.20	0.41
20:o:494:PHE:HD1	20:o:494:PHE:HA	1.68	0.41
20:o:549:ARG:HA	20:o:549:ARG:HD3	1.84	0.41
20:p:257:SER:N	20:p:272:SER:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:s:66:LEU:HD23	22:s:66:LEU:HA	1.87	0.41
1:D:159:ASP:OD1	1:D:159:ASP:N	2.50	0.41
1:D:245:ASP:OD1	1:D:246:GLY:N	2.53	0.41
1:G:143:ALA:HA	1:G:157:VAL:HG11	2.03	0.41
3:J:307:GLY:O	3:J:310:SER:OG	2.38	0.41
19:f:670:GLY:O	19:f:673:TRP:NE1	2.48	0.41
21:j:70:LEU:HA	21:j:70:LEU:HD12	1.80	0.41
19:m:238:ASP:HB2	19:m:241:PHE:HB3	2.02	0.41
19:m:613:LYS:HE3	19:m:613:LYS:HB2	1.91	0.41
19:n:438:VAL:HG13	19:n:443:GLU:OE2	2.20	0.41
20:o:283:PRO:HB2	20:o:305:CYS:H	1.85	0.41
1:F:219:GLU:HG2	25:F:800:ADP:C4	2.55	0.41
2:H:21:PHE:HB2	2:H:24:ASP:OD2	2.20	0.41
5:L:54:VAL:HG23	5:L:55:VAL:HG23	2.02	0.41
20:g:521:GLY:N	20:g:545:PRO:O	2.54	0.41
21:j:119:LEU:HD23	21:j:119:LEU:HA	1.92	0.41
19:m:644:VAL:O	19:m:647:SER:OG	2.37	0.41
19:m:666:GLU:OE2	19:m:673:TRP:CE2	2.73	0.41
1:B:236:THR:HG23	1:B:238:LYS:H	1.85	0.41
1:E:18:SER:OG	1:E:163:GLY:N	2.54	0.41
4:K:93:LYS:HE2	4:K:93:LYS:HB2	1.89	0.41
7:N:603:UNK:N	9:R:38:UNK:O	2.54	0.41
19:e:114:ASN:HA	19:e:141:SER:HA	2.02	0.41
19:f:204:GLU:OE1	19:f:287:ARG:NH1	2.53	0.41
19:f:402:MET:O	19:f:527:TYR:OH	2.25	0.41
19:f:813:GLN:HA	19:f:816:ILE:HB	2.02	0.41
20:h:456:ILE:HG13	20:h:473:THR:HG22	2.02	0.41
21:j:157:ARG:HA	21:j:160:ILE:HD12	2.03	0.41
22:l:22:VAL:HA	22:l:88:LEU:HA	2.03	0.41
22:l:72:ARG:HA	22:l:77:GLU:HA	2.02	0.41
19:m:403:HIS:HA	19:m:531:LYS:NZ	2.35	0.41
19:m:454:PRO:O	19:m:457:ARG:HG2	2.21	0.41
19:m:473:HIS:CE1	19:m:477:ARG:HG2	2.54	0.41
19:n:443:GLU:OE1	19:n:443:GLU:N	2.52	0.41
19:n:567:ARG:O	19:n:571:GLN:HG2	2.20	0.41
20:o:563:ASP:HB2	20:o:567:GLN:O	2.20	0.41
1:A:40:GLY:HA3	1:A:69:LEU:HB3	2.03	0.41
1:D:267:LEU:O	1:E:178:HIS:NE2	2.53	0.41
1:E:145:LEU:O	1:E:343:GLY:HA3	2.20	0.41
1:G:205:PHE:HD1	1:G:210:GLU:OE2	2.02	0.41
5:L:111:TYR:OH	5:L:218:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:297:VAL:O	19:f:300:THR:OG1	2.38	0.41
21:j:86:LEU:HD22	21:j:118:LEU:HB3	2.02	0.41
19:m:542:GLY:O	19:m:546:TRP:CB	2.49	0.41
20:o:265:TYR:OH	20:p:219:PHE:HD2	2.04	0.41
3:J:381:THR:HG22	3:J:383:ARG:H	1.86	0.41
4:K:87:PHE:HB2	4:K:96:PHE:CZ	2.56	0.41
5:L:66:ARG:NH2	5:L:69:ASP:OD1	2.53	0.41
6:M:1:UNK:O	6:M:5:UNK:N	2.54	0.41
19:f:919:LEU:O	19:f:923:THR:HG23	2.20	0.41
19:m:523:VAL:HG22	19:m:560:VAL:HG21	2.02	0.41
20:o:428:GLY:HA2	20:o:449:HIS:HB3	2.01	0.41
21:r:57:ILE:N	21:r:105:ASN:O	2.51	0.41
22:s:70:ARG:HA	22:s:79:MET:HA	2.02	0.41
1:B:13:VAL:HG22	1:B:109:LEU:HD23	2.02	0.41
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.91	0.41
1:D:38:TYR:HB2	1:D:71:ILE:HG23	2.02	0.41
1:D:107:PRO:HB3	1:D:136:ALA:HB3	2.02	0.41
1:F:257:ARG:NE	16:b:73:ASP:O	2.53	0.41
1:G:62:ALA:HA	1:G:69:LEU:HD21	2.02	0.41
1:G:323:PRO:HG2	1:G:326:VAL:HG21	2.02	0.41
3:J:23:ALA:HB3	25:J:800:ADP:H5'1	2.02	0.41
19:f:447:LYS:HA	19:f:447:LYS:HD3	1.83	0.41
19:f:747:SER:O	19:f:751:ARG:HD3	2.21	0.41
21:j:247:ARG:HB3	21:j:250:HIS:ND1	2.35	0.41
20:o:239:LEU:HD23	20:o:239:LEU:HA	1.75	0.41
20:o:459:HIS:HA	20:o:506:TRP:CE3	2.55	0.41
1:B:270:GLU:HG2	1:B:272:SER:H	1.86	0.41
1:C:205:PHE:HD1	1:C:210:GLU:OE2	2.04	0.41
1:D:185:ILE:HA	1:D:189:ASP:OD2	2.21	0.41
1:D:284:GLN:O	1:D:291:ARG:NH2	2.54	0.41
1:D:318:VAL:HG12	1:D:328:ILE:HD13	2.02	0.41
1:E:158:LEU:HG	1:E:279:LEU:HD12	2.03	0.41
1:E:160:SER:H	1:E:302:GLY:HA3	1.86	0.41
1:F:199:ARG:HG2	1:F:204:ASP:HA	2.03	0.41
1:G:13:VAL:HA	1:G:109:LEU:HB3	2.03	0.41
2:H:36:GLY:HA3	2:H:65:LEU:HD13	2.03	0.41
4:K:272:ASN:O	4:K:276:SER:CB	2.69	0.41
5:L:107:TYR:OH	5:L:221:GLU:OE1	2.33	0.41
19:e:162:LYS:O	19:e:166:ARG:CB	2.68	0.41
19:f:354:ARG:HB2	19:f:419:VAL:HG22	2.02	0.41
19:f:373:PRO:HG2	19:f:376:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:f:607:GLN:HB3	19:f:611:ARG:NH1	2.36	0.41
19:f:726:ARG:NH2	19:f:727:GLY:O	2.54	0.41
20:h:380:LYS:HA	20:h:397:GLU:HA	2.02	0.41
20:h:481:LYS:HA	20:h:493:SER:HA	2.02	0.41
20:h:510:HIS:CD2	20:h:579:VAL:H	2.38	0.41
21:j:95:ASP:H	21:j:99:ASP:HA	1.85	0.41
19:m:264:ARG:HH22	19:m:273:GLN:HB3	1.86	0.41
19:m:454:PRO:HB2	19:m:456:HIS:CE1	2.55	0.41
19:m:583:ARG:HD3	19:m:583:ARG:HA	1.75	0.41
19:n:556:ARG:HA	19:n:556:ARG:HD2	1.82	0.41
20:o:261:TRP:HZ2	20:o:560:ALA:HB2	1.85	0.41
20:o:290:TRP:CE2	20:o:299:PRO:HB3	2.56	0.41
20:o:332:VAL:HB	20:o:343:PRO:HB3	2.03	0.41
1:A:219:GLU:HG2	25:A:800:ADP:C4	2.56	0.41
1:C:263:PHE:HD2	1:C:313:ARG:HE	1.69	0.41
1:D:327:LYS:NZ	17:c:24:ASP:OD1	2.44	0.41
1:E:323:PRO:HG2	1:E:326:VAL:HG21	2.01	0.41
3:J:59:ILE:HG13	3:J:60:ASN:H	1.86	0.41
4:K:233:GLU:O	4:K:237:ASN:ND2	2.53	0.41
16:b:72:SER:OG	16:b:73:ASP:N	2.53	0.41
17:c:9:LEU:HA	17:c:10:PRO:HD3	1.86	0.41
19:e:216:VAL:HG13	19:e:231:ASP:OD2	2.21	0.41
19:e:252:TRP:HH2	19:e:300:THR:HG21	1.86	0.41
19:f:704:ARG:O	19:f:708:GLN:HG2	2.21	0.41
19:f:842:ASN:O	19:f:846:LYS:HG2	2.21	0.41
21:j:239:VAL:HA	21:j:242:LYS:HE2	2.02	0.41
21:j:329:THR:O	21:j:332:PRO:HD3	2.21	0.41
19:m:239:PRO:O	19:m:243:ASN:HB2	2.21	0.41
19:m:438:VAL:HG21	19:m:450:TRP:HZ2	1.86	0.41
19:m:577:ASN:OD1	19:m:578:ALA:N	2.53	0.41
20:o:516:CYS:HA	20:o:550:VAL:HG21	2.04	0.41
22:s:58:ARG:HG3	22:s:62:PRO:HA	2.03	0.41
1:C:207:SER:HB3	1:C:210:GLU:HB2	2.02	0.40
2:H:105:LEU:HD11	2:H:123:MET:HE3	2.03	0.40
5:L:149:ASP:HB2	5:L:174:MET:HB2	2.03	0.40
19:e:205:ILE:HD12	19:e:259:VAL:HG23	2.03	0.40
19:f:683:LYS:HE2	19:f:683:LYS:HB3	1.75	0.40
21:j:101:HIS:O	21:j:103:ARG:N	2.54	0.40
21:j:143:TRP:NE1	21:j:344:PRO:HB3	2.36	0.40
19:m:568:LEU:HD23	19:m:568:LEU:HA	1.70	0.40
20:o:430:VAL:N	20:o:446:PHE:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:o:457:HIS:HD2	20:o:506:TRP:H	1.69	0.40
20:o:518:ASP:OD2	20:o:522:ARG:HB2	2.21	0.40
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.86	0.40
1:F:48:MET:HB3	2:H:168:GLY:HA2	2.03	0.40
1:F:52:LEU:HG	2:H:167:GLU:HB3	2.03	0.40
1:I:41:ARG:HG2	1:I:55:ASP:O	2.22	0.40
1:I:335:GLU:HA	16:b:12:ILE:HD12	2.03	0.40
4:K:240:GLN:OE1	5:L:244:ARG:NH1	2.54	0.40
5:L:62:CYS:SG	5:L:63:ASP:N	2.94	0.40
5:L:177:LEU:HD12	5:L:189:LEU:HD23	2.03	0.40
8:O:28:UNK:N	8:O:33:UNK:O	2.54	0.40
19:f:451:ARG:HD3	19:f:451:ARG:HA	1.84	0.40
20:h:398:LEU:HD23	20:h:398:LEU:HA	1.89	0.40
22:k:57:VAL:O	22:k:61:ASP:N	2.34	0.40
19:m:267:ALA:HA	19:m:379:ARG:HB3	2.04	0.40
19:m:749:GLU:O	19:m:753:LEU:HG	2.21	0.40
19:n:368:ARG:O	19:n:440:ARG:NH1	2.55	0.40
20:o:552:TRP:CD2	20:o:559:ILE:HD12	2.57	0.40
1:C:275:ILE:HD13	1:C:275:ILE:HG21	1.91	0.40
2:H:8:LEU:HD22	2:H:94:LEU:HD13	2.04	0.40
2:H:267:LEU:HD23	2:H:267:LEU:HA	1.96	0.40
3:J:36:ARG:NH1	13:Y:321:UNK:O	2.53	0.40
4:K:40:LEU:HB3	4:K:46:LEU:HD23	2.04	0.40
4:K:223:GLN:O	4:K:227:GLU:CB	2.67	0.40
19:f:462:ARG:HH12	19:f:542:GLY:HA2	1.85	0.40
19:f:578:ALA:O	19:f:582:PHE:HB2	2.21	0.40
20:h:411:MET:HE1	20:h:413:PHE:CE2	2.56	0.40
21:j:62:GLU:OE1	21:j:151:LYS:NZ	2.55	0.40
19:m:588:PHE:HD1	19:m:591:LEU:HD12	1.86	0.40
21:r:170:MET:O	21:r:174:GLU:CB	2.69	0.40
1:D:48:MET:HB3	1:F:173:GLY:HA2	2.03	0.40
3:J:247:ASP:HB3	3:J:257:HIS:CD2	2.56	0.40
3:J:247:ASP:OD1	3:J:247:ASP:N	2.53	0.40
4:K:186:ALA:HB2	4:K:218:VAL:HG23	2.04	0.40
18:d:20:TYR:HD1	18:d:20:TYR:HA	1.73	0.40
19:m:473:HIS:NE2	19:m:527:TYR:HB2	2.35	0.40
19:n:466:MET:O	19:n:470:ARG:HG2	2.22	0.40
20:o:209:ARG:HE	20:p:217:ILE:HA	1.87	0.40
22:t:35:ASP:OD1	22:t:35:ASP:N	2.54	0.40
1:D:95:SER:OG	1:D:96:LYS:N	2.55	0.40
1:F:148:TYR:CE2	1:F:347:LEU:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:PRO:HG3	1:G:313:ARG:HH22	1.87	0.40
2:H:183:ARG:HH11	2:H:183:ARG:HD2	1.77	0.40
4:K:120:TRP:CH2	4:K:221:GLU:HA	2.55	0.40
5:L:70:SER:OG	5:L:81:PRO:O	2.30	0.40
10:U:143:ILE:HA	10:U:150:ARG:O	2.21	0.40
19:f:726:ARG:HD2	19:f:726:ARG:HA	1.80	0.40
20:g:446:PHE:HA	20:g:488:ASN:HA	2.02	0.40
20:h:387:ASP:HA	19:m:677:VAL:HG23	2.04	0.40
20:h:460:ALA:H	20:h:508:PRO:HB3	1.87	0.40
21:j:268:ALA:HB1	21:j:310:ILE:O	2.21	0.40
19:m:252:TRP:CZ3	19:m:297:VAL:HG13	2.57	0.40
19:m:271:ALA:O	19:m:275:ILE:HG12	2.22	0.40
20:o:257:SER:HB3	20:o:310:MET:HA	2.03	0.40
20:o:274:ASN:OD1	20:o:275:ASN:N	2.54	0.40
20:p:187:LYS:HD2	22:s:30:ILE:CG1	2.52	0.40
23:x:194:ALA:O	23:x:198:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	334 (91%)	34 (9%)	0	100	100
1	B	368/376 (98%)	338 (92%)	30 (8%)	0	100	100
1	C	368/376 (98%)	341 (93%)	27 (7%)	0	100	100
1	D	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	E	368/376 (98%)	335 (91%)	33 (9%)	0	100	100
1	F	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	G	368/376 (98%)	342 (93%)	26 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	368/376 (98%)	342 (93%)	26 (7%)	0	100	100
2	H	368/375 (98%)	345 (94%)	23 (6%)	0	100	100
3	J	363/390 (93%)	336 (93%)	27 (7%)	0	100	100
4	K	276/286 (96%)	244 (88%)	32 (12%)	0	100	100
5	L	267/272 (98%)	233 (87%)	34 (13%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	10	41
11	V	163/182 (90%)	125 (77%)	36 (22%)	2 (1%)	10	41
12	X	220/389 (57%)	216 (98%)	4 (2%)	0	100	100
15	a	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
16	b	71/89 (80%)	58 (82%)	13 (18%)	0	100	100
17	c	33/50 (66%)	26 (79%)	7 (21%)	0	100	100
18	d	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
19	e	868/1053 (82%)	807 (93%)	60 (7%)	1 (0%)	48	79
19	f	871/1053 (83%)	796 (91%)	75 (9%)	0	100	100
19	m	868/1053 (82%)	797 (92%)	70 (8%)	1 (0%)	48	79
19	n	870/1053 (83%)	797 (92%)	73 (8%)	0	100	100
20	g	393/612 (64%)	314 (80%)	77 (20%)	2 (0%)	24	57
20	h	394/612 (64%)	332 (84%)	59 (15%)	3 (1%)	16	49
20	o	393/612 (64%)	321 (82%)	70 (18%)	2 (0%)	24	57
20	p	397/612 (65%)	329 (83%)	68 (17%)	0	100	100
21	i	258/492 (52%)	226 (88%)	32 (12%)	0	100	100
21	j	280/492 (57%)	216 (77%)	60 (21%)	4 (1%)	9	38
21	q	258/492 (52%)	215 (83%)	43 (17%)	0	100	100
21	r	258/492 (52%)	217 (84%)	41 (16%)	0	100	100
22	k	91/96 (95%)	72 (79%)	19 (21%)	0	100	100
22	l	91/96 (95%)	76 (84%)	14 (15%)	1 (1%)	11	43
22	s	91/96 (95%)	82 (90%)	9 (10%)	0	100	100
22	t	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
23	x	220/392 (56%)	218 (99%)	2 (1%)	0	100	100
All	All	11636/14727 (79%)	10362 (89%)	1256 (11%)	18 (0%)	44	74

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	79	PRO
20	o	467	PHE
20	h	491	LEU
21	j	246	TYR
20	o	469	HIS
19	e	537	ASP
20	h	511	PRO
21	j	103	ARG
19	m	455	ALA
20	g	404	LYS
20	g	469	HIS
22	l	82	PRO
11	V	72	PRO
11	V	84	PRO
20	h	490	PRO
21	j	342	LYS
21	j	341	VAL
10	U	78	GLU

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	318/324 (98%)	318 (100%)	0	100	100
1	B	318/324 (98%)	315 (99%)	3 (1%)	70	76
1	C	318/324 (98%)	316 (99%)	2 (1%)	78	79
1	D	318/324 (98%)	317 (100%)	1 (0%)	86	83
1	E	318/324 (98%)	316 (99%)	2 (1%)	78	79
1	F	318/324 (98%)	317 (100%)	1 (0%)	86	83
1	G	318/324 (98%)	316 (99%)	2 (1%)	78	79
1	I	318/324 (98%)	317 (100%)	1 (0%)	86	83
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	323/338 (96%)	323 (100%)	0	100	100
4	K	247/254 (97%)	246 (100%)	1 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L	238/241 (99%)	238 (100%)	0	100	100
12	X	74/282 (26%)	74 (100%)	0	100	100
15	a	45/57 (79%)	44 (98%)	1 (2%)	45	65
16	b	64/76 (84%)	63 (98%)	1 (2%)	55	70
17	c	22/44 (50%)	22 (100%)	0	100	100
18	d	21/22 (96%)	21 (100%)	0	100	100
19	e	125/891 (14%)	125 (100%)	0	100	100
19	f	643/891 (72%)	643 (100%)	0	100	100
19	m	453/891 (51%)	449 (99%)	4 (1%)	70	76
19	n	307/891 (34%)	305 (99%)	2 (1%)	76	78
20	h	307/531 (58%)	306 (100%)	1 (0%)	86	83
20	o	344/531 (65%)	341 (99%)	3 (1%)	70	76
20	p	37/531 (7%)	35 (95%)	2 (5%)	20	46
21	j	244/422 (58%)	242 (99%)	2 (1%)	73	77
22	s	87/89 (98%)	87 (100%)	0	100	100
22	t	87/89 (98%)	87 (100%)	0	100	100
23	x	64/282 (23%)	64 (100%)	0	100	100
All	All	6589/10263 (64%)	6560 (100%)	29 (0%)	81	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	TYR
1	B	197	TYR
1	B	245	ASP
1	C	38	TYR
1	C	249	ILE
1	D	261	LEU
1	E	158	LEU
1	E	256	PHE
1	F	245	ASP
1	G	69	LEU
1	G	197	TYR
1	I	38	TYR
4	K	254	THR
15	a	50	VAL

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Mol	Chain	Res	Type
16	b	37	LEU
20	h	472	VAL
21	j	59	VAL
21	j	218	VAL
19	m	438	VAL
19	m	658	LEU
19	m	743	ILE
19	m	760	VAL
19	n	329	VAL
19	n	561	GLU
20	o	462	VAL
20	o	465	VAL
20	o	550	VAL
20	p	185	GLU
20	p	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	106	HIS
1	B	133	ASN
1	C	16	ASN
1	C	133	ASN
1	D	10	GLN
1	D	65	HIS
1	D	133	ASN
1	E	9	ASN
1	E	98	GLN
1	E	120	ASN
1	F	9	ASN
1	F	44	HIS
1	F	297	ASN
1	G	98	GLN
1	G	116	ASN
1	G	334	GLN
2	H	12	ASN
2	H	41	GLN
2	H	49	GLN
2	H	88	HIS
2	H	161	HIS
2	H	246	GLN

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Mol	Chain	Res	Type
1	I	98	GLN
1	I	178	HIS
1	I	372	HIS
3	J	58	ASN
3	J	257	HIS
3	J	273	GLN
4	K	58	ASN
4	K	100	HIS
4	K	147	ASN
4	K	167	ASN
4	K	248	GLN
5	L	20	GLN
5	L	229	ASN
5	L	255	GLN
12	X	161	ASN
19	f	215	ASN
19	f	653	GLN
19	f	708	GLN
19	f	731	ASN
19	f	772	ASN
19	f	773	GLN
19	f	891	HIS
19	f	901	ASN
20	h	264	GLN
20	h	276	ASN
20	h	306	GLN
20	h	320	ASN
20	h	330	GLN
20	h	345	GLN
20	h	371	ASN
20	h	497	ASN
20	h	544	ASN
21	j	94	HIS
21	j	105	ASN
21	j	115	HIS
21	j	150	GLN
21	j	159	HIS
21	j	221	HIS
21	j	326	ASN
21	j	360	GLN
21	j	366	GLN
19	m	280	ASN

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Mol	Chain	Res	Type
19	m	391	GLN
19	m	472	GLN
19	m	524	ASN
19	m	529	ASN
19	m	589	ASN
19	m	772	ASN
19	n	243	ASN
19	n	475	GLN
19	n	529	ASN
19	n	571	GLN
20	o	345	GLN
20	o	368	ASN
20	o	370	HIS
20	o	436	HIS
20	p	189	GLN
20	p	216	ASN
22	s	12	GLN
22	s	24	ASN
22	s	36	ASN
22	s	41	GLN
22	s	47	HIS
22	s	93	ASN
22	t	18	GLN
22	t	36	ASN
22	t	93	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 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$
25	ADP	F	800	-	28,29,29	1.66	5 (17%)	43,45,45	1.88	11 (25%)
25	ADP	I	800	-	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)
25	ADP	B	800	-	28,29,29	1.53	5 (17%)	43,45,45	1.99	13 (30%)
26	ATP	H	401	-	32,33,33	1.37	5 (15%)	48,52,52	1.75	10 (20%)
25	ADP	C	800	-	28,29,29	1.45	4 (14%)	43,45,45	1.88	10 (23%)
25	ADP	D	800	-	28,29,29	1.54	3 (10%)	43,45,45	1.65	7 (16%)
25	ADP	J	800	-	28,29,29	1.43	4 (14%)	43,45,45	1.82	12 (27%)
25	ADP	A	800	-	28,29,29	1.40	5 (17%)	43,45,45	1.79	12 (27%)
25	ADP	G	800	-	28,29,29	1.40	4 (14%)	43,45,45	1.76	8 (18%)
25	ADP	E	800	-	28,29,29	1.38	5 (17%)	43,45,45	1.90	12 (27%)

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
25	ADP	F	800	-	-	4/16/32/32	0/3/3/3
25	ADP	I	800	-	-	0/16/32/32	0/3/3/3
25	ADP	B	800	-	-	3/16/32/32	0/3/3/3
26	ATP	H	401	-	-	7/22/38/38	0/3/3/3
25	ADP	C	800	-	-	4/16/32/32	0/3/3/3
25	ADP	D	800	-	-	4/16/32/32	0/3/3/3
25	ADP	J	800	-	-	6/16/32/32	0/3/3/3
25	ADP	A	800	-	-	4/16/32/32	0/3/3/3
25	ADP	G	800	-	-	0/16/32/32	0/3/3/3
25	ADP	E	800	-	-	1/16/32/32	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	800	ADP	C5-C4	4.81	1.47	1.39
25	J	800	ADP	C5-C4	4.80	1.47	1.39
26	H	401	ATP	C5-C4	4.47	1.47	1.39
25	F	800	ADP	C4-N9	-4.24	1.28	1.37
25	D	800	ADP	C5-N7	-3.65	1.32	1.39
25	D	800	ADP	C5-C4	3.61	1.45	1.39
25	A	800	ADP	C5-C4	3.54	1.45	1.39
25	G	800	ADP	C5-C4	3.53	1.45	1.39
25	F	800	ADP	C5-N7	-3.45	1.32	1.39
25	B	800	ADP	C5-N7	-3.38	1.32	1.39
25	B	800	ADP	C5-C4	3.31	1.45	1.39
25	C	800	ADP	C5-C4	3.30	1.45	1.39
25	C	800	ADP	C5-N7	-3.20	1.33	1.39
25	B	800	ADP	C4-N9	-3.18	1.31	1.37
25	A	800	ADP	C5-N7	-3.15	1.33	1.39
25	D	800	ADP	C4-N9	-3.14	1.31	1.37
25	E	800	ADP	C5-N7	-3.08	1.33	1.39
25	E	800	ADP	C5-C4	3.04	1.44	1.39
25	F	800	ADP	C8-N9	-2.97	1.32	1.37
25	F	800	ADP	C5-C4	2.96	1.44	1.39
25	A	800	ADP	C4-N9	-2.96	1.31	1.37
25	C	800	ADP	C4-N9	-2.93	1.31	1.37
25	G	800	ADP	C4-N9	-2.89	1.31	1.37
25	G	800	ADP	C5-N7	-2.88	1.33	1.39
25	J	800	ADP	C5-C6	2.73	1.48	1.41
25	I	800	ADP	C5-C6	2.73	1.48	1.41
25	E	800	ADP	C4-N9	-2.72	1.32	1.37
25	C	800	ADP	C8-N9	-2.72	1.32	1.37
25	E	800	ADP	C8-N9	-2.69	1.33	1.37
26	H	401	ATP	C5-C6	2.67	1.48	1.41
25	B	800	ADP	C8-N9	-2.62	1.33	1.37
25	F	800	ADP	PA-O3A	-2.53	1.56	1.59
25	B	800	ADP	PA-O3A	-2.38	1.56	1.59
26	H	401	ATP	C8-N7	2.37	1.36	1.31
26	H	401	ATP	C4-N9	-2.35	1.32	1.37
26	H	401	ATP	C5-N7	-2.32	1.34	1.39
25	A	800	ADP	C8-N9	-2.31	1.33	1.37
25	J	800	ADP	C8-N7	2.29	1.36	1.31
25	I	800	ADP	C5-N7	-2.28	1.34	1.39
25	G	800	ADP	C8-N9	-2.26	1.33	1.37
25	J	800	ADP	C5-N7	-2.17	1.35	1.39
25	E	800	ADP	C5-C6	2.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	I	800	ADP	C8-N7	2.16	1.35	1.31
25	A	800	ADP	C8-N7	2.03	1.35	1.31

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	800	ADP	C5-C4-N3	-5.88	118.62	126.72
25	I	800	ADP	C5-C4-N3	-5.86	118.64	126.72
25	E	800	ADP	C5-C4-N3	-5.68	118.89	126.72
25	C	800	ADP	C5-C4-N3	-5.60	119.01	126.72
25	D	800	ADP	C5-C4-N3	-5.55	119.07	126.72
25	J	800	ADP	C5-C4-N3	-5.53	119.10	126.72
25	G	800	ADP	C5-C4-N3	-5.46	119.19	126.72
26	H	401	ATP	C5-C4-N3	-5.15	119.62	126.72
25	A	800	ADP	C5-C4-N3	-4.99	119.84	126.72
25	F	800	ADP	C5-C4-N3	-4.76	120.16	126.72
25	I	800	ADP	N3-C4-N9	4.74	135.22	127.17
25	J	800	ADP	N3-C4-N9	4.58	134.95	127.17
25	B	800	ADP	N3-C4-N9	4.50	134.83	127.17
25	E	800	ADP	N3-C4-N9	4.44	134.72	127.17
25	C	800	ADP	N3-C4-N9	4.34	134.54	127.17
25	G	800	ADP	N3-C4-N9	4.19	134.30	127.17
25	D	800	ADP	N3-C4-N9	4.02	134.00	127.17
26	H	401	ATP	N3-C4-N9	4.00	133.96	127.17
25	F	800	ADP	C4-C5-N7	-3.79	106.24	110.58
25	C	800	ADP	C2-N3-C4	3.67	120.80	111.83
25	B	800	ADP	C2-N3-C4	3.65	120.74	111.83
26	H	401	ATP	C4-C5-N7	-3.62	106.44	110.58
25	F	800	ADP	C4-N9-C8	3.62	109.54	105.74
25	A	800	ADP	N3-C2-N1	-3.61	123.12	128.58
25	A	800	ADP	N3-C4-N9	3.59	133.27	127.17
25	J	800	ADP	C2-N3-C4	3.57	120.55	111.83
25	E	800	ADP	C2-N3-C4	3.52	120.43	111.83
25	A	800	ADP	C2-N3-C4	3.51	120.41	111.83
25	E	800	ADP	C4-C5-N7	-3.47	106.62	110.58
25	A	800	ADP	C4-C5-N7	-3.47	106.62	110.58
25	I	800	ADP	C2-N3-C4	3.45	120.25	111.83
25	F	800	ADP	N3-C4-N9	3.43	133.00	127.17
25	F	800	ADP	C2'-C1'-N9	-3.41	104.83	113.30
26	H	401	ATP	C2-N3-C4	3.38	120.10	111.83
25	I	800	ADP	C4-C5-N7	-3.38	106.72	110.58
25	C	800	ADP	C4-C5-N7	-3.37	106.73	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	800	ADP	N3-C2-N1	-3.37	123.49	128.58
25	J	800	ADP	C4-C5-N7	-3.35	106.75	110.58
25	B	800	ADP	C4-C5-N7	-3.31	106.80	110.58
25	G	800	ADP	C4-C5-N7	-3.25	106.86	110.58
25	F	800	ADP	C2-N3-C4	3.23	119.72	111.83
25	J	800	ADP	N3-C2-N1	-3.21	123.72	128.58
26	H	401	ATP	C4-N9-C8	3.13	109.02	105.74
25	F	800	ADP	N3-C2-N1	-3.06	123.96	128.58
25	J	800	ADP	C4-N9-C8	3.04	108.93	105.74
25	G	800	ADP	C2-N3-C4	3.03	119.23	111.83
25	E	800	ADP	C4-N9-C8	3.03	108.92	105.74
25	B	800	ADP	N3-C2-N1	-3.00	124.03	128.58
25	D	800	ADP	C2-N3-C4	3.00	119.16	111.83
26	H	401	ATP	N3-C2-N1	-3.00	124.04	128.58
25	C	800	ADP	C4-N9-C8	2.95	108.84	105.74
25	B	800	ADP	C2'-C1'-N9	-2.89	106.13	113.30
25	G	800	ADP	C4-N9-C8	2.87	108.75	105.74
25	B	800	ADP	C4-N9-C8	2.77	108.65	105.74
25	E	800	ADP	N3-C2-N1	-2.76	124.41	128.58
25	F	800	ADP	N9-C8-N7	-2.72	110.07	113.94
25	D	800	ADP	C3'-C2'-C1'	2.69	106.56	101.46
25	I	800	ADP	N3-C2-N1	-2.64	124.58	128.58
26	H	401	ATP	C5-N7-C8	2.64	107.59	103.45
25	I	800	ADP	C4-N9-C8	2.63	108.50	105.74
25	B	800	ADP	C3'-C2'-C1'	2.61	106.40	101.46
25	E	800	ADP	C3'-C2'-C1'	2.61	106.40	101.46
25	E	800	ADP	C5-N7-C8	2.60	107.54	103.45
25	I	800	ADP	C3'-C2'-C1'	2.56	106.31	101.46
25	A	800	ADP	C4-N9-C8	2.56	108.43	105.74
25	D	800	ADP	O2'-C2'-C3'	-2.50	103.79	111.82
25	I	800	ADP	C5-N7-C8	2.50	107.38	103.45
25	J	800	ADP	C5-N7-C8	2.49	107.36	103.45
25	B	800	ADP	O2A-PA-O1A	2.49	124.03	112.44
25	F	800	ADP	C5-N7-C8	2.46	107.31	103.45
26	H	401	ATP	N9-C8-N7	-2.40	110.53	113.94
25	E	800	ADP	N9-C8-N7	-2.40	110.54	113.94
25	D	800	ADP	C4-C5-N7	-2.39	107.86	110.58
25	A	800	ADP	O4'-C1'-N9	2.38	112.66	108.09
25	F	800	ADP	C6-C5-N7	2.38	136.67	132.09
25	C	800	ADP	C5-N7-C8	2.37	107.18	103.45
25	C	800	ADP	O2A-PA-O1A	2.36	123.44	112.44
26	H	401	ATP	C6-C5-N7	2.35	136.62	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	800	ADP	C5-N7-C8	2.34	107.13	103.45
25	E	800	ADP	O2A-PA-O1A	2.34	123.32	112.44
25	B	800	ADP	C5-N7-C8	2.29	107.04	103.45
25	B	800	ADP	C2'-C3'-C4'	2.27	107.00	102.61
25	F	800	ADP	O3B-PB-O1B	2.25	119.61	110.83
25	A	800	ADP	C6-C5-N7	2.25	136.42	132.09
25	G	800	ADP	C5-N7-C8	2.23	106.96	103.45
25	E	800	ADP	C2'-C1'-N9	-2.21	107.80	113.30
25	C	800	ADP	N9-C8-N7	-2.21	110.80	113.94
25	E	800	ADP	O3A-PA-O1A	-2.17	104.16	110.70
25	A	800	ADP	C2-N1-C6	2.17	122.29	118.73
25	G	800	ADP	C3'-C2'-C1'	2.17	105.56	101.46
25	G	800	ADP	N9-C8-N7	-2.12	110.93	113.94
25	A	800	ADP	N9-C8-N7	-2.12	110.93	113.94
25	B	800	ADP	N9-C8-N7	-2.11	110.95	113.94
25	J	800	ADP	C6-C5-N7	2.09	136.11	132.09
25	B	800	ADP	O3B-PB-O2B	2.08	115.59	107.80
25	J	800	ADP	N9-C8-N7	-2.06	111.01	113.94
25	C	800	ADP	O3B-PB-O2B	2.04	115.44	107.80
25	D	800	ADP	O2A-PA-O1A	2.03	121.87	112.44
26	H	401	ATP	O3G-PG-O2G	2.02	115.39	107.80
25	J	800	ADP	C2'-C3'-C4'	2.02	106.52	102.61
25	J	800	ADP	C2-N1-C6	2.01	122.03	118.73
25	J	800	ADP	C3'-C2'-C1'	2.01	105.26	101.46
25	A	800	ADP	C2'-C3'-C4'	2.00	106.48	102.61

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	800	ADP	C5'-O5'-PA-O2A
25	A	800	ADP	C5'-O5'-PA-O3A
25	A	800	ADP	O4'-C4'-C5'-O5'
25	A	800	ADP	C3'-C4'-C5'-O5'
25	C	800	ADP	C5'-O5'-PA-O3A
25	D	800	ADP	C5'-O5'-PA-O1A
25	D	800	ADP	C5'-O5'-PA-O3A
25	E	800	ADP	C5'-O5'-PA-O1A
25	F	800	ADP	C5'-O5'-PA-O2A
25	F	800	ADP	C5'-O5'-PA-O3A
25	J	800	ADP	PA-O3A-PB-O3B
25	J	800	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
25	J	800	ADP	C5'-O5'-PA-O2A
25	J	800	ADP	C5'-O5'-PA-O3A
26	H	401	ATP	C5'-O5'-PA-O1A
26	H	401	ATP	C5'-O5'-PA-O2A
26	H	401	ATP	C5'-O5'-PA-O3A
25	B	800	ADP	C3'-C4'-C5'-O5'
25	F	800	ADP	C3'-C4'-C5'-O5'
26	H	401	ATP	O4'-C4'-C5'-O5'
26	H	401	ATP	C3'-C4'-C5'-O5'
25	D	800	ADP	O4'-C4'-C5'-O5'
25	F	800	ADP	O4'-C4'-C5'-O5'
25	D	800	ADP	C3'-C4'-C5'-O5'
25	B	800	ADP	O4'-C4'-C5'-O5'
25	C	800	ADP	C3'-C4'-C5'-O5'
25	J	800	ADP	C3'-C4'-C5'-O5'
26	H	401	ATP	PA-O3A-PB-O1B
25	C	800	ADP	O4'-C4'-C5'-O5'
25	J	800	ADP	O4'-C4'-C5'-O5'
25	B	800	ADP	C5'-O5'-PA-O1A
25	C	800	ADP	C5'-O5'-PA-O1A
26	H	401	ATP	PA-O3A-PB-O2B

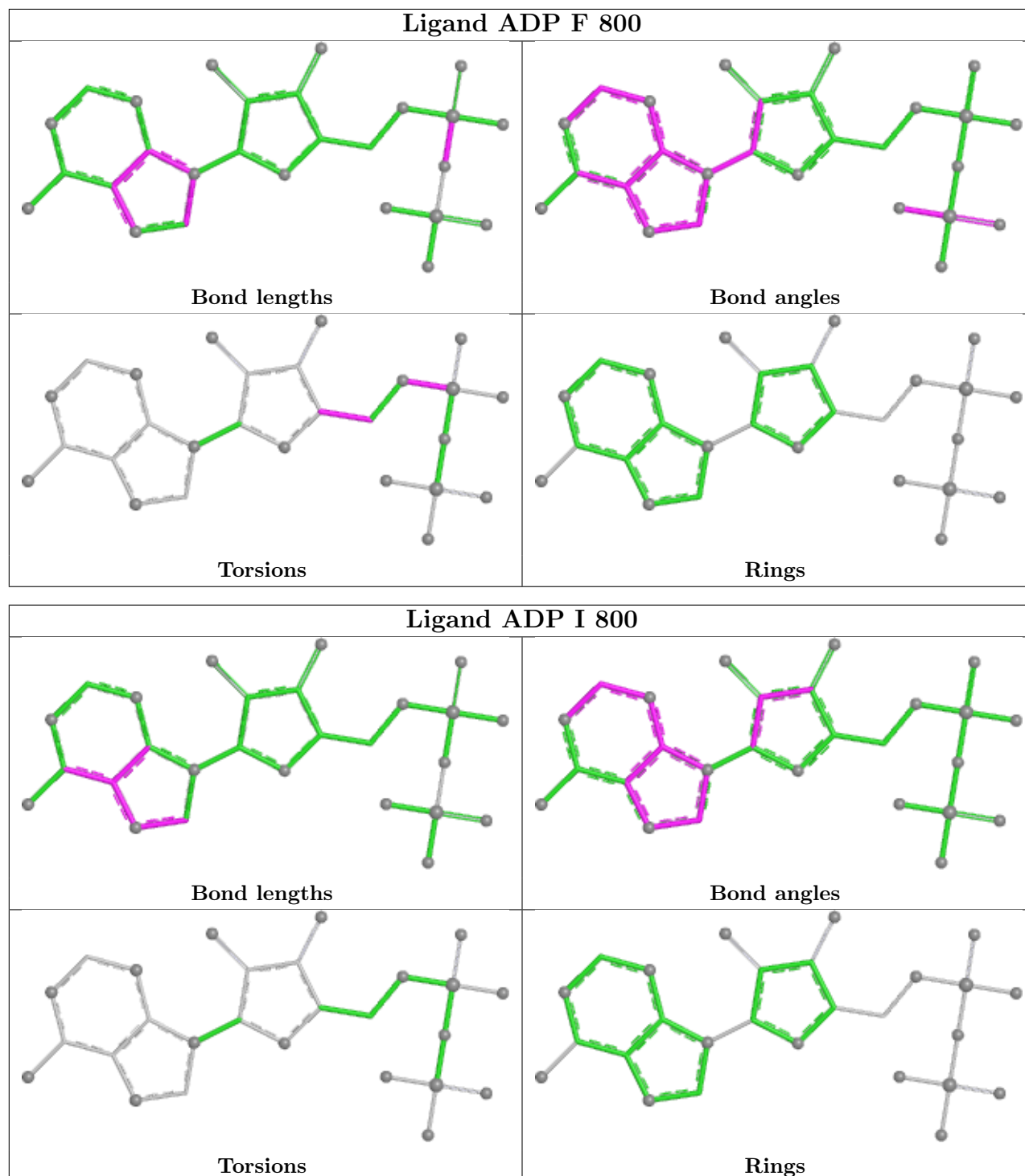
There are no ring outliers.

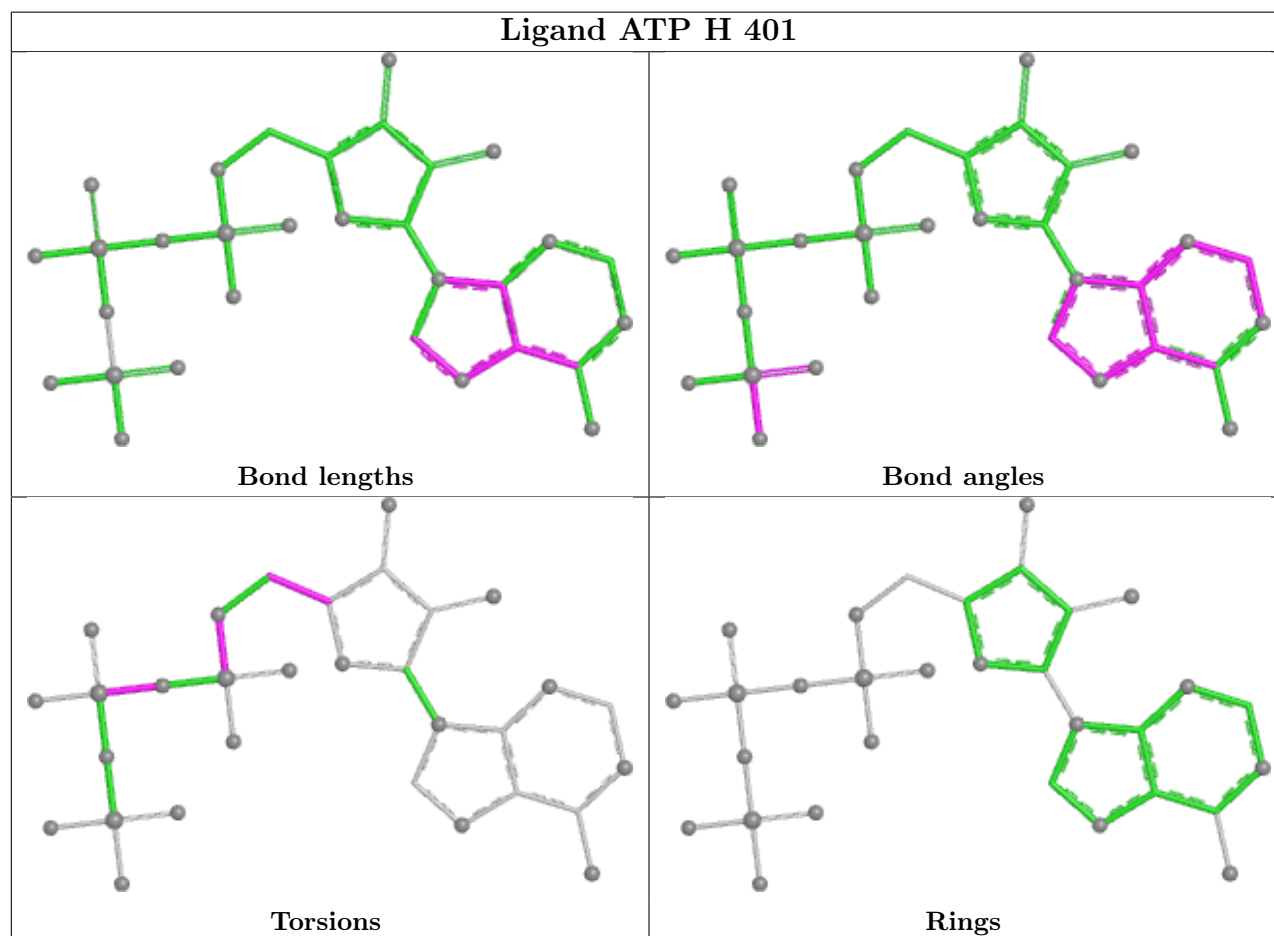
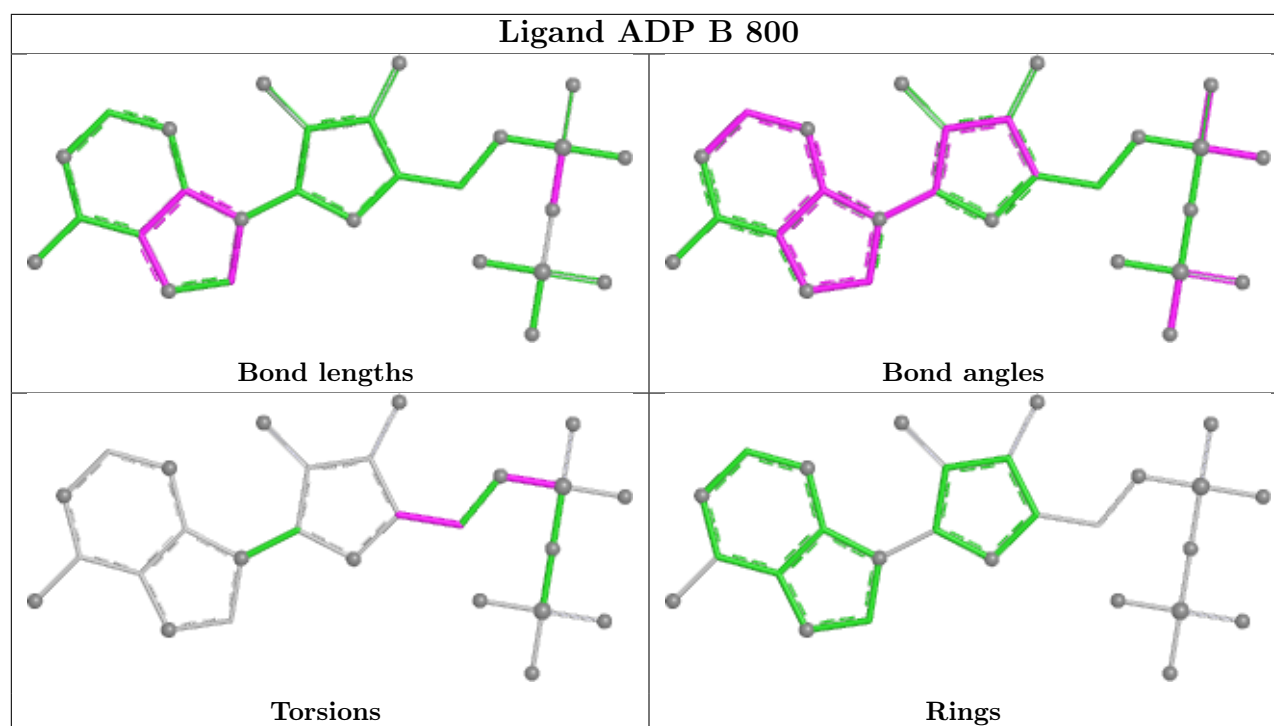
8 monomers are involved in 16 short contacts:

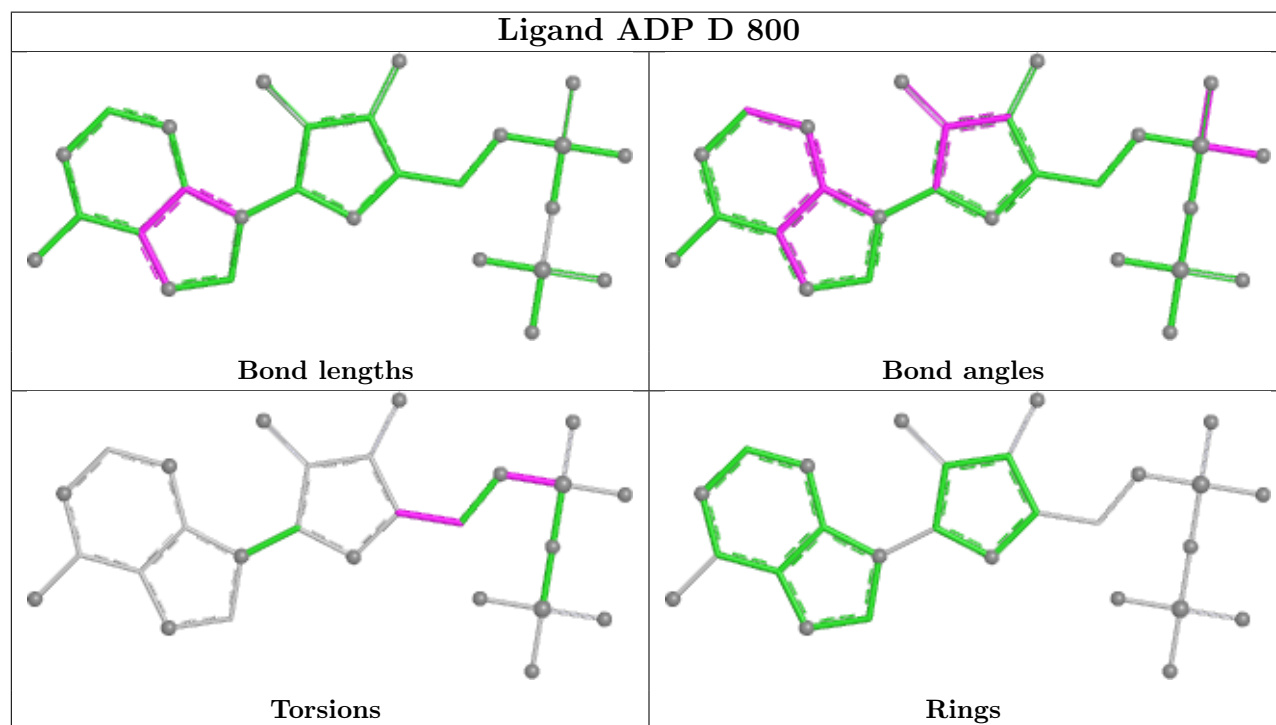
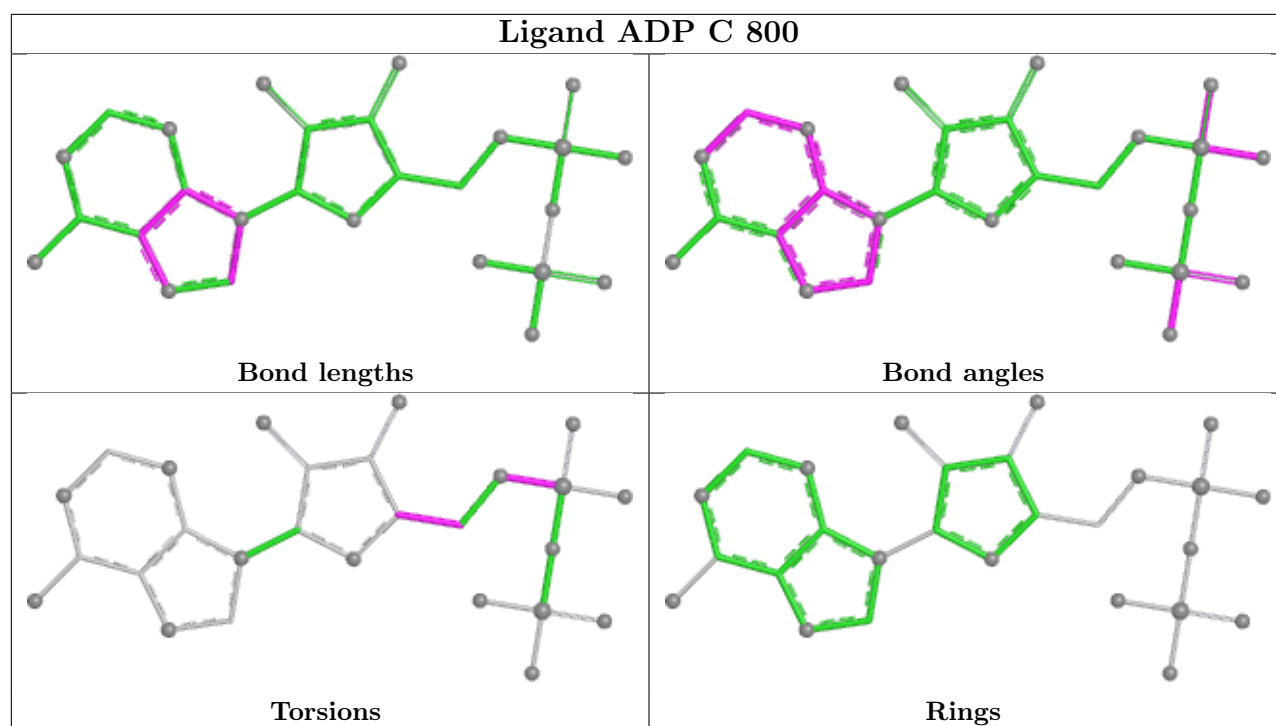
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	800	ADP	3	0
26	H	401	ATP	1	0
25	C	800	ADP	2	0
25	D	800	ADP	2	0
25	J	800	ADP	1	0
25	A	800	ADP	2	0
25	G	800	ADP	3	0
25	E	800	ADP	2	0

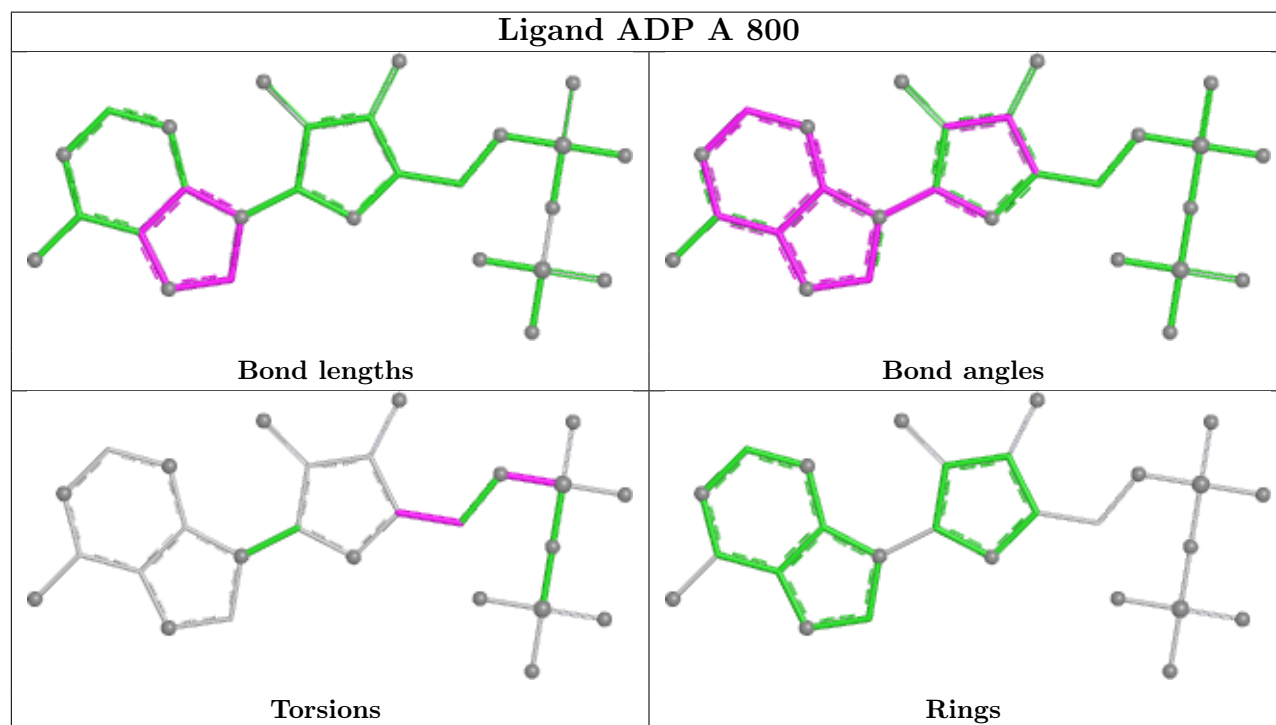
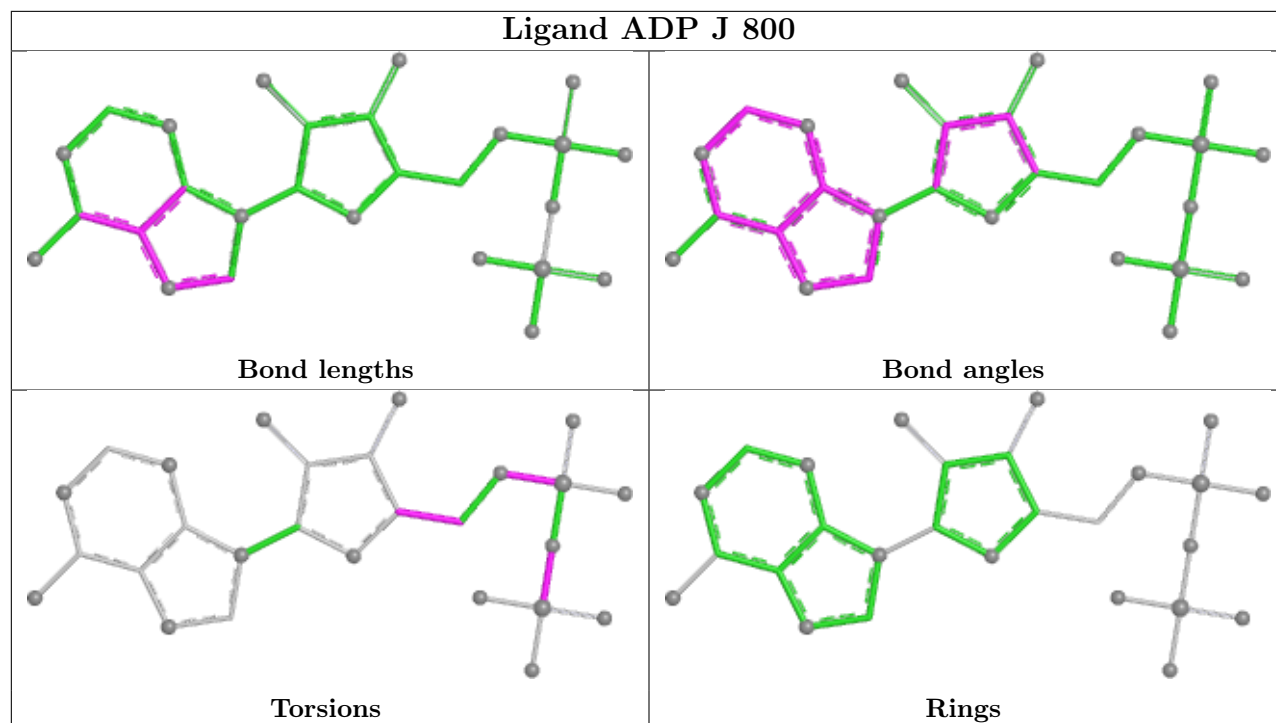
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

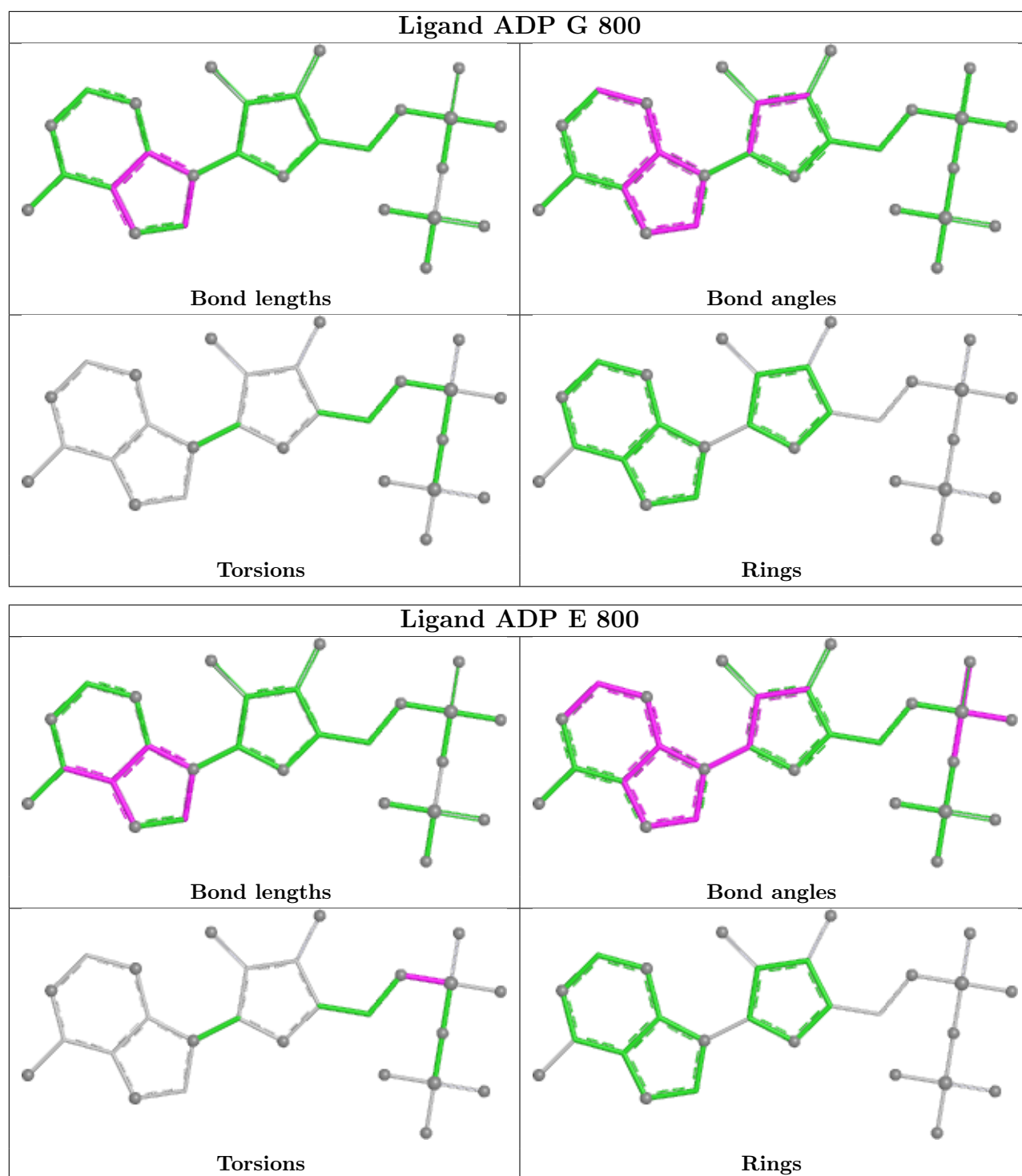
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	Y	11
7	N	5
6	M	5
8	O	3
8	P	3
9	R	2
9	Q	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	99.45
1	M	171:UNK	C	201:UNK	N	95.63
1	N	367:UNK	C	401:UNK	N	94.83
1	M	367:UNK	C	401:UNK	N	83.96
1	M	625:UNK	C	701:UNK	N	67.24
1	N	634:UNK	C	701:UNK	N	66.59
1	Y	26:UNK	C	155:UNK	N	62.21
1	Y	500:UNK	C	508:UNK	N	61.14
1	R	38:UNK	C	42:UNK	N	56.24
1	Q	38:UNK	C	42:UNK	N	55.28
1	Y	359:UNK	C	415:UNK	N	40.71
1	M	741:UNK	C	801:UNK	N	36.38
1	N	768:UNK	C	801:UNK	N	34.80
1	Y	193:UNK	C	282:UNK	N	28.70
1	N	559:UNK	C	602:UNK	N	26.73
1	O	41:UNK	C	64:UNK	N	26.59
1	M	559:UNK	C	601:UNK	N	23.98
1	P	41:UNK	C	64:UNK	N	22.87
1	Y	160:UNK	C	181:UNK	N	21.87
1	Y	620:UNK	C	703:UNK	N	21.61
1	P	78:UNK	C	80:UNK	N	17.18
1	O	78:UNK	C	80:UNK	N	16.31
1	O	94:UNK	C	96:UNK	N	15.75
1	P	94:UNK	C	96:UNK	N	15.58
1	R	62:UNK	C	64:UNK	N	15.43
1	Q	62:UNK	C	64:UNK	N	13.22
1	Y	535:UNK	C	580:UNK	N	12.88
1	Y	611:UNK	C	615:UNK	N	12.25
1	Y	421:UNK	C	423:UNK	N	8.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	586:UNK	C	588:UNK	N	6.92
1	Y	597:UNK	C	601:UNK	N	4.97

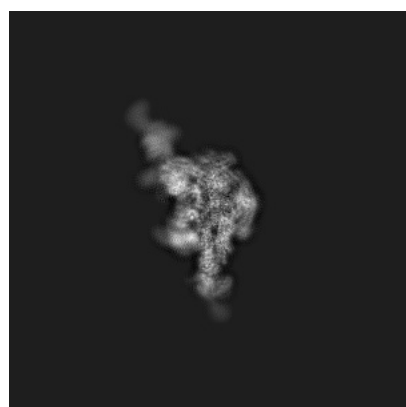
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4168. These allow visual inspection of the internal detail of the map and identification of artifacts.

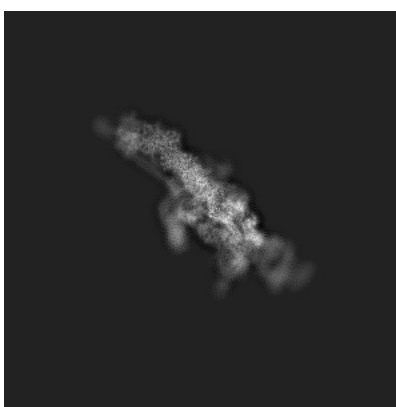
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

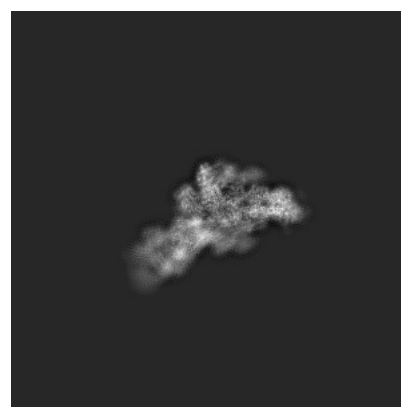
6.1.1 Primary map



X



Y

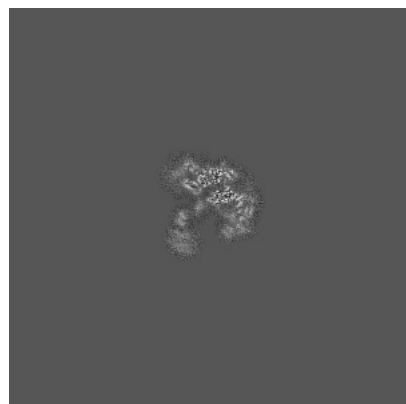


Z

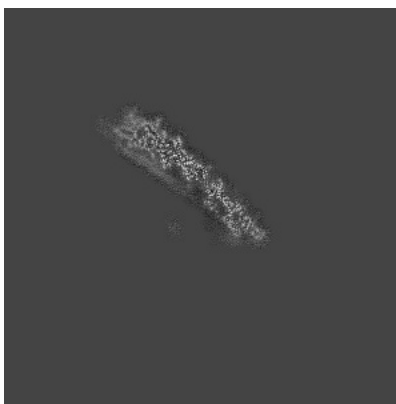
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

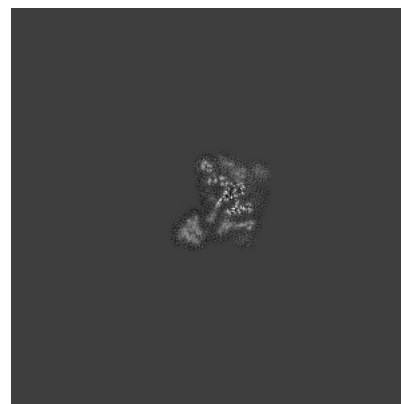
6.2.1 Primary map



X Index: 300



Y Index: 300

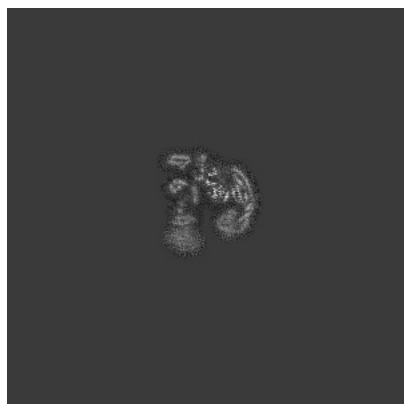


Z Index: 300

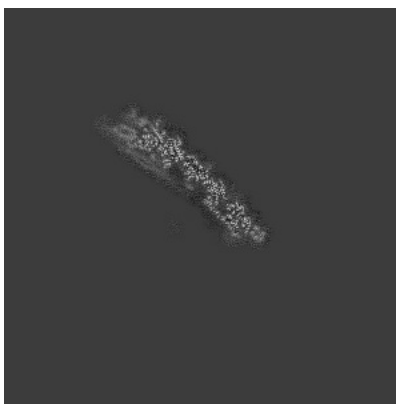
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

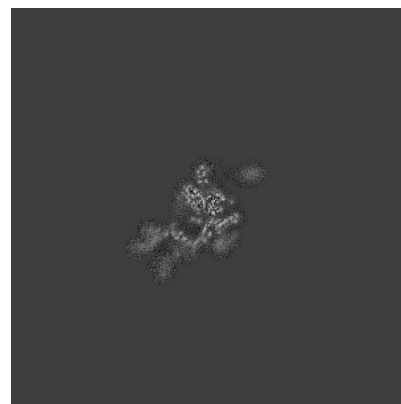
6.3.1 Primary map



X Index: 288



Y Index: 302

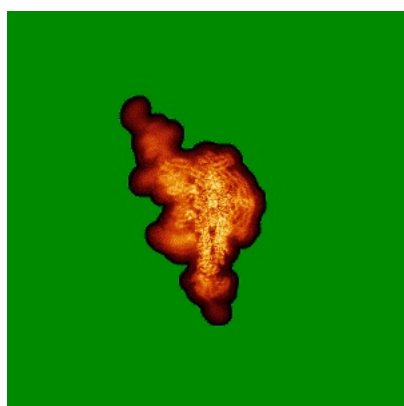


Z Index: 336

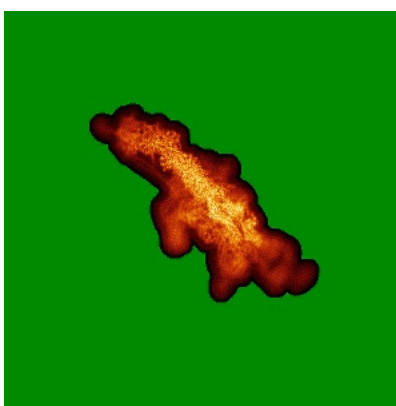
The images above show the largest variance slices of the map in three orthogonal directions.

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

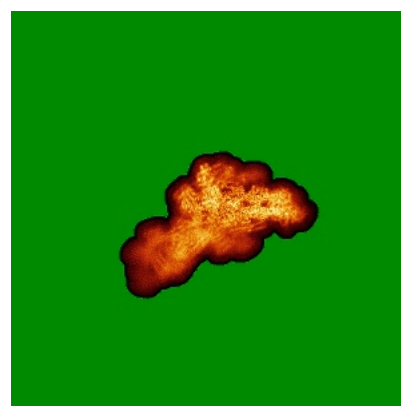
6.4.1 Primary map



X



Y

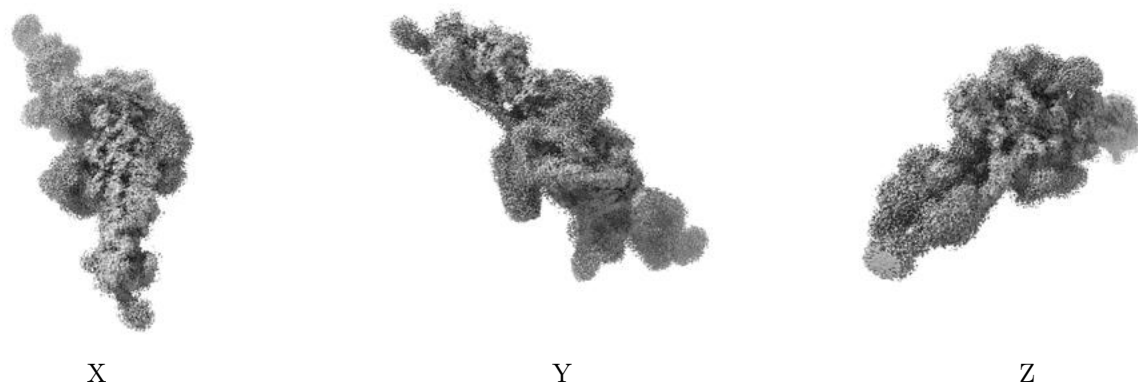


Z

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 0.046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

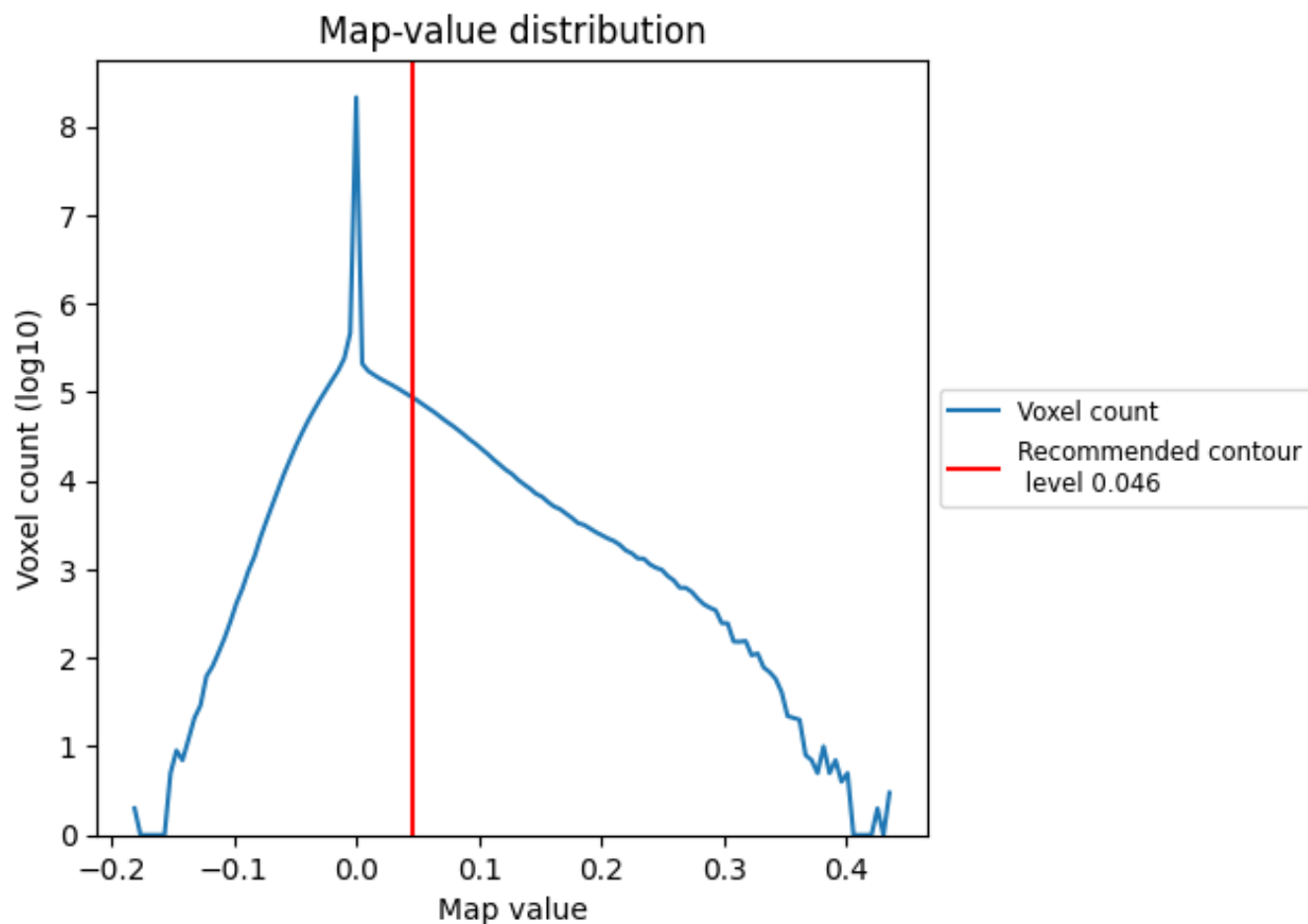
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

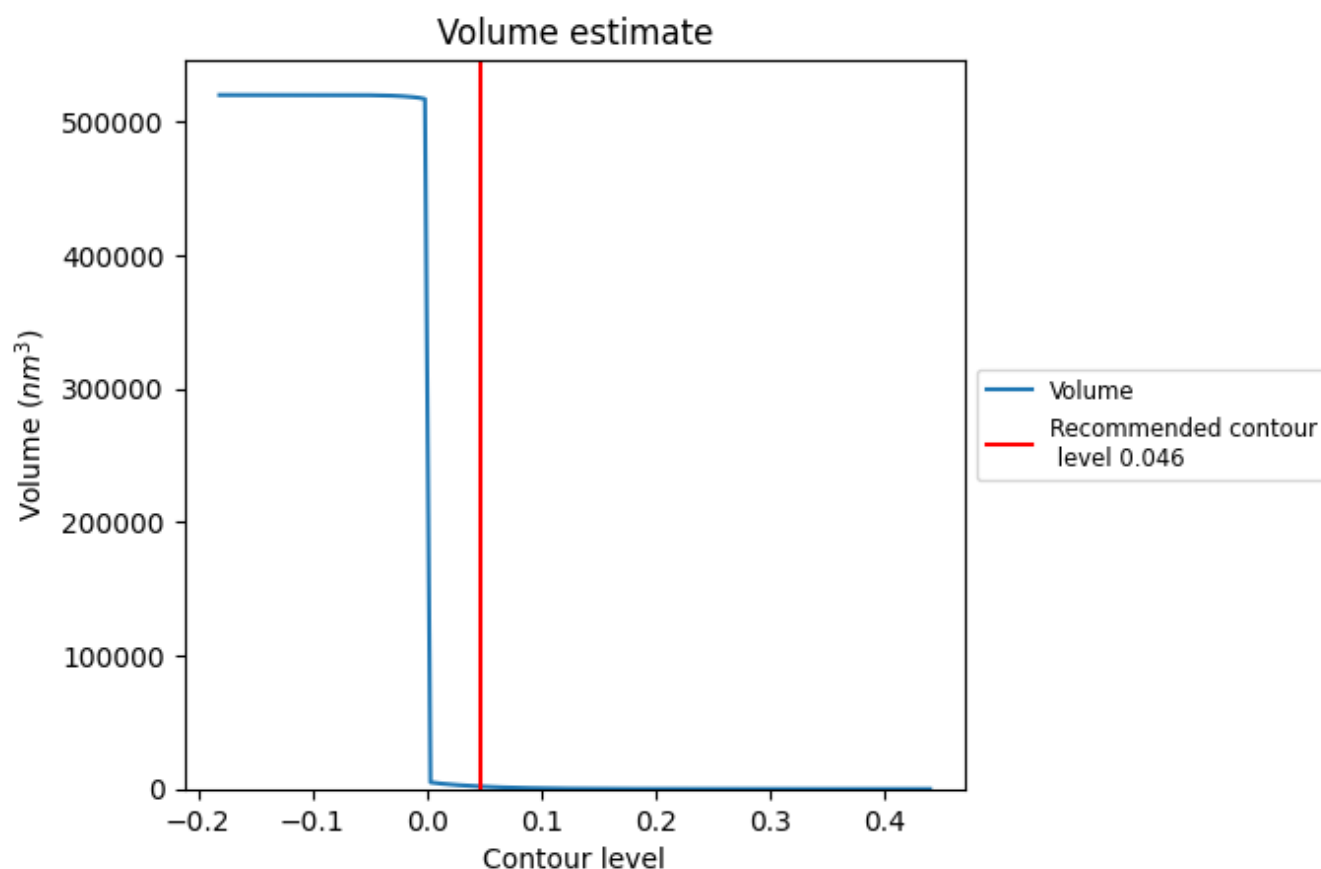
This section contains the results of statistical analysis of the map.

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.

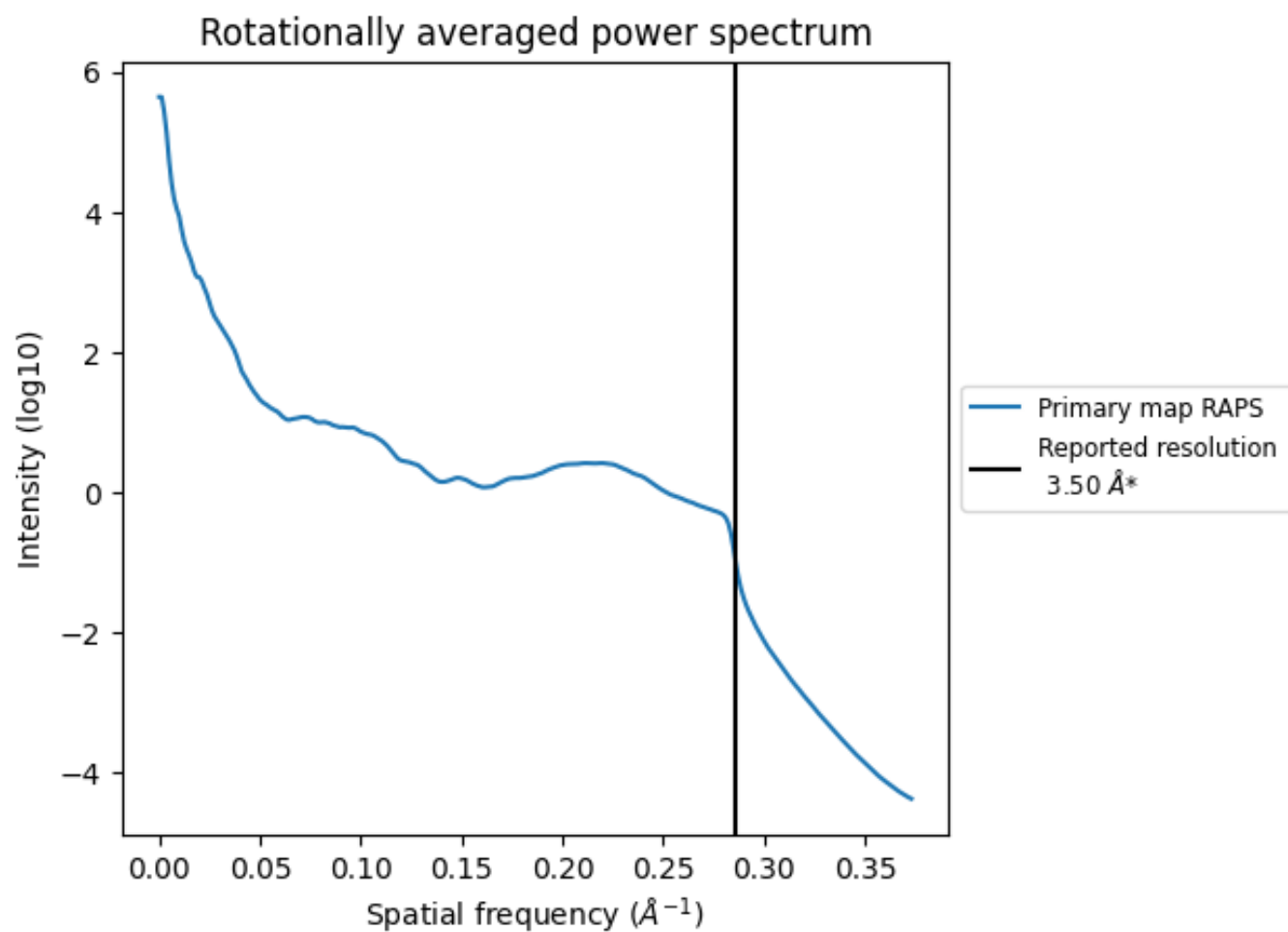
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1916 nm³; this corresponds to an approximate mass of 1731 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

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

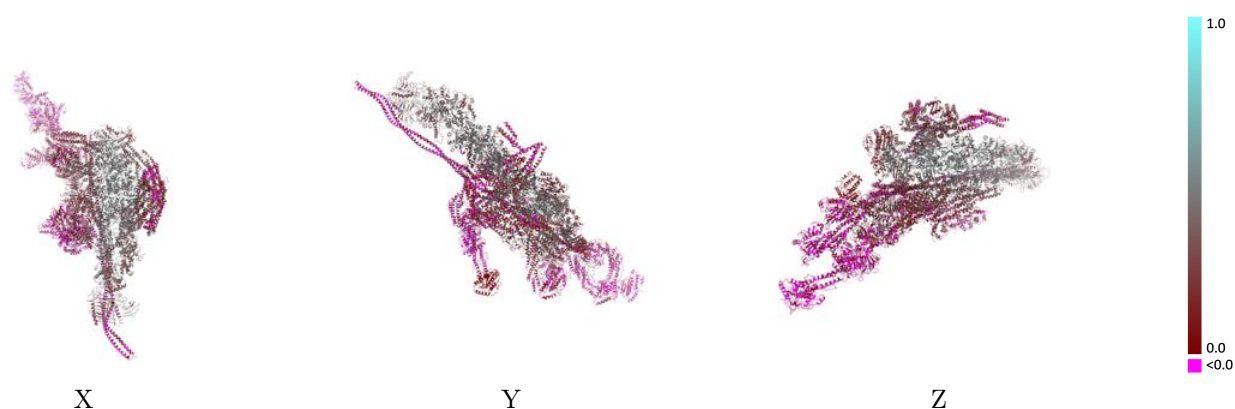
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4168 and PDB model 6F1T. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

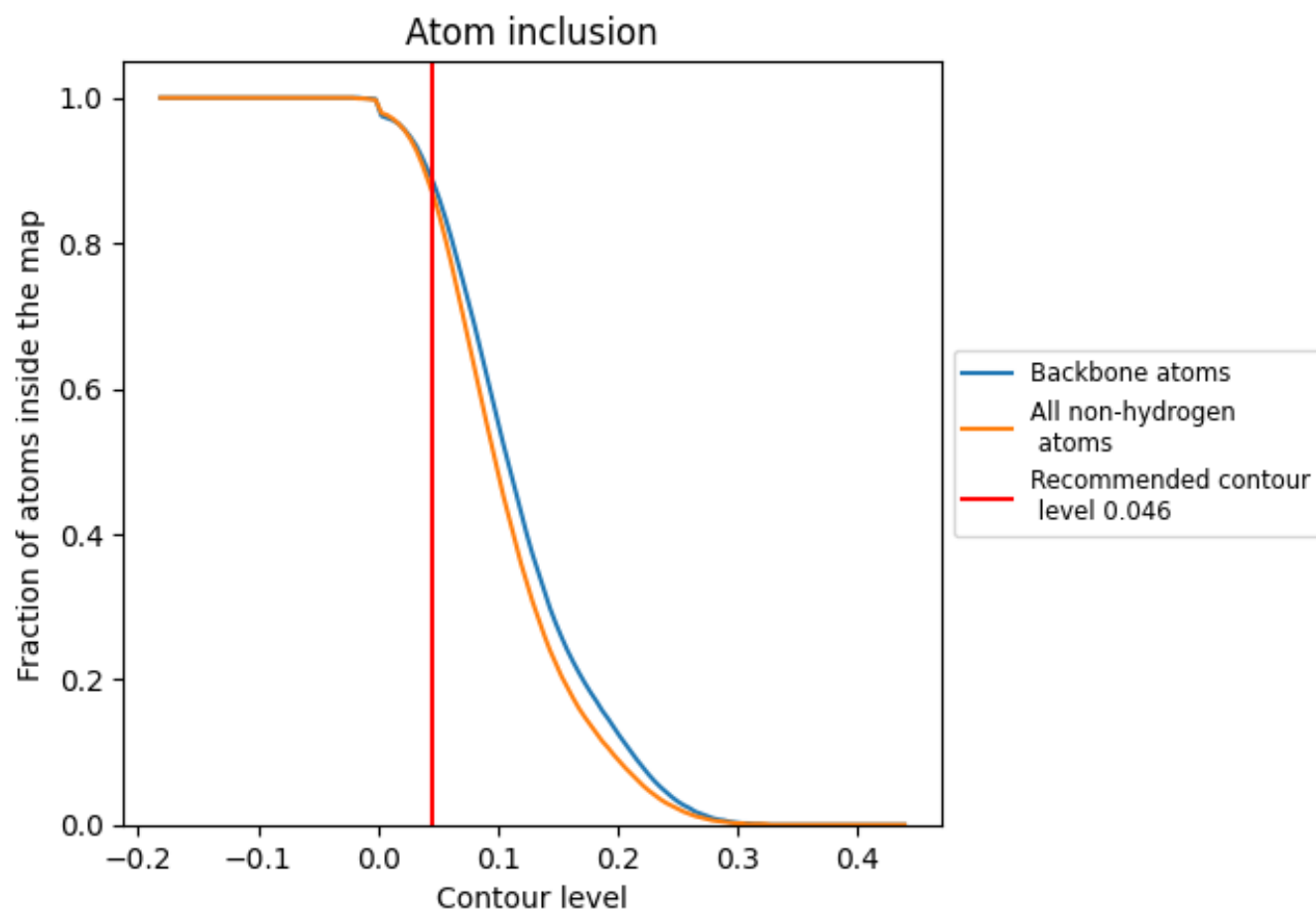


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.046) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.2690
A	 0.9400	 0.4110
B	 0.9630	 0.4730
C	 0.9460	 0.4780
D	 0.9600	 0.4650
E	 0.9520	 0.4730
F	 0.9570	 0.4600
G	 0.9600	 0.4500
H	 0.9620	 0.4520
I	 0.9460	 0.3910
J	 0.9490	 0.3890
K	 0.9480	 0.2900
L	 0.9410	 0.3630
M	 0.9640	 0.1830
N	 0.9720	 0.2050
O	 0.9910	 0.1940
P	 0.9880	 0.2470
Q	 0.4940	 0.1760
R	 0.9930	 0.4040
U	 0.9620	 0.3030
V	 0.9990	 0.3820
X	 0.7120	 0.1100
Y	 0.9880	 0.3960
Z	 0.9920	 0.3400
a	 0.9250	 0.4390
b	 0.9320	 0.4050
c	 0.9440	 0.4200
d	 0.9130	 0.3730
e	 0.7290	 0.1310
f	 0.9010	 0.2120
g	 0.8230	 0.0460
h	 0.9150	 0.2420
i	 0.0230	 -0.0000
j	 0.8070	 0.0720
k	 0.6510	 0.0120



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Chain	Atom inclusion	Q-score
l	 0.6910	 0.0350
m	 0.8990	 0.2480
n	 0.7840	 0.1680
o	 0.9150	 0.2180
p	 0.8290	 0.0500
q	 0.6220	 0.0260
r	 0.2970	 0.0000
s	 0.7740	 0.0320
t	 0.7900	 0.0600
x	 0.6840	 0.1050
z	 0.9320	 0.3110