



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 11:13 PM EST

PDB ID : 7KZM
EMDB ID : EMD-23082
Title : Outer dynein arm bound to doublet microtubules from *C. reinhardtii*
Authors : Walton, T.; Wu, H.; Brown, A.B.
Deposited on : 2020-12-10
Resolution : 7.50 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

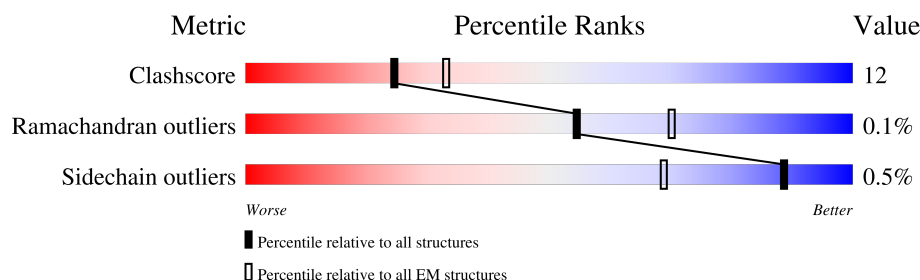
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A1	443	
1	A3	443	
1	A5	443	
1	A7	443	
1	B1	443	
1	B3	443	
1	B5	443	
1	B7	443	

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Mol	Chain	Length	Quality of chain
2	A2	451	
2	A4	451	
2	A6	451	
2	B2	451	
2	B4	451	
2	B6	451	
3	A	4503	
4	B	4568	
5	C	4485	
6	D	683	
7	E	567	
8	F	136	
9	G	159	
10	H	120	
11	I	105	
12	J	100	
13	K	91	
13	L	91	
13	M	91	
13	N	91	
14	O	117	
15	P	103	
16	X	749	
16	X1	749	
17	X0	162	

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Mol	Chain	Length	Quality of chain
18	Y	552	<div><div><div></div><div></div><div></div></div><div>8%5%87%</div></div>
18	Y1	552	<div><div><div></div><div></div><div></div></div><div>19%7%73%</div></div>
19	Y0	168	<div><div><div></div><div></div><div></div></div><div>11%99%</div></div>
20	Z	184	<div><div><div></div><div></div><div></div></div><div>20%60%31%8%</div></div>

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 124943 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 Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	419	Total	C	N	O	S	0	0
			3298	2077	563	628	30		
1	B3	410	Total	C	N	O	S	0	0
			3227	2030	553	614	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	430	Total	C	N	O	S	0	0
			3339	2114	568	636	21		
2	A4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	A6	429	Total	C	N	O	S	0	0
			3335	2112	567	635	21		
2	B2	411	Total	C	N	O	S	0	0
			3204	2035	544	605	20		
2	B4	409	Total	C	N	O	S	0	0
			3193	2028	542	603	20		
2	B6	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called Heavy chain alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	3275	Total	C	N	O	0	0
			16173	9623	3275	3275		

- Molecule 4 is a protein called Flagellar outer dynein arm heavy chain beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	3540	Total	C	N	O	S	0	0
			19163	11601	3735	3803	24		

- Molecule 5 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	3890	Total	C	N	O	S	0	0
			21756	13184	4221	4314	37		

- Molecule 6 is a protein called Dynein, 78 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	456	Total	C	N	O	S	0	0
			3609	2297	610	678	24		

- Molecule 7 is a protein called Dynein, 70 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	474	Total	C	N	O	S	0	0
			3697	2332	623	725	17		

- Molecule 8 is a protein called Flagellar outer dynein arm light chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	100	Total	C	N	O	0	0
			495	295	100	100		

- Molecule 9 is a protein called Dynein 18 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		

- Molecule 10 is a protein called Dynein 11 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	H	91	Total	C	N	O	0	0
			451	269	91	91		

- Molecule 11 is a protein called Dynein light chain roadblock LC7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	103	Total	C	N	O	S	0	0
			827	525	148	153	1		

- Molecule 12 is a protein called Dynein light chain roadblock LC7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	94	Total	C	N	O	S	0	0
			741	466	133	140	2		

- Molecule 13 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	L	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	M	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
13	N	82	Total	C	N	O		0	0
			407	243	82	82			

- Molecule 14 is a protein called Dynein light chain 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	97	Total	C	N	O	0	0
			481	286	97	98		

- Molecule 15 is a protein called Dynein light chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	98	Total	C	N	O	S	0	0
			805	523	128	146	8		

- Molecule 16 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	56	Total	C	N	O	S	0	0
			481	292	97	89	3		
16	X1	142	Total	C	N	O	S	0	0
			1178	715	223	235	5		

- Molecule 17 is a protein called DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X0	162	Total	C	N	O		0	0
			810	486	162	162			

- Molecule 18 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	73	Total	C	N	O	S	0	0
			595	360	112	120	3		
18	Y1	147	Total	C	N	O	S	0	0
			1185	729	223	224	9		

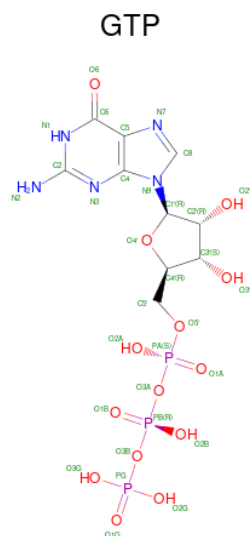
- Molecule 19 is a protein called DC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y0	168	Total	C	N	O		0	0
			840	504	168	168			

- Molecule 20 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
21	A1	1	Total 32	C 10	N 5	O 14	P 3	0
21	A3	1	Total 32	C 10	N 5	O 14	P 3	0
21	A5	1	Total 32	C 10	N 5	O 14	P 3	0
21	A7	1	Total 32	C 10	N 5	O 14	P 3	0
21	B2	1	Total 32	C 10	N 5	O 14	P 3	0
21	B5	1	Total 32	C 10	N 5	O 14	P 3	0
21	B7	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

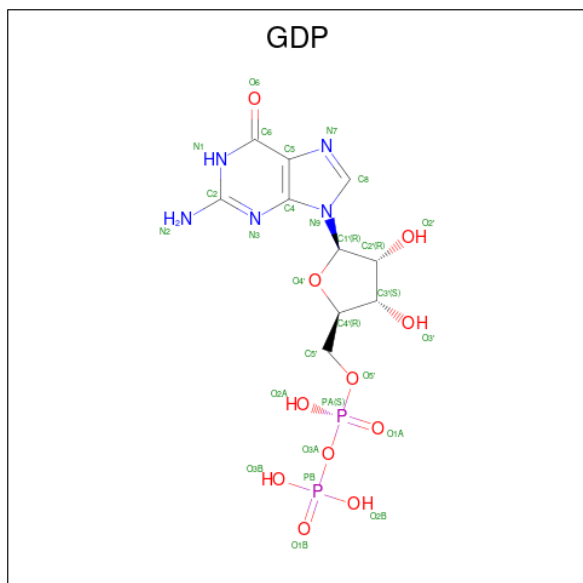
Mol	Chain	Residues	Atoms	AltConf
22	A1	1	Total Mg 1 1	0
22	A2	1	Total Mg 1 1	0
22	A4	1	Total Mg 1 1	0
22	A6	1	Total Mg 1 1	0
22	B3	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
22	B4	1	Total	Mg	0
			1	1	
22	B6	1	Total	Mg	0
			1	1	

- Molecule 23 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

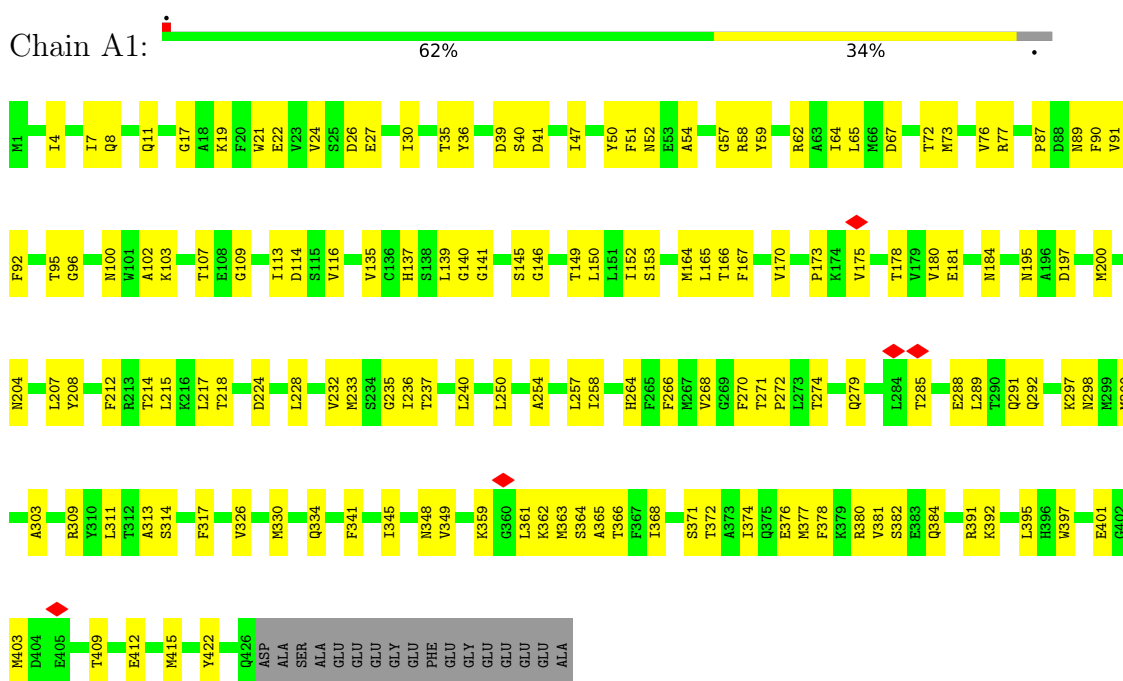


Mol	Chain	Residues	Atoms					AltConf
23	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	

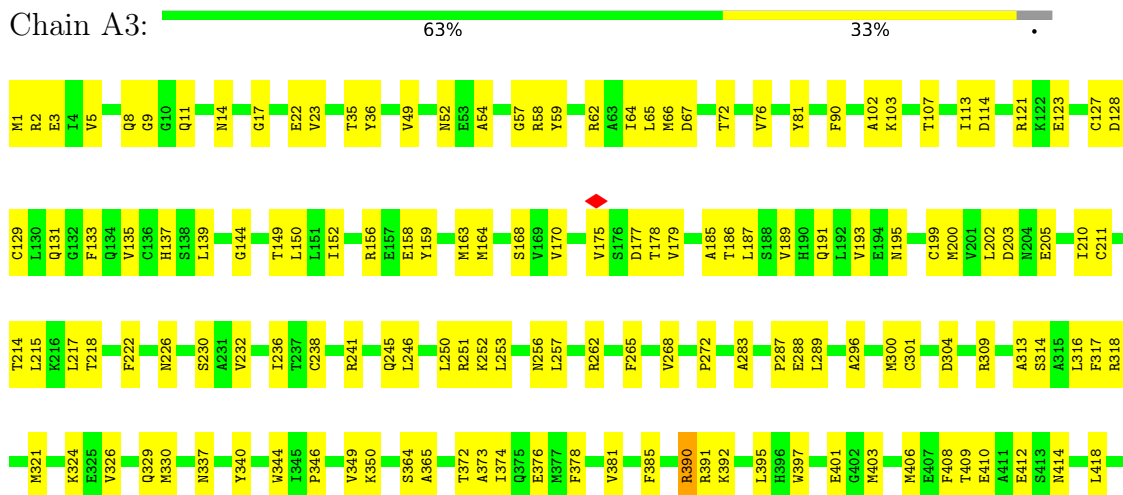
3 Residue-property plots

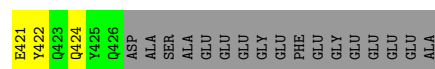
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Tubulin beta



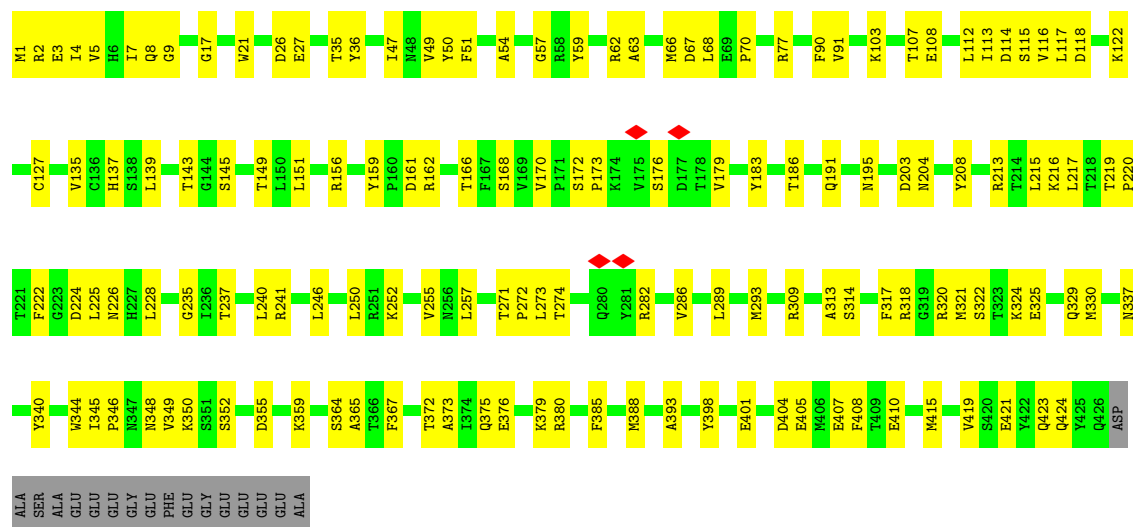
• Molecule 1: Tubulin beta





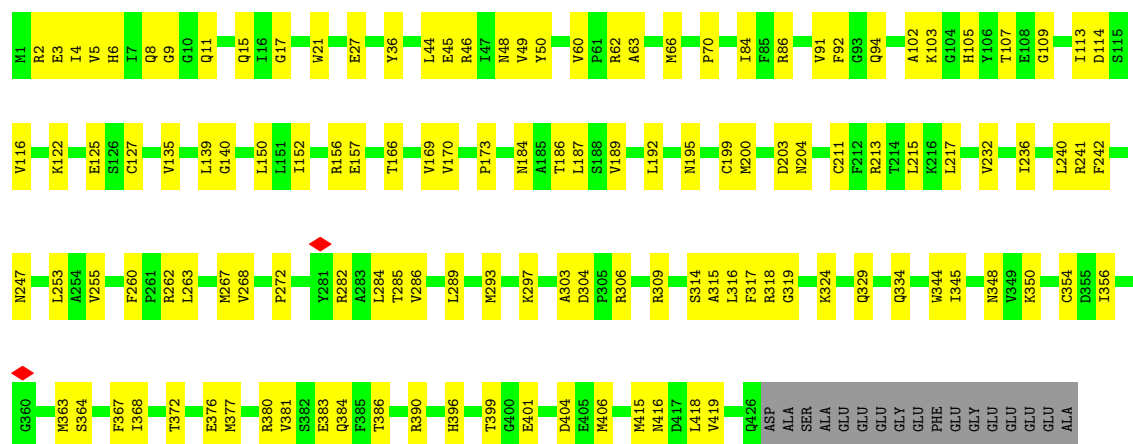
• Molecule 1: Tubulin beta

Chain A5: 64% 32%



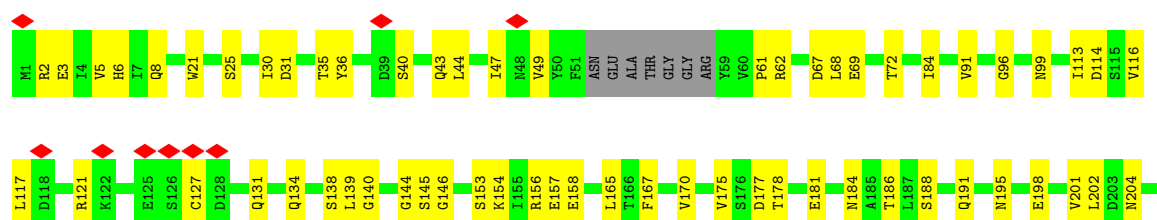
• Molecule 1: Tubulin beta

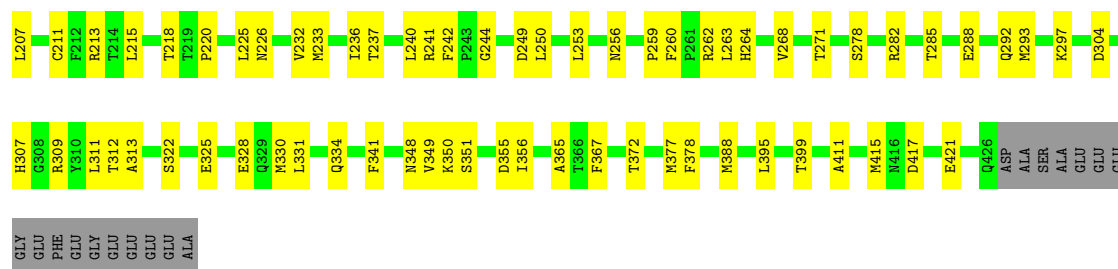
Chain A7: 67% 29%



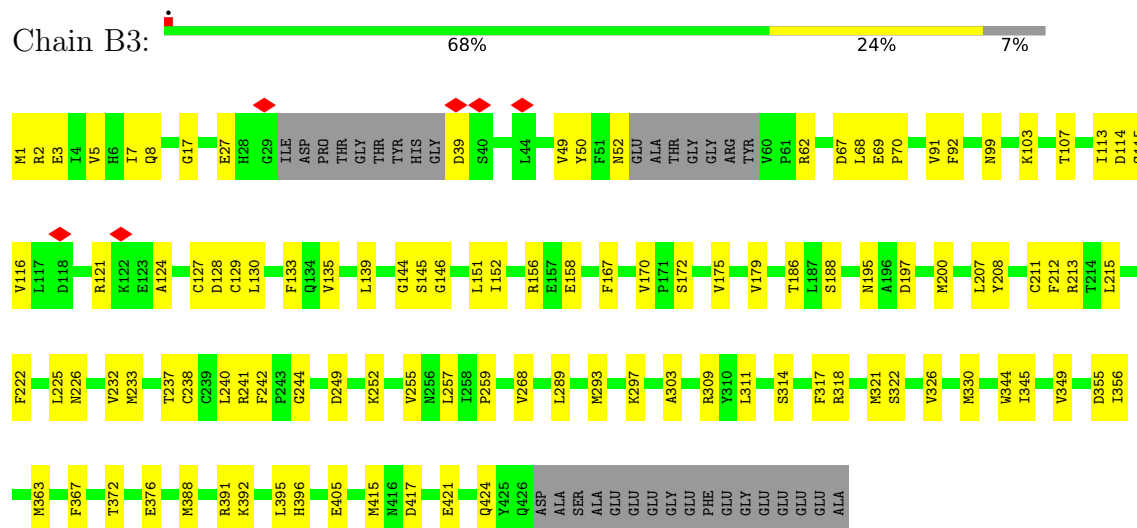
• Molecule 1: Tubulin beta

Chain B1: 66% 28% 5%

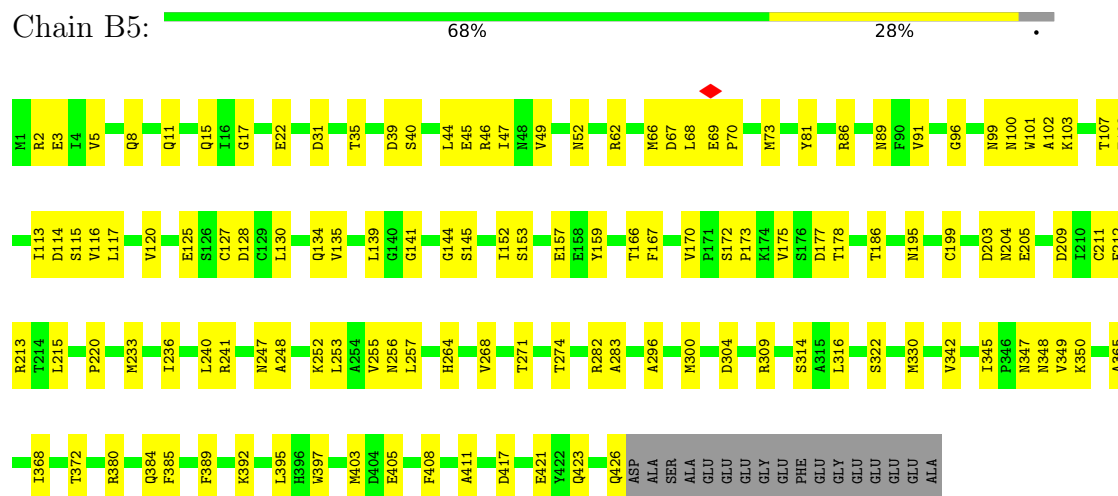




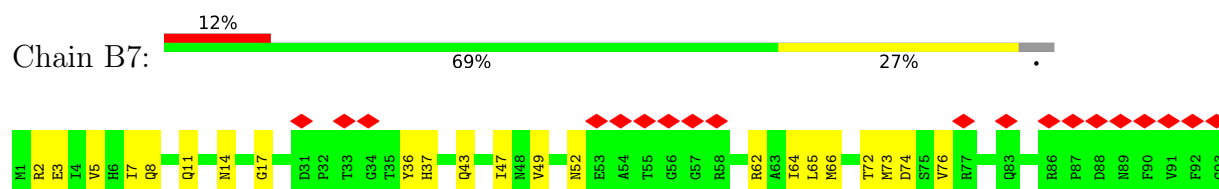
• Molecule 1: Tubulin beta

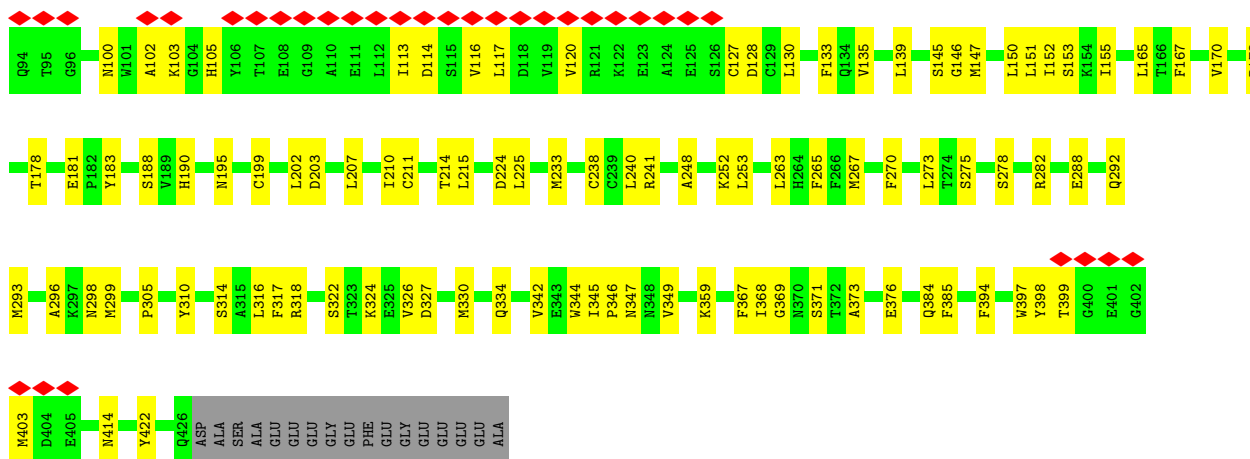


• Molecule 1: Tubulin beta



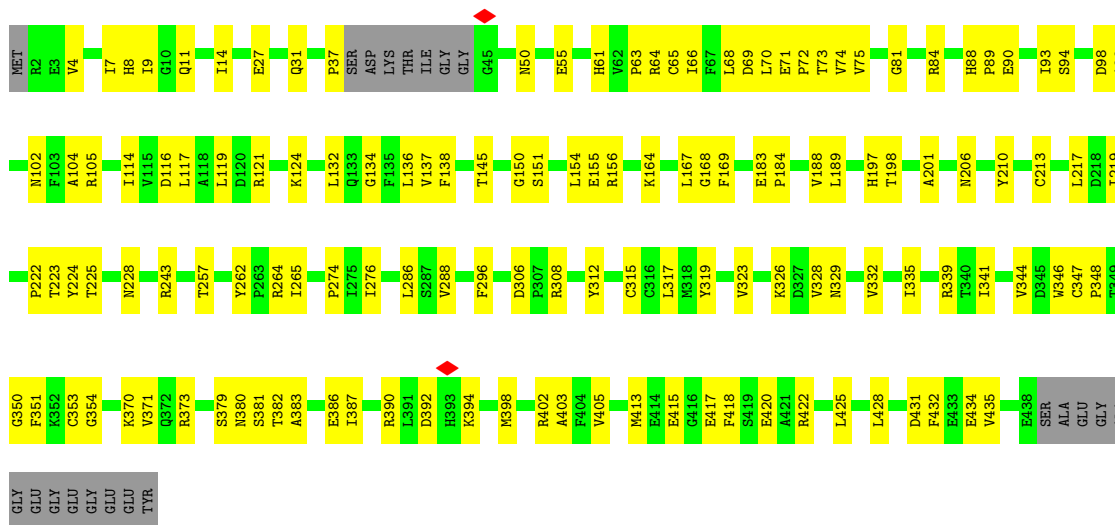
• Molecule 1: Tubulin beta





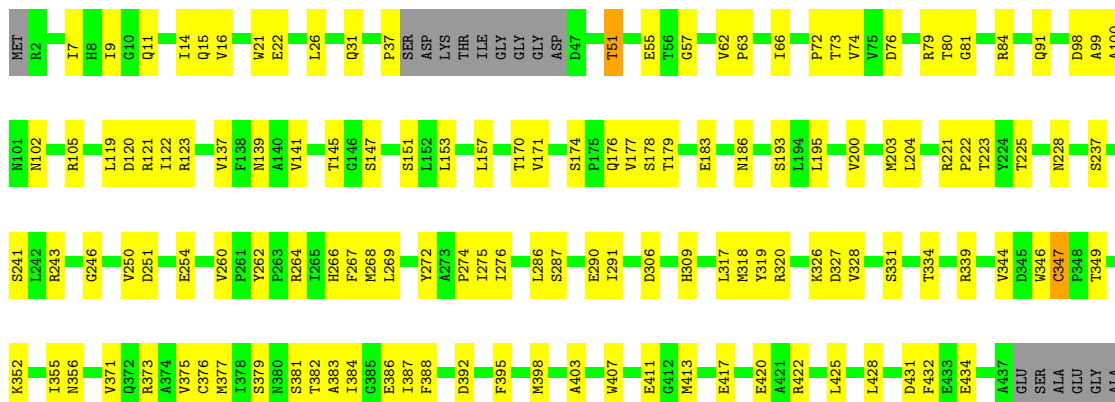
• Molecule 2: Tubulin alpha

Chain A2:



• Molecule 2: Tubulin alpha

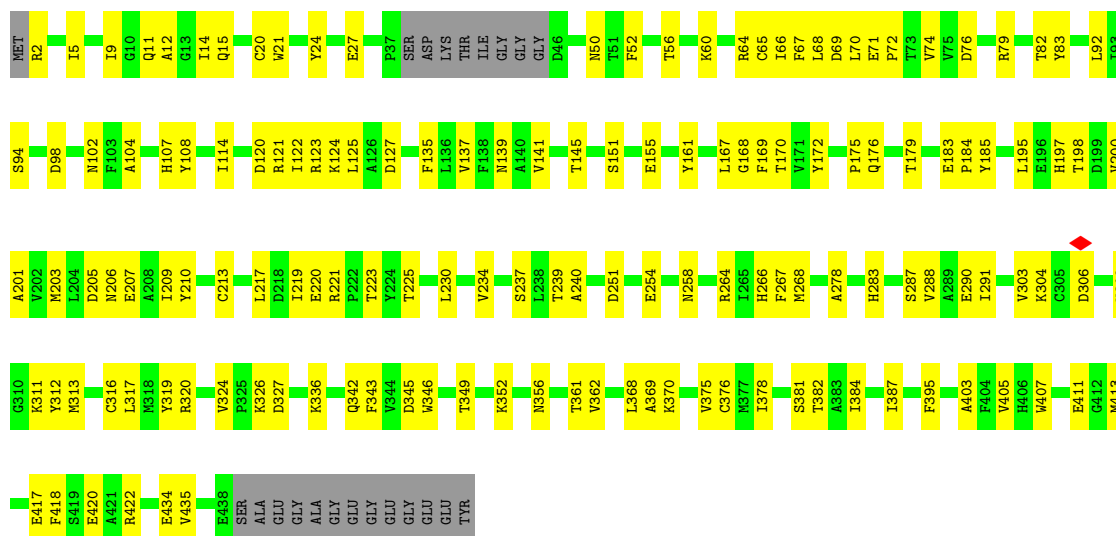
Chain A4:



GLY
GLU
GLY
GLY
GLY
GLY
GLY
TYR

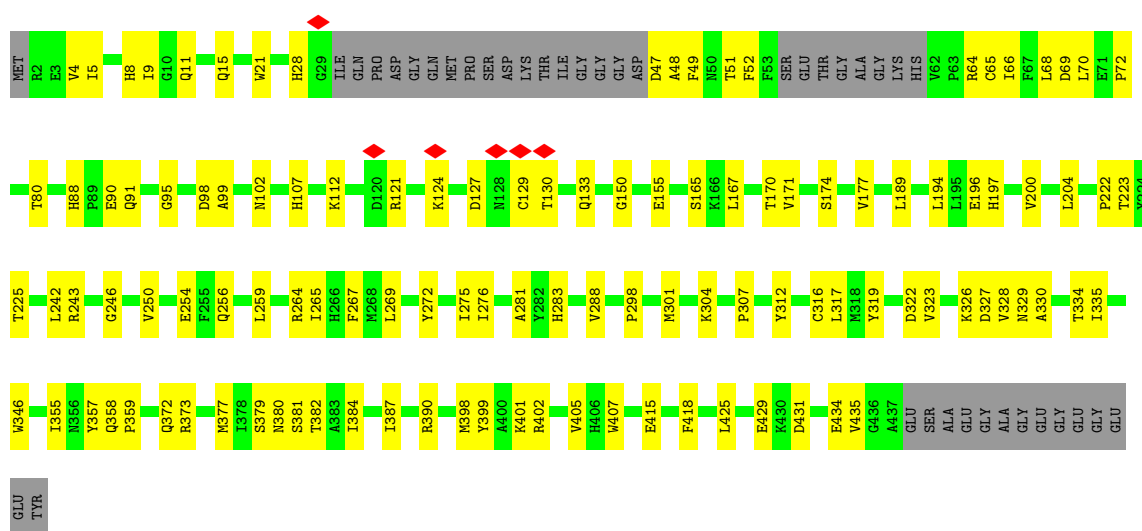
• Molecule 2: Tubulin alpha

Chain A6: 63% 32% 5%



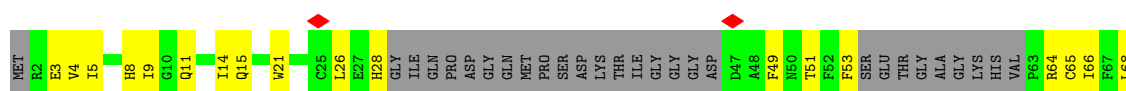
• Molecule 2: Tubulin alpha

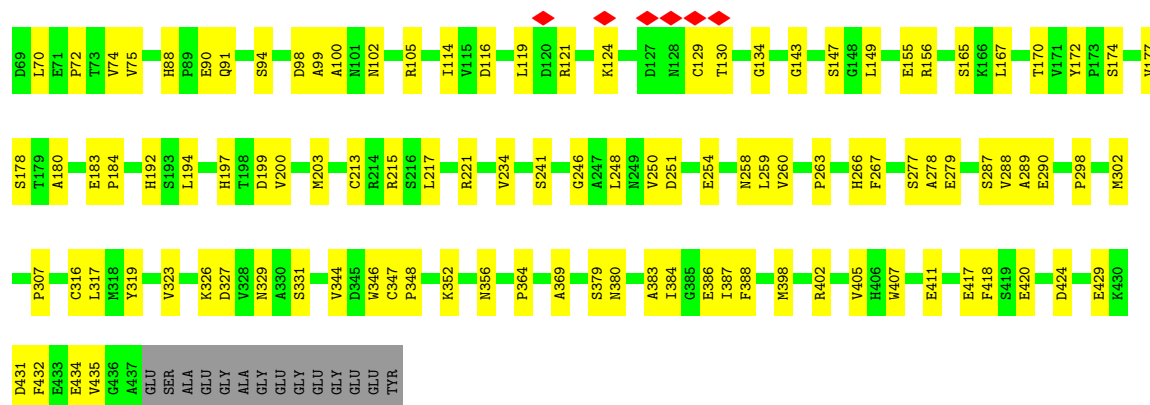
Chain B2: 66% 25% 9%



• Molecule 2: Tubulin alpha

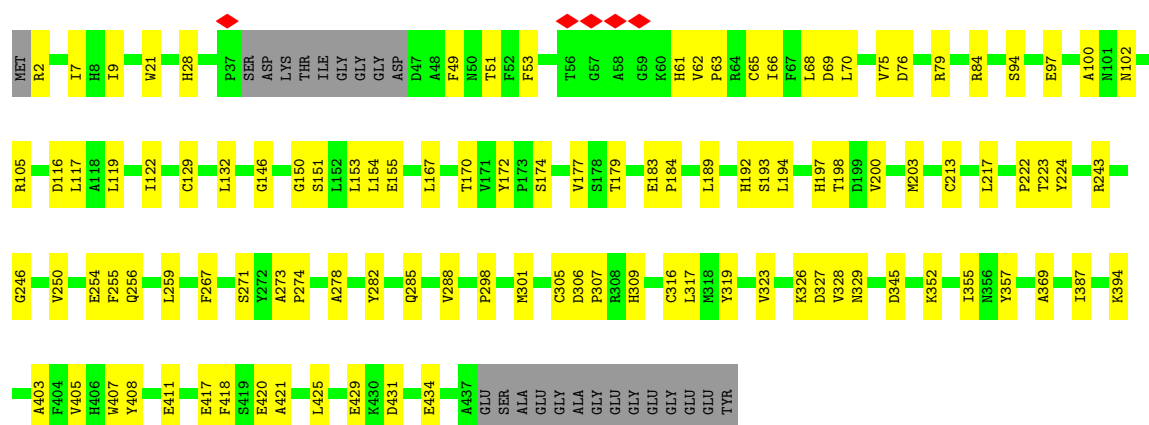
Chain B4: 63% 27% 9%





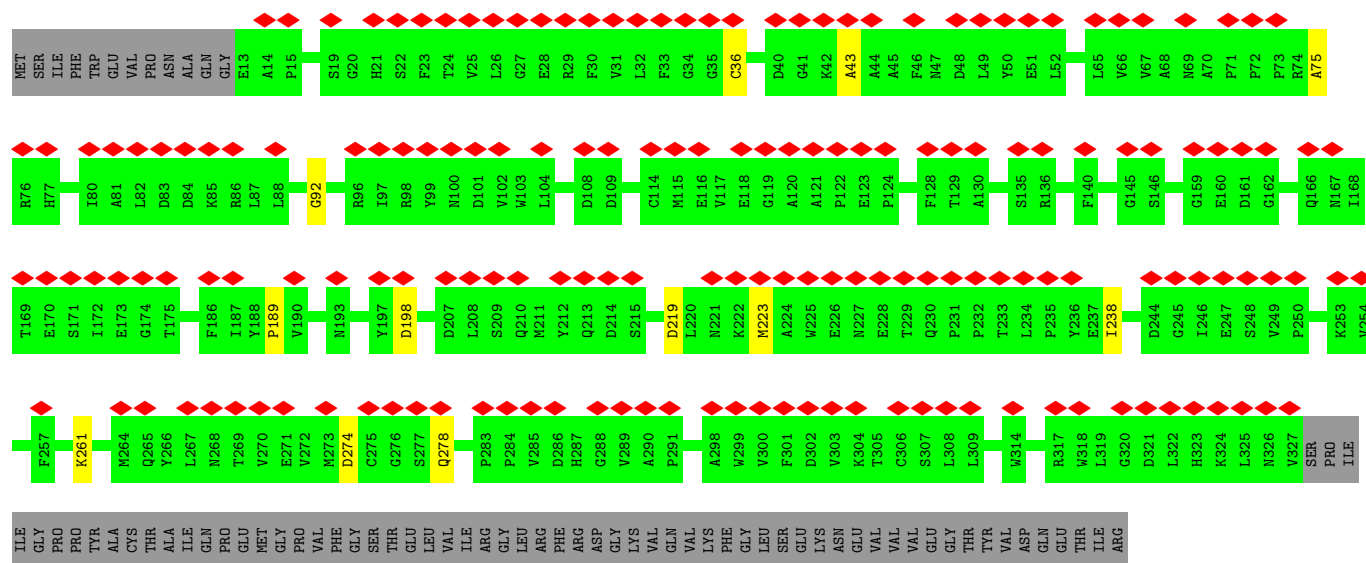
• Molecule 2: Tubulin alpha

Chain B6: 71% 24% 5%



• Molecule 3: Heavy chain alpha

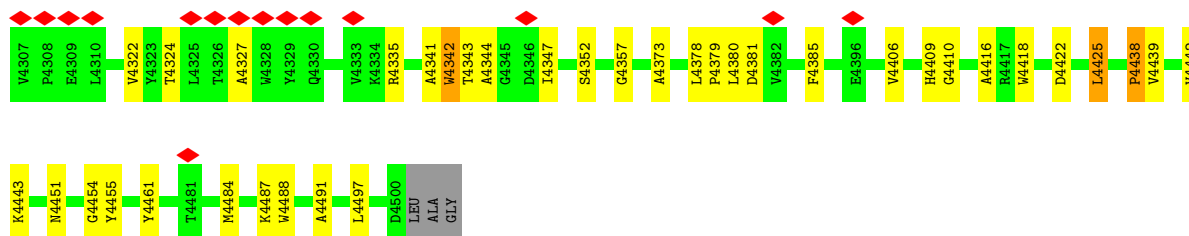
Chain A: 16% 58% 14% 27%



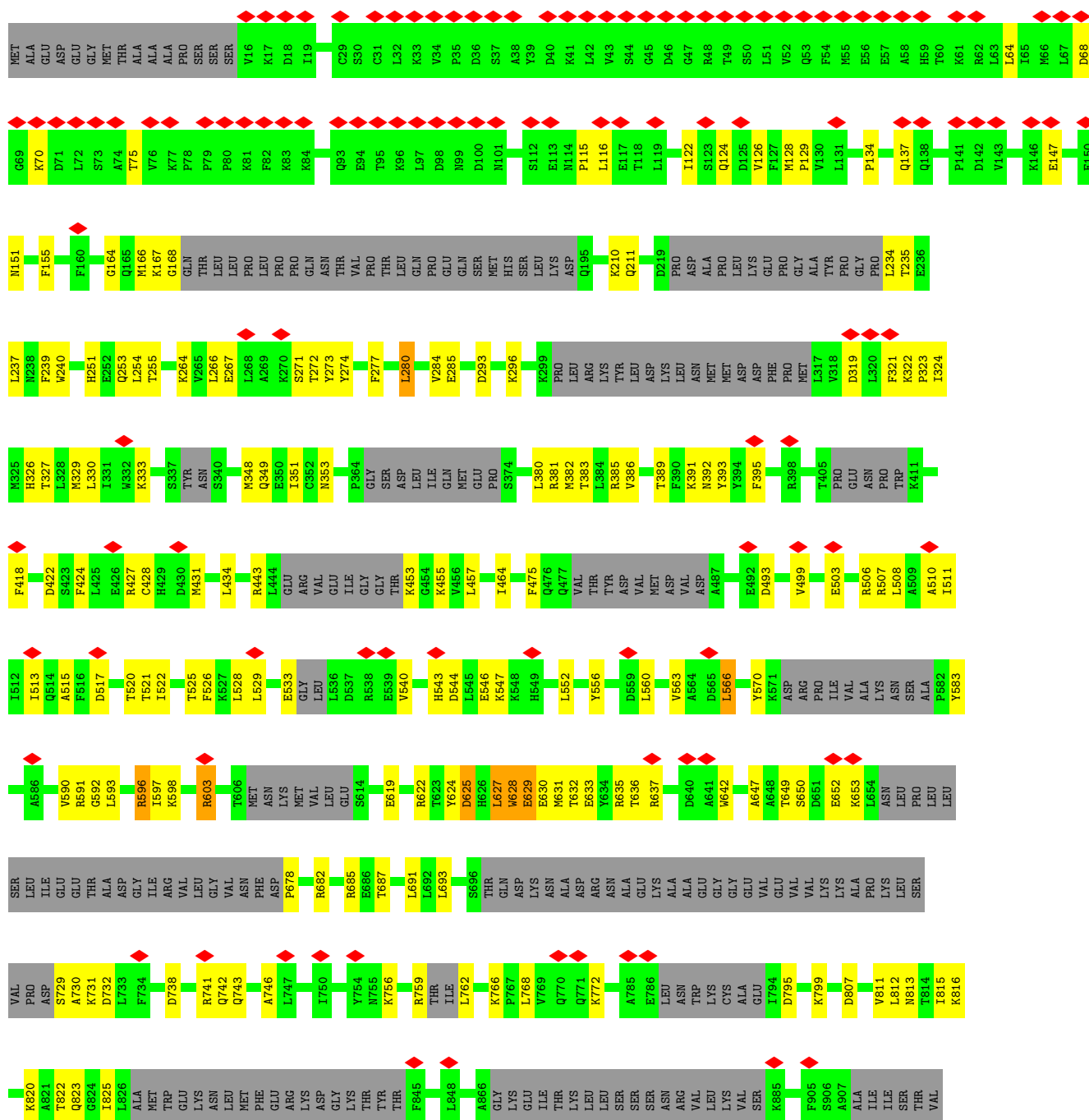
C1509	K1437	M1331	ASP	LEU	ALA	VAL	VAL	MET	VAL	GLN	TYR	GLU	LEU	SER	GLY	THR	VAL	GLN	VAL
P1516	A1438	K1341	HIS	SER	LEU	GLY	SER	ASP	GLN	ASN	VAL	GLY	ARG	PHE	VAL	THR	ALA	GLN	THR
F1517	D1342	D1342	TRP	ILE	GLU	VAL	ASP	ALA	PHE	ALA	GLY	GLY	ASP	GLY	VAL	THR	ASN	GLN	ASN
S1518	M1440	E1343	ARG	THR	GLN	GLY	GLY	LEU	GLN	GLY	ASP	ALA	ASP	GLY	LEU	GLY	GLY	LEU	TYR
S1519	I1344	I1344	LEU	THR	CYS	PRO	CYS	PRO	VAL	PRO	LEU	ASP	PRO	LEU	ASP	ASP	ASP	ASP	GLY
P1520	Y1442	L1346	ALA	ILE	ASP	ILE	ASP	GLN	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
P1522	M1443	G1346	THR	ILE	ARG	GLN	ARG	GLY	GLY	VAL	ASP	ASP	TRP	ASP	GLY	THR	ASP	ASP	GLY
L1523	E1444	Q1347	THR	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
E1524	S1445	K1349	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N1525	K1446	L1351	THR	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PHE	GLY	GLY	GLY	GLY	GLY	GLY
K1526		D1352	PHE	THR	SER	ASP	ASP	ASP	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
Q1529	S1458	D1353	ASN	GLN	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
Y1530	A1459	Q1359	VAL	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
M1531	D1460	I1360	ASP	PRO	PRO	PHE	PHE	PHE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
N1532	L1461	M1361	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
D1533	L1462	E1363	PHE	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
A1536	D1463	Y1370	LEU	HIS	PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
K1537	L1464	L1465	ASP	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
N1540	S1466	S1373	LEU	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
Y1553	M1467	L1374	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
P1554	G1468	F1375	ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
S1555	M1469	I1376	LEU	ASP	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
R1558	M1470	H1377	GLY	GLY	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
L1562	P1471	S1378	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Q1568	M1472	E1379	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
V1572	R1473	E1380	GLY	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
I1576	V1474	V1381	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
Y1577	Q1475	K1382	ASP	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
W1578	I1476	E1383	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E1583	M1479	E1384	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
F1586	F1482	L1385	ASN	PHE	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
T1587	I1485	P1386	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E1588	D1486	Q1387	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
F1586	D1487	T1388	VAL	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
T1587	K1487	F1392	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
E1588	L1488	I1395	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
M1589	R1489	T1395	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
A1590	L1490	V1399	VAL	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
R1591	D1491	K1400	ASP	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
G1592	S1492	K1401	ARG	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
G1595	E1493	V1402	SER	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
Y1600	E1494	K1410	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
Q1607	V1495	N1411	ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
I1612	P1496	S1414	MET	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
K1621	P1497	G1420	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	Q1607	N1424																	
	I1612																		
	K1621																		





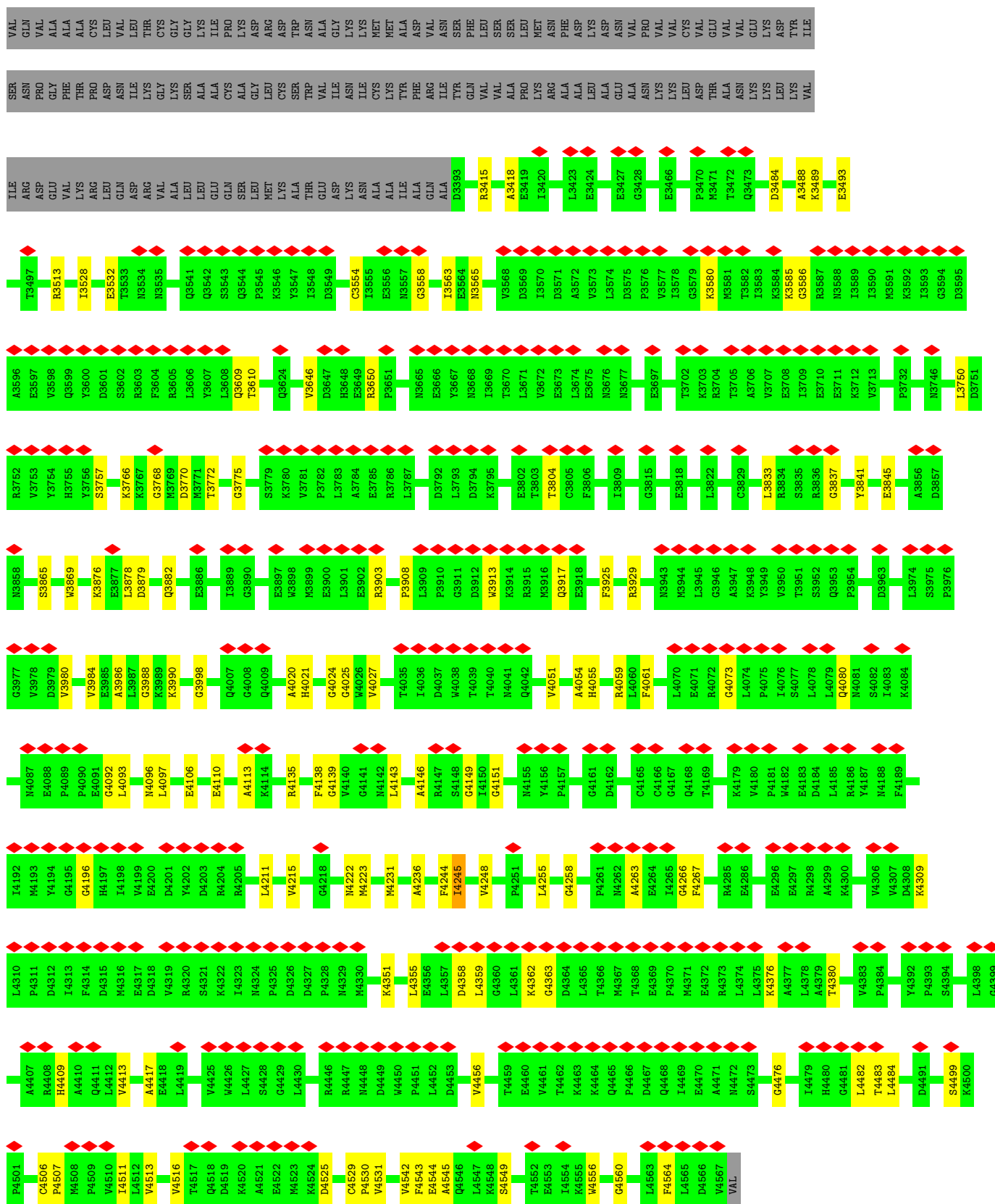


• Molecule 4: Flagellar outer dynein arm heavy chain beta

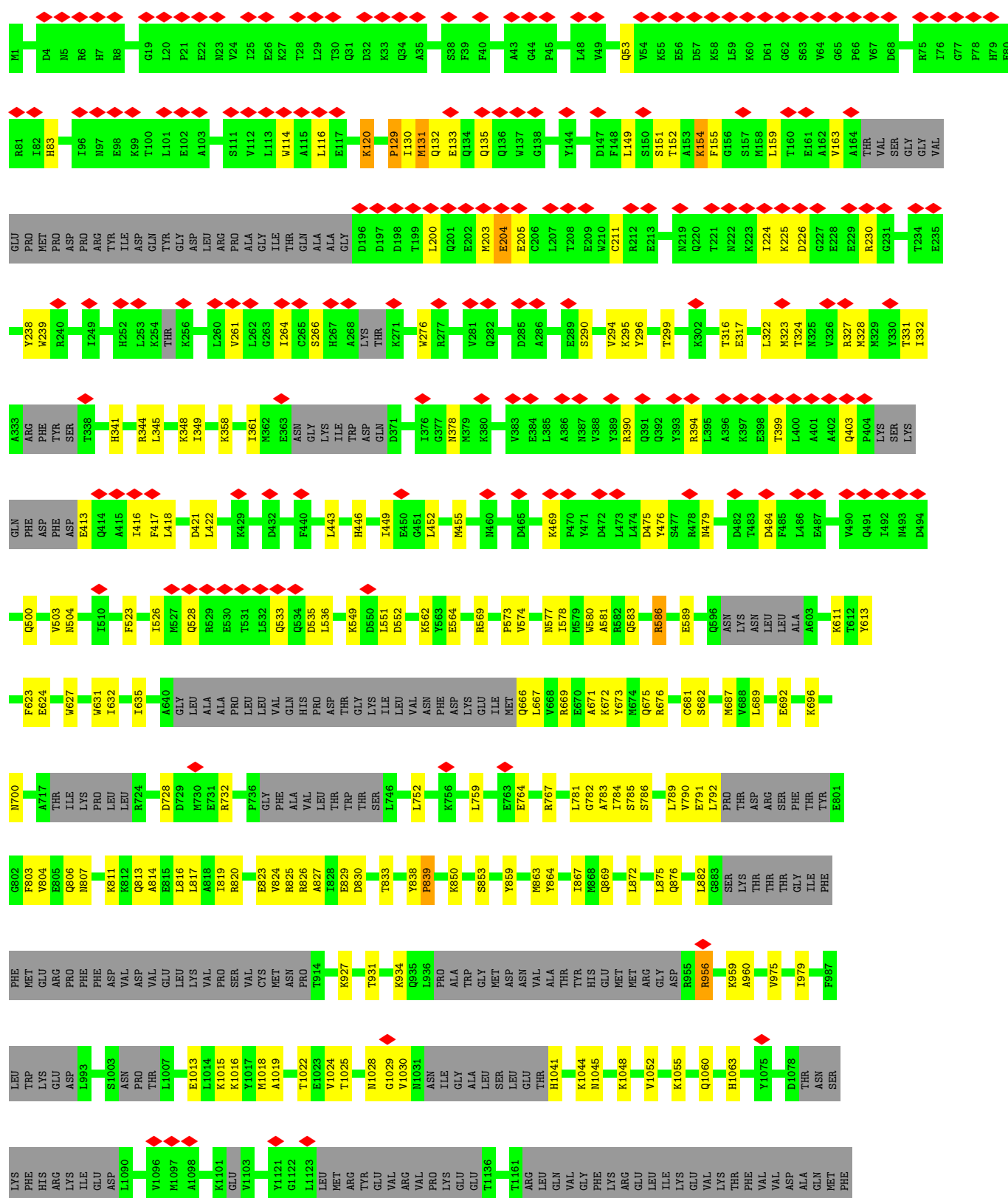
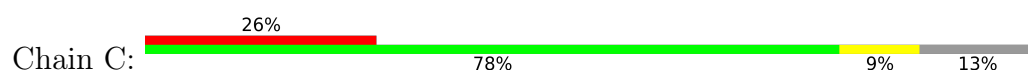






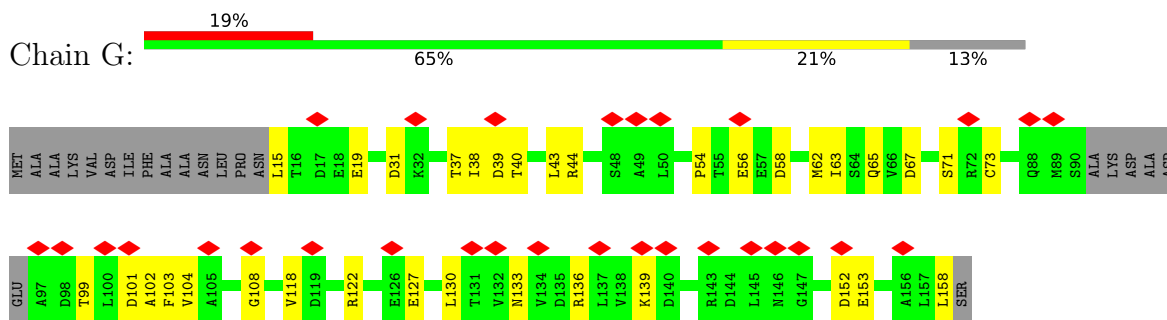
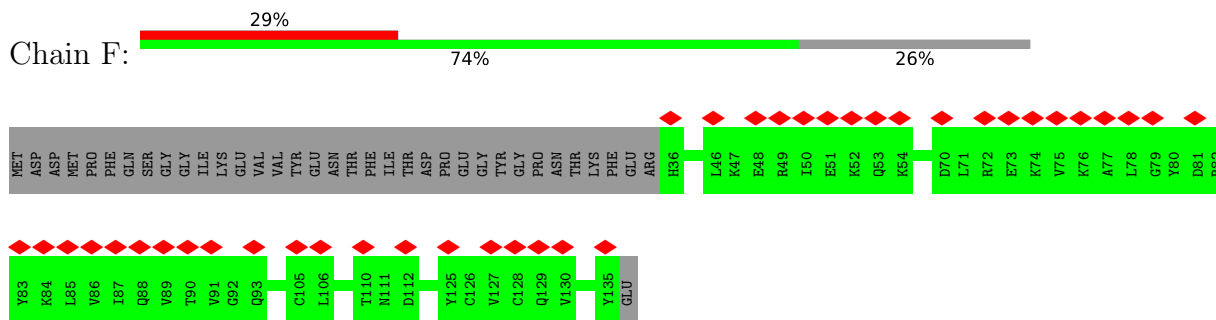
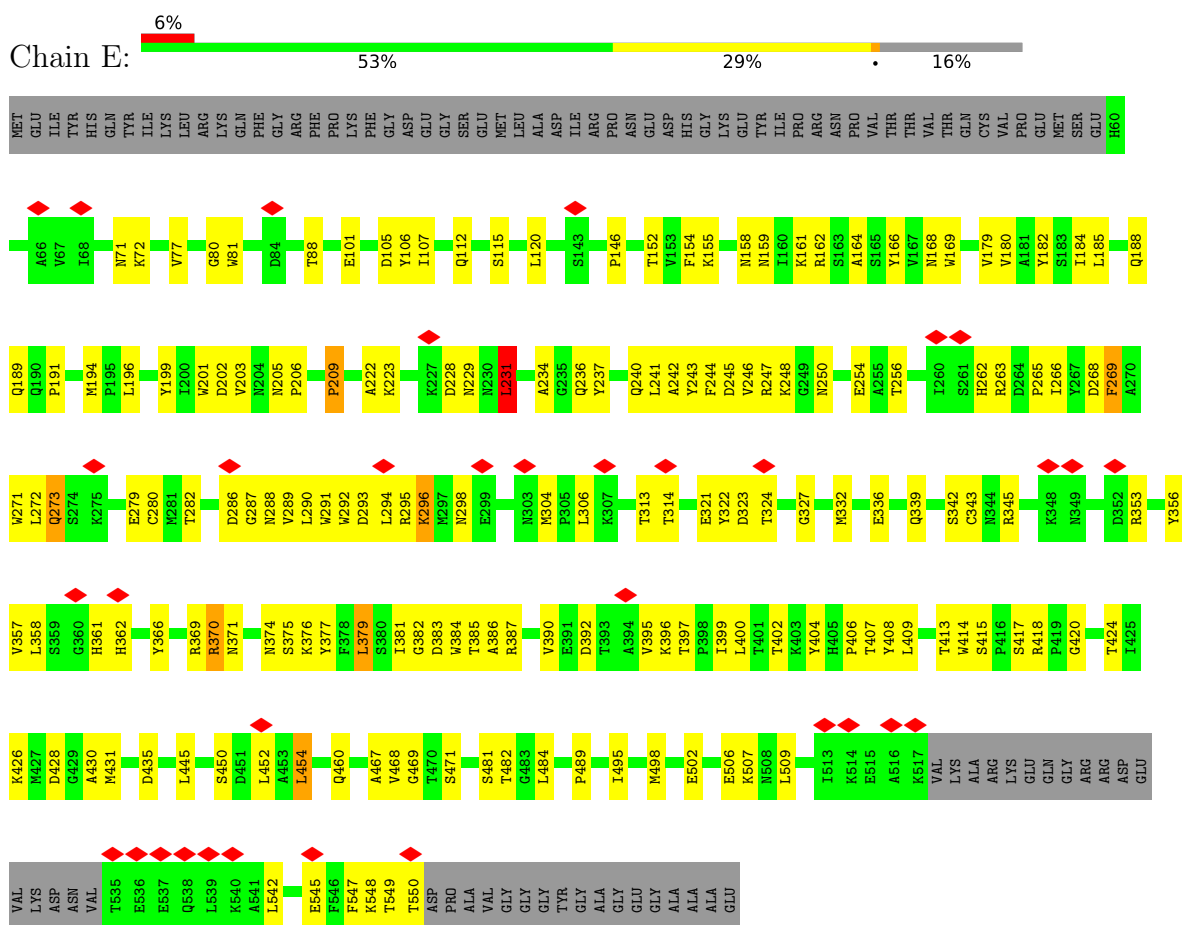


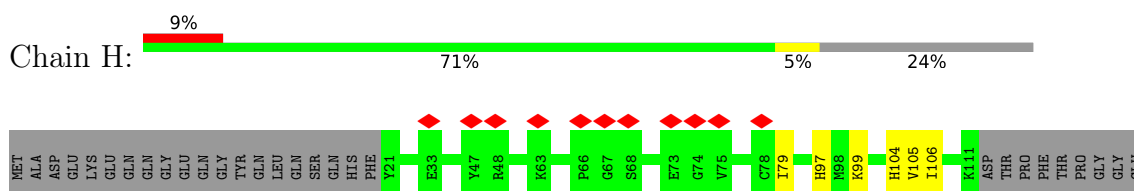
- Molecule 5: Dynein gamma chain, flagellar outer arm



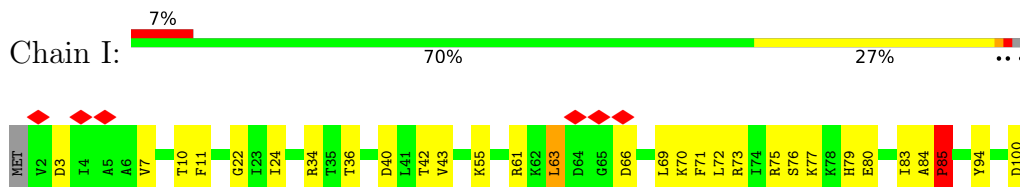




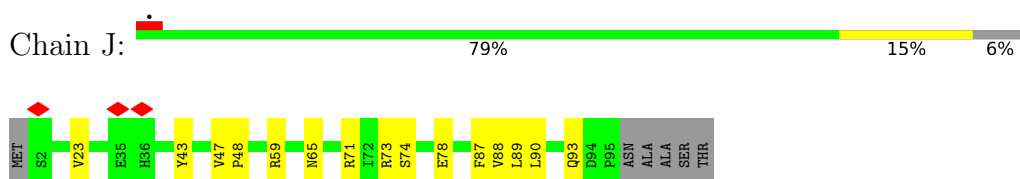




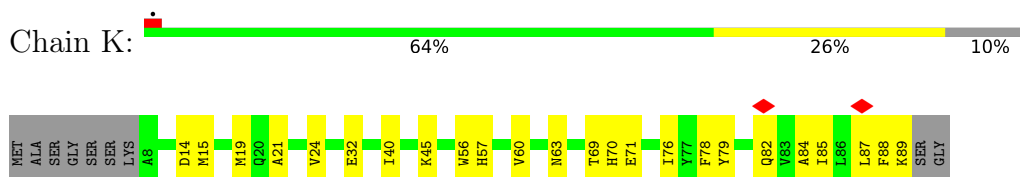
- Molecule 11: Dynein light chain roadblock LC7a



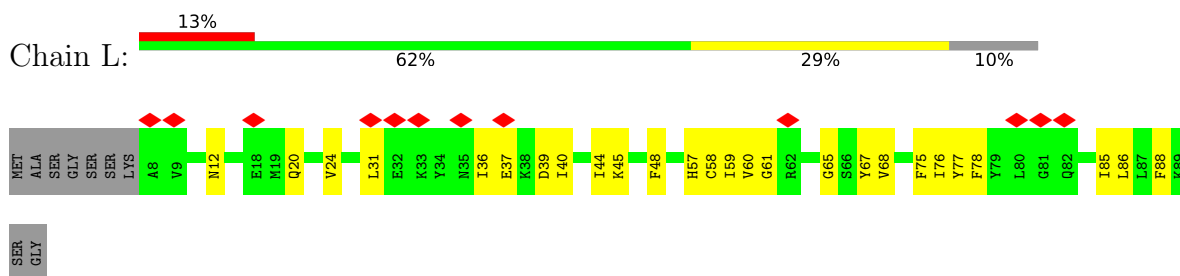
- Molecule 12: Dynein light chain roadblock LC7b



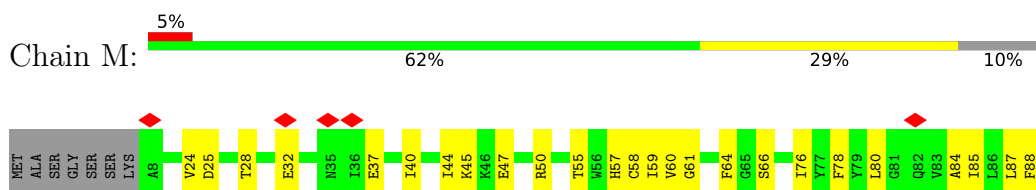
- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



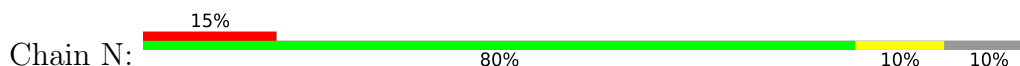
- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 13: Dynein 8 kDa light chain, flagellar outer arm



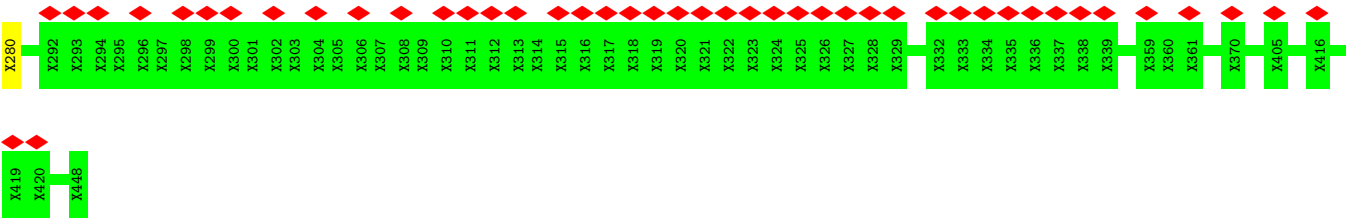
[illegible]

- Molecule 16: Outer dynein arm-docking complex subunit 1

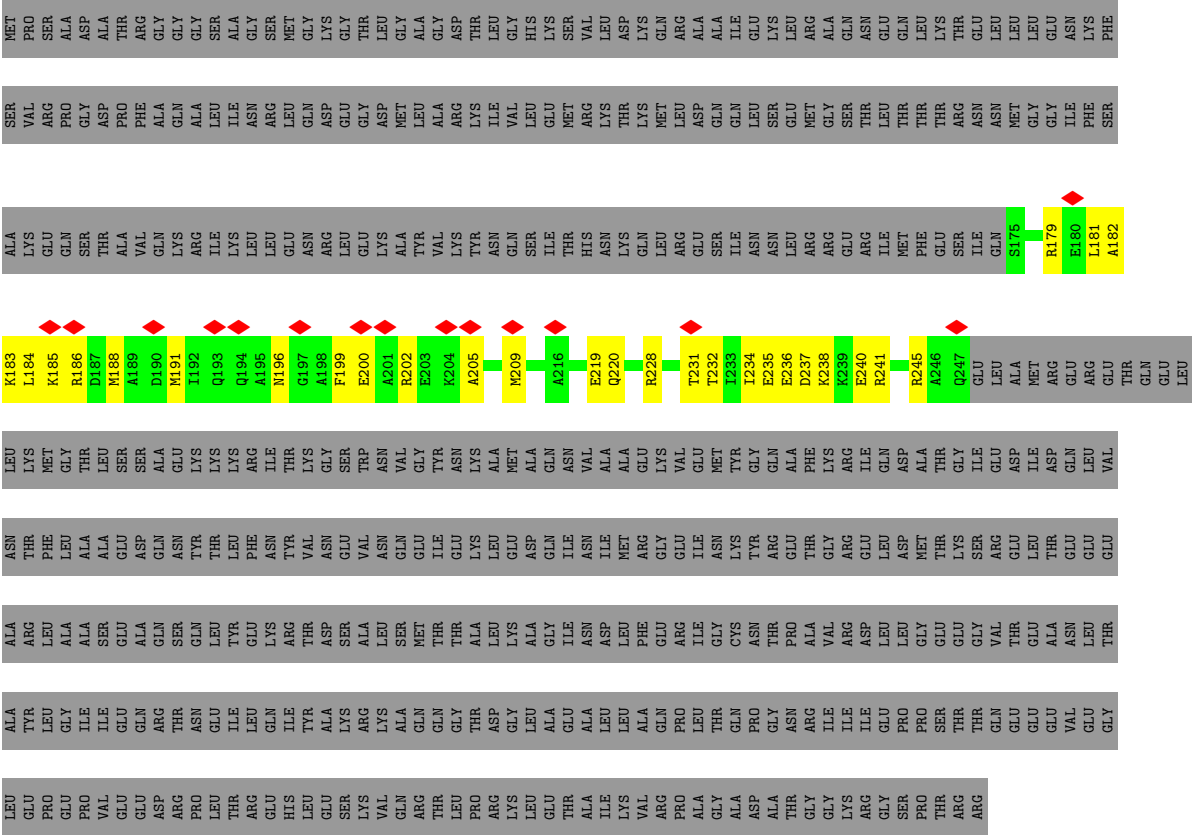
[illegible]

- Molecule 17: DC1

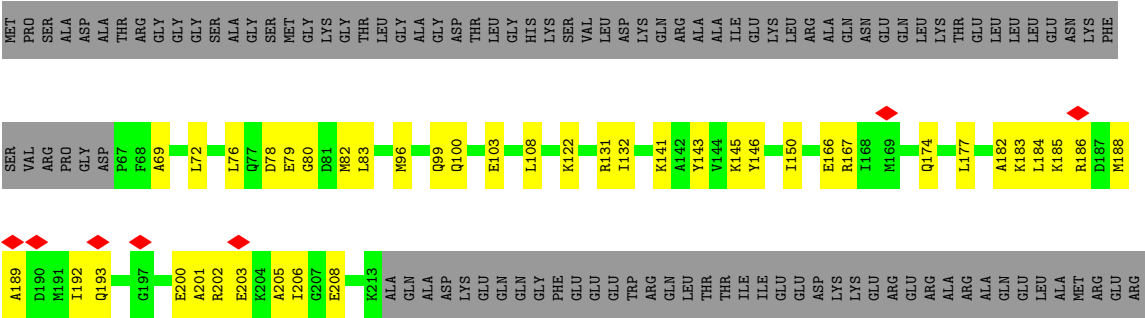




• Molecule 18: Outer dynein arm protein 1

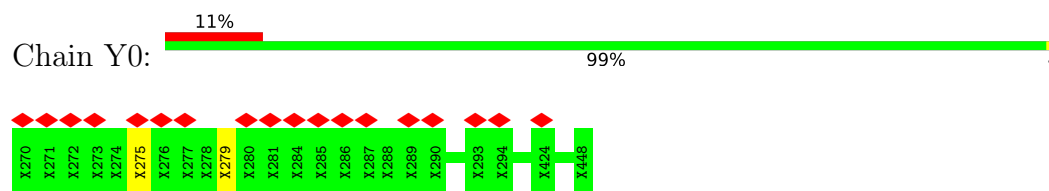


• Molecule 18: Outer dynein arm protein 1

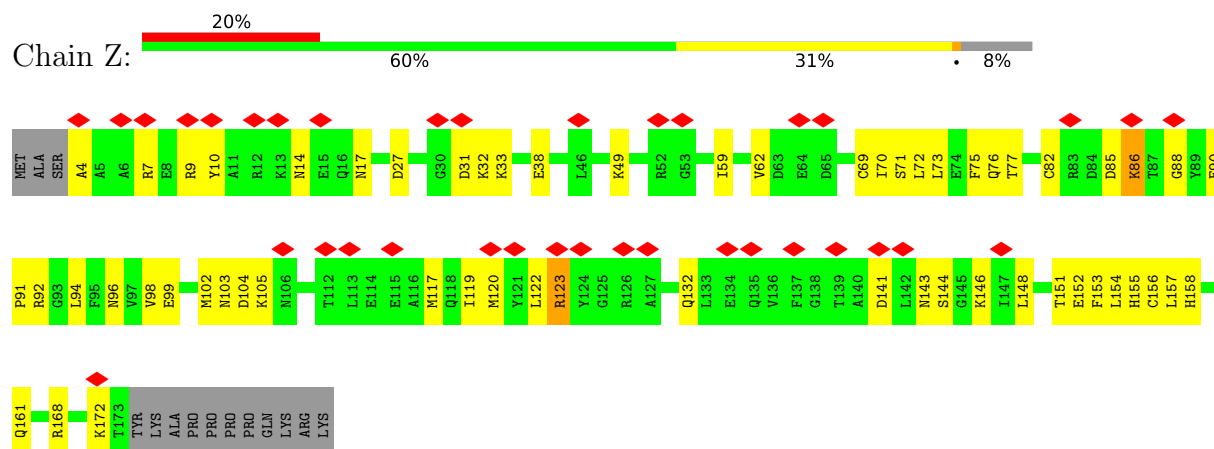




- Molecule 19: DC2



- Molecule 20: Outer dynein arm-docking complex protein DC3



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The composite map was assembled on a box 700 reference map (7.5 Å) using the ODA-DC and ODA core composite maps (deposited separately), and maps targeting the aHC AAA+ domain (4.5 Å), bHC AAA+ domain (6.2 Å), aHC AAA+ domain (11.4 Å), and aHC tail domain (5.3 Å). A second conformation of bHC AAA+ domain (9.8 Å) is also provided.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	952.0, 952.0, 952.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A1	0.28	0/3420	0.53	0/4628
1	A3	0.31	0/3420	0.54	0/4628
1	A5	0.30	0/3420	0.52	0/4628
1	A7	0.28	0/3420	0.51	0/4628
1	B1	0.29	0/3371	0.49	0/4561
1	B3	0.32	0/3295	0.49	0/4454
1	B5	0.31	0/3420	0.51	0/4628
1	B7	0.29	0/3420	0.50	0/4628
2	A2	0.31	0/3410	0.53	0/4623
2	A4	0.34	0/3389	0.58	0/4595
2	A6	0.31	0/3406	0.54	0/4618
2	B2	0.31	0/3271	0.52	0/4434
2	B4	0.32	0/3260	0.52	0/4418
2	B6	0.29	0/3389	0.50	0/4595
3	A	0.32	0/16168	0.55	0/22506
4	B	0.34	1/19223 (0.0%)	0.61	7/26574 (0.0%)
5	C	0.34	0/21839	0.57	7/30089 (0.0%)
6	D	0.70	2/3699 (0.1%)	0.88	6/5023 (0.1%)
7	E	0.71	1/3784 (0.0%)	0.90	7/5152 (0.1%)
8	F	0.24	0/494	0.52	0/687
9	G	0.34	0/1098	0.63	0/1471
10	H	0.26	0/450	0.46	0/626
11	I	0.56	0/840	0.85	3/1133 (0.3%)
12	J	0.55	0/752	0.78	0/1019
13	K	0.53	0/687	0.70	0/926
13	L	0.56	0/687	0.74	0/926
13	M	0.43	0/687	0.73	0/926
13	N	0.25	0/406	0.49	0/565
14	O	0.26	0/480	0.56	0/666
15	P	0.58	0/823	0.87	1/1108 (0.1%)
16	X	0.29	0/485	0.57	0/642
16	X1	0.32	0/1186	0.51	0/1582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Y	0.30	0/598	0.52	0/793
18	Y1	0.29	0/1192	0.52	0/1585
20	Z	0.34	0/1403	0.67	0/1885
All	All	0.36	4/124292 (0.0%)	0.59	31/169950 (0.0%)

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
3	A	0	21
4	B	0	15
5	C	0	7
All	All	0	43

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	314	SER	CA-CB	-5.69	1.44	1.52
4	B	3908	PRO	C-N	-5.56	1.21	1.34
7	E	336	GLU	CA-C	-5.46	1.38	1.52
6	D	378	VAL	CB-CG2	-5.19	1.42	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	376	LEU	CB-CG-CD1	8.76	125.90	111.00
4	B	4073	GLY	C-N-CA	8.14	142.06	121.70
4	B	4499	SER	C-N-CA	7.97	141.63	121.70
5	C	129	PRO	CA-N-CD	-7.73	100.68	111.50
7	E	370	ARG	C-N-CA	-7.37	103.28	121.70
5	C	455	MET	CB-CG-SD	-6.88	91.76	112.40
4	B	552	LEU	CA-CB-CG	6.71	130.75	115.30
7	E	379	LEU	CB-CG-CD1	-6.70	99.62	111.00
5	C	586	ARG	CA-CB-CG	6.59	127.89	113.40
6	D	184	ARG	N-CA-CB	6.39	122.10	110.60
6	D	543	LEU	CB-CG-CD2	-6.05	100.72	111.00
4	B	795	ASP	CB-CG-OD1	6.00	123.70	118.30
4	B	603	ARG	CB-CG-CD	5.93	127.03	111.60
6	D	537	LEU	CA-CB-CG	5.82	128.68	115.30
7	E	454	LEU	CB-CG-CD1	-5.71	101.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	439	LEU	CA-CB-CG	5.69	128.38	115.30
6	D	376	LEU	CB-CG-CD2	-5.67	101.37	111.00
7	E	379	LEU	CA-CB-CG	5.65	128.29	115.30
7	E	231	LEU	CB-CG-CD2	-5.63	101.42	111.00
7	E	293	ASP	CB-CG-OD2	-5.54	113.32	118.30
5	C	586	ARG	CB-CA-C	5.53	121.46	110.40
4	B	566	LEU	CB-CG-CD1	-5.48	101.68	111.00
15	P	58	ASP	CB-CG-OD1	5.40	123.16	118.30
5	C	418	LEU	CA-CB-CG	5.28	127.43	115.30
7	E	431	MET	CA-CB-CG	5.24	122.20	113.30
4	B	280	LEU	CA-CB-CG	-5.18	103.37	115.30
11	I	61	ARG	NE-CZ-NH2	5.17	122.88	120.30
11	I	63	LEU	CA-CB-CG	5.16	127.18	115.30
5	C	323	MET	CG-SD-CE	5.06	108.30	100.20
11	I	85	PRO	N-CA-C	5.06	125.26	112.10
5	C	131	MET	CA-CB-CG	5.06	121.90	113.30

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1300	PHE	Peptide
3	A	1482	PHE	Peptide
3	A	1508	SER	Peptide
3	A	1633	ILE	Peptide
3	A	1654	SER	Peptide
3	A	1660	GLN	Peptide
3	A	1676	ILE	Peptide
3	A	1677	CYS	Peptide
3	A	1792	CYS	Peptide
3	A	1815	VAL	Peptide
3	A	2044	GLY	Peptide
3	A	2804	LEU	Peptide
3	A	2879	PRO	Peptide
3	A	3589	SER	Peptide
3	A	3740	LEU	Peptide
3	A	4137	GLY	Peptide
3	A	4147	ALA	Peptide
3	A	4234	LYS	Peptide
3	A	4342	TRP	Peptide
3	A	4347	ILE	Peptide
3	A	4425	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	B	1611	ASN	Peptide
4	B	1875	CYS	Peptide
4	B	2473	TYR	Peptide
4	B	2498	ASP	Peptide
4	B	2744	LYS	Peptide
4	B	2850	ASP	Peptide
4	B	2959	ILE	Peptide
4	B	3036	HIS	Peptide
4	B	3513	ARG	Peptide
4	B	3580	LYS	Peptide
4	B	3750	LEU	Peptide
4	B	3903	ARG	Peptide
4	B	4143	LEU	Peptide
4	B	4245	ILE	Peptide
4	B	4511	ILE	Peptide
5	C	1414	LYS	Peptide
5	C	1524	LEU	Peptide
5	C	1686	SER	Peptide
5	C	1768	ASP	Peptide
5	C	2568	PRO	Peptide
5	C	2730	MET	Peptide
5	C	3819	TYR	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	A1	3346	0	3238	102	0
1	A3	3346	0	3238	110	0
1	A5	3346	0	3238	102	0
1	A7	3346	0	3238	88	0
1	B1	3298	0	3196	83	0
1	B3	3227	0	3134	80	0
1	B5	3346	0	3238	106	0
1	B7	3346	0	3238	91	0
2	A2	3339	0	3272	102	0
2	A4	3318	0	3259	94	0
2	A6	3335	0	3269	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B2	3204	0	3152	84	0
2	B4	3193	0	3141	107	0
2	B6	3318	0	3259	80	0
3	A	16173	0	7306	417	0
4	B	19163	0	10961	281	0
5	C	21756	0	13263	244	0
6	D	3609	0	3534	90	0
7	E	3697	0	3534	133	0
8	F	495	0	221	0	0
9	G	1089	0	1072	24	0
10	H	451	0	204	3	0
11	I	827	0	841	24	0
12	J	741	0	750	12	0
13	K	671	0	654	20	0
13	L	671	0	654	20	0
13	M	671	0	654	23	0
13	N	407	0	192	5	0
14	O	481	0	230	1	0
15	P	805	0	801	19	0
16	X	481	0	488	19	0
16	X1	1178	0	1179	27	0
17	X0	810	0	170	1	0
18	Y	595	0	586	22	0
18	Y1	1185	0	1230	35	0
19	Y0	840	0	181	1	0
20	Z	1384	0	1359	46	0
21	A1	32	0	12	0	0
21	A3	32	0	12	1	0
21	A5	32	0	12	1	0
21	A7	32	0	12	4	0
21	B2	32	0	12	1	0
21	B5	32	0	12	1	0
21	B7	32	0	12	0	0
22	A1	1	0	0	0	0
22	A2	1	0	0	0	0
22	A4	1	0	0	0	0
22	A6	1	0	0	0	0
22	B3	1	0	0	0	0
22	B4	1	0	0	0	0
22	B6	1	0	0	0	0
23	A1	28	0	12	0	0
23	A3	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A5	28	0	12	0	0
23	A7	28	0	12	2	0
23	B1	28	0	12	3	0
23	B3	28	0	12	2	0
23	B5	28	0	12	1	0
23	B7	28	0	12	1	0
All	All	124943	0	95354	2603	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 12.

All (2603) 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)
4:B:3879:ASP:HA	5:C:1534:GLU:CB	1.40	1.48
4:B:3879:ASP:CB	5:C:1530:PRO:O	1.86	1.23
4:B:3879:ASP:CA	5:C:1534:GLU:CB	2.17	1.23
3:A:1676:ILE:O	3:A:1679:ALA:HB3	1.56	1.05
3:A:2399:SER:HA	3:A:2438:PHE:O	1.57	1.03
10:H:79:ILE:O	10:H:105:VAL:HA	1.63	0.99
3:A:3420:ILE:HA	3:A:3443:TYR:HA	1.45	0.98
3:A:1764:ALA:HB1	3:A:1835:LEU:HA	1.47	0.95
3:A:1344:ILE:O	3:A:1348:GLN:N	1.98	0.95
3:A:4031:ALA:HB1	3:A:4034:ALA:HB3	1.48	0.94
5:C:4360:HIS:HA	5:C:4387:GLU:HA	1.47	0.94
3:A:3880:ILE:O	3:A:3970:PHE:HA	1.68	0.92
4:B:382:MET:O	4:B:386:VAL:HG23	1.69	0.92
1:A3:215:LEU:HB3	1:A3:217:LEU:HD13	1.54	0.90
3:A:2604:SER:O	3:A:2608:TYR:CB	2.20	0.90
3:A:3396:ARG:O	3:A:3400:ALA:N	2.06	0.89
1:B5:175:VAL:HG22	2:B6:329:ASN:HD21	1.35	0.89
3:A:4125:LEU:O	3:A:4129:ILE:N	2.06	0.89
3:A:3724:PHE:O	3:A:3728:LYS:N	2.06	0.88
3:A:4031:ALA:O	3:A:4035:ILE:N	2.07	0.88
4:B:503:GLU:HG2	6:D:510:SER:HB2	1.56	0.88
1:B3:330:MET:HE2	1:B3:349:VAL:HG11	1.57	0.86
3:A:1655:PHE:O	3:A:1659:SER:N	2.09	0.86
1:A3:121:ARG:HD2	18:Y1:141:LYS:HZ2	1.41	0.85
1:B7:113:ILE:HD13	1:B7:150:LEU:HD11	1.55	0.85
4:B:627:LEU:HG	4:B:631:MET:HE2	1.57	0.85
3:A:3616:PRO:HA	3:A:3623:LYS:HA	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2372:PHE:N	3:A:2486:ALA:O	2.10	0.85
4:B:2885:LYS:O	4:B:2889:ALA:HB2	1.76	0.84
1:A1:215:LEU:HB3	1:A1:217:LEU:HD13	1.59	0.84
3:A:4185:MET:HA	3:A:4491:ALA:HA	1.60	0.84
3:A:1788:VAL:O	3:A:1792:CYS:N	2.10	0.84
1:B7:113:ILE:HD11	1:B7:147:MET:HG3	1.58	0.83
20:Z:59:ILE:HG13	20:Z:70:ILE:HD11	1.60	0.83
3:A:2316:TYR:HA	3:A:2327:PRO:HA	1.60	0.83
1:B5:256:ASN:HD22	1:B5:350:LYS:HD2	1.44	0.82
1:B5:173:PRO:HB3	1:B5:384:GLN:HE22	1.40	0.82
3:A:2514:GLY:O	3:A:2518:LEU:N	2.10	0.82
3:A:2540:MET:O	3:A:2544:ILE:N	2.11	0.82
2:A2:417:GLU:HA	2:A2:420:GLU:HG2	1.62	0.82
3:A:2029:GLY:O	3:A:2033:CYS:N	2.13	0.82
3:A:2401:SER:HA	3:A:2440:ASP:H	1.45	0.82
3:A:1347:TRP:O	3:A:1351:LEU:N	2.12	0.81
3:A:2350:THR:O	3:A:2354:SER:N	2.13	0.81
3:A:2439:VAL:H	3:A:2486:ALA:HA	1.45	0.81
20:Z:32:LYS:NZ	20:Z:71:SER:OG	2.13	0.81
2:A2:402:ARG:HH11	20:Z:168:ARG:HH22	1.29	0.80
1:A3:218:THR:O	2:A4:326:LYS:NZ	2.14	0.80
1:B3:175:VAL:HG12	2:B4:329:ASN:HD21	1.45	0.80
13:M:61:GLY:O	13:M:84:ALA:HB3	1.80	0.80
1:A1:73:MET:HE1	1:A1:92:PHE:HB2	1.64	0.80
1:A5:156:ARG:NH1	1:A5:195:ASN:O	2.14	0.80
3:A:3976:ILE:H	3:A:3982:ALA:HB1	1.47	0.79
3:A:2910:PHE:O	3:A:2914:SER:N	2.15	0.79
3:A:1290:ASN:O	3:A:1294:THR:N	2.13	0.78
1:A5:309:ARG:H	1:A5:372:THR:HG22	1.44	0.78
3:A:2441:ASP:HA	3:A:2488:MET:HA	1.63	0.78
2:B4:155:GLU:HG2	2:B4:197:HIS:CE1	2.19	0.78
1:B1:218:THR:O	2:B2:326:LYS:NZ	2.16	0.78
3:A:3987:GLU:O	3:A:3991:GLN:N	2.13	0.78
6:D:318:ASN:HD21	6:D:321:TYR:HB2	1.49	0.78
3:A:4151:GLU:HA	3:A:4157:PHE:HA	1.64	0.78
3:A:2437:TYR:H	3:A:2484:TYR:HA	1.48	0.78
6:D:200:CYS:SG	15:P:89:TYR:OH	2.41	0.78
1:B7:100:ASN:HD22	1:B7:103:LYS:HG3	1.47	0.77
3:A:2719:LEU:O	3:A:2851:ALA:N	2.18	0.77
2:B4:88:HIS:CD2	2:B4:90:GLU:HG3	2.19	0.77
3:A:3390:MET:O	3:A:3394:MET:N	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:75:VAL:HG11	2:A2:94:SER:HB2	1.67	0.77
3:A:3721:ARG:O	3:A:3997:SER:N	2.14	0.77
3:A:2231:HIS:HA	3:A:2282:LEU:HA	1.66	0.77
2:A4:11:GLN:OE1	2:A4:15:GLN:NE2	2.18	0.77
2:A6:82:THR:HG23	2:A6:83:TYR:HD1	1.48	0.77
1:A3:397:TRP:HH2	2:A4:260:VAL:HG23	1.51	0.76
6:D:520:HIS:H	6:D:542:ARG:HD2	1.49	0.76
1:A1:377:MET:SD	1:A1:380:ARG:NH2	2.58	0.76
1:B5:2:ARG:HE	1:B5:240:LEU:HD22	1.50	0.76
3:A:2218:ILE:O	3:A:2222:LEU:CB	2.33	0.76
2:A6:71:GLU:OE1	1:A7:247:ASN:ND2	2.19	0.76
3:A:2707:SER:O	3:A:2711:SER:N	2.17	0.76
1:B3:5:VAL:HG23	1:B3:62:ARG:HG2	1.65	0.76
3:A:3793:HIS:O	3:A:3797:ASP:N	2.18	0.76
3:A:3915:MET:N	3:A:3940:ASP:O	2.19	0.76
2:B2:91:GLN:HG3	2:B2:121:ARG:HH21	1.51	0.76
3:A:1298:PHE:N	3:A:1410:LYS:O	2.19	0.76
5:C:1877:ASN:O	5:C:1881:LEU:N	2.17	0.75
3:A:2466:GLY:O	3:A:2479:ILE:N	2.18	0.75
3:A:3358:SER:HA	3:A:3469:THR:O	1.86	0.75
3:A:1805:GLY:HA2	3:A:1827:ALA:HA	1.67	0.75
1:A1:268:VAL:HG23	1:A1:300:MET:HB2	1.69	0.75
2:B4:11:GLN:OE1	2:B4:15:GLN:NE2	2.20	0.75
3:A:1359:GLN:O	3:A:1363:GLU:N	2.17	0.75
4:B:743:GLN:HE22	7:E:263:ARG:HD2	1.51	0.75
1:B7:275:SER:HG	1:B7:278:SER:HG	1.35	0.74
2:B4:88:HIS:HD2	2:B4:90:GLU:HG3	1.53	0.74
1:A7:139:LEU:HD12	1:A7:170:VAL:HG12	1.70	0.74
18:Y:182:ALA:O	18:Y:186:ARG:HD3	1.86	0.74
1:A3:139:LEU:HD12	1:A3:170:VAL:HG12	1.70	0.74
2:B4:178:SER:HB3	1:B5:347:ASN:HD21	1.52	0.74
3:A:1327:GLN:O	3:A:1331:MET:N	2.21	0.74
3:A:2794:ASP:O	3:A:2799:GLY:N	2.21	0.74
3:A:1420:GLY:O	3:A:1424:ASN:N	2.19	0.73
3:A:1745:PHE:O	3:A:1772:PHE:HA	1.88	0.73
3:A:1968:ASN:HA	3:A:1972:PRO:HA	1.69	0.73
2:A6:69:ASP:OD1	2:A6:70:LEU:N	2.22	0.73
2:B6:259:LEU:HD11	2:B6:316:CYS:HB2	1.71	0.73
3:A:3926:VAL:O	3:A:3930:TYR:N	2.18	0.73
1:B5:107:THR:OG1	1:B5:108:GLU:OE1	2.06	0.73
4:B:4529:CYS:O	4:B:4545:ALA:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:819:ILE:HG21	7:E:205:ASN:HB3	1.71	0.73
1:B3:99:ASN:ND2	2:B4:254:GLU:OE1	2.22	0.73
4:B:2751:VAL:HA	4:B:2795:GLY:HA2	1.71	0.73
2:B4:116:ASP:OD1	2:B4:156:ARG:NH1	2.22	0.72
7:E:168:ASN:ND2	7:E:222:ALA:O	2.21	0.72
1:A3:131:GLN:HE21	1:A3:250:LEU:HB2	1.54	0.72
1:B3:2:ARG:HE	1:B3:240:LEU:HD22	1.55	0.72
2:B4:278:ALA:HA	2:B4:369:ALA:HB2	1.71	0.72
3:A:2592:SER:O	3:A:2596:TRP:N	2.17	0.72
2:A2:98:ASP:O	2:A2:105:ARG:NH2	2.21	0.72
3:A:3752:GLU:O	3:A:3756:ARG:N	2.20	0.72
2:A4:102:ASN:ND2	2:A4:411:GLU:OE1	2.23	0.72
3:A:3959:ALA:O	3:A:3963:ALA:HB2	1.90	0.72
3:A:3740:LEU:O	3:A:3746:VAL:N	2.21	0.72
3:A:4135:PRO:HA	3:A:4148:PRO:HA	1.71	0.72
6:D:319:PRO:HG2	6:D:370:PRO:HA	1.72	0.72
2:B4:75:VAL:HG11	2:B4:94:SER:HB2	1.72	0.71
3:A:1717:THR:O	3:A:1842:PHE:HA	1.90	0.71
3:A:2696:PHE:H	3:A:2699:ALA:HB3	1.54	0.71
7:E:286:ASP:OD2	7:E:288:ASN:ND2	2.23	0.71
1:B1:99:ASN:ND2	2:B2:254:GLU:OE1	2.23	0.71
3:A:2542:THR:O	3:A:2545:LEU:CB	2.39	0.71
5:C:813:GLN:O	5:C:816:LEU:HB2	1.89	0.71
7:E:158:ASN:ND2	7:E:199:TYR:OH	2.23	0.71
3:A:4484:MET:O	3:A:4488:TRP:N	2.19	0.71
16:X1:216:MET:HE1	18:Y1:167:ARG:HA	1.73	0.71
3:A:2178:GLN:O	3:A:2182:MET:N	2.22	0.71
3:A:3956:LEU:HA	3:A:3959:ALA:HB3	1.71	0.71
5:C:2137:GLN:O	5:C:2153:ILE:N	2.20	0.71
5:C:2411:LEU:O	5:C:2415:TYR:N	2.20	0.71
7:E:266:ILE:HG22	7:E:268:ASP:H	1.55	0.71
1:B1:30:ILE:HD11	1:B1:47:ILE:HD11	1.72	0.70
3:A:1341:LYS:O	3:A:1345:LEU:N	2.24	0.70
5:C:569:ARG:NH1	6:D:614:THR:OG1	2.24	0.70
1:A3:36:TYR:HB2	1:A3:59:TYR:HE2	1.56	0.70
3:A:4451:ASN:O	3:A:4455:TYR:N	2.23	0.70
1:A1:175:VAL:HG13	2:A2:329:ASN:HD21	1.56	0.70
5:C:2153:ILE:HA	5:C:2528:GLY:HA3	1.73	0.70
2:B6:192:HIS:HD2	2:B6:421:ALA:HA	1.57	0.70
20:Z:152:GLU:O	20:Z:155:HIS:ND1	2.25	0.70
1:A5:375:GLN:HB2	1:A5:419:VAL:HG23	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:82:THR:HG23	2:A6:83:TYR:CD1	2.25	0.70
1:B3:52:ASN:OD1	1:B3:62:ARG:NH2	2.24	0.70
5:C:3812:ASP:O	5:C:3816:ARG:N	2.25	0.70
2:A6:11:GLN:OE1	2:A6:15:GLN:NE2	2.24	0.70
3:A:1735:SER:O	3:A:1739:GLY:N	2.25	0.70
6:D:282:TRP:O	6:D:638:LYS:NZ	2.23	0.70
3:A:2334:ASP:N	3:A:2349:PRO:O	2.25	0.69
7:E:162:ARG:HD3	7:E:196:LEU:HD22	1.74	0.69
2:B2:288:VAL:HG13	2:B2:319:TYR:HE2	1.57	0.69
4:B:1918:ALA:N	4:B:2042:VAL:O	2.25	0.69
1:A7:396:HIS:HA	1:A7:399:THR:HG22	1.74	0.69
3:A:2552:HIS:O	3:A:2556:SER:N	2.17	0.69
3:A:2689:ALA:HB3	3:A:3425:THR:H	1.58	0.69
3:A:3370:TRP:O	3:A:3374:ARG:CB	2.41	0.69
4:B:1961:LEU:HA	4:B:1966:ALA:HB3	1.74	0.69
2:A4:317:LEU:HB3	2:A4:319:TYR:HE1	1.57	0.69
2:B6:405:VAL:HG13	2:B6:418:PHE:HE2	1.55	0.69
1:B3:293:MET:HG3	1:B3:367:PHE:HB2	1.74	0.69
5:C:666:GLN:HG2	5:C:667:LEU:HD23	1.74	0.69
1:B7:113:ILE:CD1	1:B7:150:LEU:HD11	2.23	0.69
3:A:3287:ALA:HB1	3:A:3295:ARG:HA	1.75	0.69
3:A:3781:ALA:HB1	3:A:3837:ALA:HB1	1.74	0.69
15:P:62:LYS:HG3	15:P:63:LYS:HD3	1.75	0.69
2:A4:51:THR:HG21	2:A4:243:ARG:HG2	1.75	0.69
1:B5:52:ASN:OD1	1:B5:62:ARG:NH2	2.26	0.69
3:A:1792:CYS:HA	3:A:1824:SER:O	1.93	0.69
3:A:3868:ALA:O	3:A:3873:GLU:N	2.24	0.69
6:D:436:ALA:HB3	6:D:454:LYS:HA	1.75	0.68
7:E:304:MET:SD	7:E:353:ARG:NH2	2.65	0.68
16:X:266:ARG:HH11	18:Y:219:GLU:HG2	1.57	0.68
20:Z:103:ASN:ND2	20:Z:117:MET:SD	2.66	0.68
2:B4:259:LEU:HD11	2:B4:316:CYS:HB2	1.75	0.68
7:E:101:GLU:OE1	11:I:34:ARG:NH2	2.24	0.68
2:A6:172:TYR:CE2	2:A6:203:MET:HG3	2.28	0.68
2:A4:195:LEU:HD21	2:A4:264:ARG:HE	1.58	0.68
6:D:503:ARG:NH1	6:D:514:SER:OG	2.26	0.68
7:E:414:TRP:CD1	7:E:420:GLY:HA2	2.28	0.68
1:B1:2:ARG:HE	1:B1:240:LEU:HD22	1.59	0.68
5:C:4356:VAL:O	5:C:4360:HIS:N	2.26	0.68
1:B1:68:LEU:HB3	1:B1:96:GLY:HA2	1.75	0.68
3:A:2439:VAL:O	3:A:2487:CYS:N	2.15	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3879:ASP:CB	5:C:1530:PRO:C	2.62	0.68
4:B:4106:GLU:O	4:B:4110:GLU:N	2.27	0.68
3:A:3401:GLY:HA2	3:A:3446:ASN:O	1.93	0.68
1:B1:139:LEU:HD12	1:B1:170:VAL:HG12	1.75	0.68
15:P:74:LYS:HE3	15:P:95:ARG:HD3	1.75	0.68
1:A5:159:TYR:HB3	1:A5:162:ARG:HD3	1.74	0.67
1:A5:172:SER:HB2	1:A5:380:ARG:HH12	1.59	0.67
6:D:286:SER:O	6:D:290:ARG:NH1	2.28	0.67
2:B2:51:THR:HG21	2:B2:243:ARG:HG2	1.76	0.67
2:B4:170:THR:HG21	2:B4:194:LEU:HD11	1.75	0.67
4:B:596:ARG:NE	7:E:404:TYR:OH	2.24	0.67
5:C:3507:PRO:O	5:C:3511:ARG:N	2.27	0.67
2:A4:403:ALA:HB2	1:A5:344:TRP:HZ3	1.59	0.67
3:A:1804:PRO:HA	3:A:1834:PRO:HA	1.76	0.67
3:A:4418:TRP:HA	3:A:4422:ASP:O	1.95	0.67
4:B:3879:ASP:N	5:C:1534:GLU:CB	2.56	0.67
1:A1:11:GLN:HG2	1:A1:72:THR:HG21	1.77	0.67
3:A:1967:LEU:O	3:A:1971:PHE:N	2.27	0.67
4:B:4483:THR:HA	4:B:4507:PRO:HA	1.76	0.67
1:B5:248:ALA:HA	1:B5:252:LYS:HD2	1.76	0.67
5:C:1595:ASP:O	5:C:1599:LYS:N	2.16	0.67
7:E:332:MET:HG3	7:E:342:SER:HB2	1.76	0.67
16:X1:216:MET:O	16:X1:220:VAL:HG23	1.94	0.67
1:A1:113:ILE:HG21	1:A1:150:LEU:HD22	1.77	0.67
5:C:3845:VAL:O	5:C:3849:ARG:N	2.27	0.67
6:D:598:LYS:O	6:D:598:LYS:NZ	2.28	0.67
7:E:375:SER:OG	7:E:376:LYS:N	2.27	0.67
1:A7:9:GLY:HA2	1:A7:66:MET:HG3	1.76	0.67
3:A:1664:TYR:O	3:A:1672:CYS:HA	1.94	0.67
5:C:1763:TRP:HA	5:C:1770:VAL:HA	1.77	0.67
1:A1:107:THR:OG1	1:A1:401:GLU:OE2	2.13	0.67
13:K:15:MET:HE1	13:K:19:MET:HG3	1.76	0.67
1:B7:330:MET:HB3	1:B7:349:VAL:HG21	1.76	0.67
3:A:3394:MET:O	3:A:3398:ILE:N	2.23	0.67
4:B:2806:TYR:HA	4:B:2824:ALA:HB2	1.77	0.67
2:A4:274:PRO:HG3	2:A4:286:LEU:HD11	1.77	0.67
1:B1:304:ASP:HB3	1:B1:307:HIS:CD2	2.30	0.67
1:B5:175:VAL:HG22	2:B6:329:ASN:ND2	2.07	0.67
20:Z:154:LEU:HB3	20:Z:158:HIS:HE1	1.60	0.67
1:A1:27:GLU:HA	1:A1:359:LYS:HD2	1.76	0.66
2:A2:50:ASN:O	2:A2:64:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:619:GLU:HA	4:B:622:ARG:HG2	1.77	0.66
3:A:2501:LEU:O	3:A:2504:LEU:N	2.20	0.66
4:B:1669:SER:HA	4:B:1722:ASP:HA	1.78	0.66
2:B4:178:SER:HB3	1:B5:347:ASN:ND2	2.09	0.66
1:B5:139:LEU:HD12	1:B5:170:VAL:HG12	1.76	0.66
7:E:454:LEU:HD13	7:E:468:VAL:HG11	1.77	0.66
2:A2:262:TYR:HB2	2:A2:265:ILE:HD12	1.76	0.66
3:A:2379:GLY:O	3:A:2383:LEU:N	2.25	0.66
2:A2:72:PRO:HG3	1:A3:1:MET:HG2	1.76	0.66
1:A3:65:LEU:HD12	1:A3:90:PHE:CE1	2.30	0.66
1:A7:45:GLU:HG3	1:A7:46:ARG:HG2	1.78	0.66
1:B1:49:VAL:HG11	1:B1:241:ARG:HG2	1.77	0.66
1:B5:114:ASP:OD1	1:B5:115:SER:N	2.28	0.66
1:B5:135:VAL:HG21	1:B5:152:ILE:HD11	1.76	0.66
2:B6:102:ASN:ND2	2:B6:105:ARG:HG3	2.11	0.66
3:A:1965:GLY:O	3:A:1969:ASP:N	2.28	0.66
3:A:3611:GLY:HA3	3:A:3711:CYS:HA	1.78	0.66
18:Y1:122:LYS:HA	18:Y1:122:LYS:HE3	1.78	0.66
1:B1:165:LEU:HD21	1:B1:250:LEU:HD11	1.78	0.66
2:B6:75:VAL:HG11	2:B6:94:SER:HB2	1.78	0.66
4:B:590:VAL:HG11	4:B:635:ARG:HB3	1.76	0.66
2:A2:27:GLU:OE1	2:A2:243:ARG:NH1	2.27	0.66
2:A6:287:SER:N	2:A6:290:GLU:OE2	2.27	0.66
1:B5:100:ASN:HD22	1:B5:103:LYS:HG3	1.61	0.66
4:B:349:GLN:NE2	4:B:353:ASN:OD1	2.29	0.66
4:B:1498:SER:N	4:B:1507:ALA:O	2.29	0.66
5:C:784:ILE:HG12	5:C:820:ARG:HD3	1.77	0.66
1:B5:220:PRO:HD2	2:B6:326:LYS:HD3	1.77	0.66
3:A:1792:CYS:O	3:A:1794:THR:N	2.29	0.66
4:B:4263:ALA:O	4:B:4267:PHE:CB	2.44	0.66
11:I:84:ALA:O	11:I:94:TYR:HA	1.96	0.66
1:A1:311:LEU:HD11	1:A1:372:THR:HB	1.78	0.66
3:A:2547:ALA:O	3:A:2551:LEU:N	2.23	0.66
2:A2:415:GLU:OE2	20:Z:168:ARG:NH1	2.29	0.65
2:A6:176:GLN:NE2	2:A6:207:GLU:OE1	2.28	0.65
1:B3:391:ARG:HH21	2:B4:346:TRP:HE1	1.44	0.65
2:B4:5:ILE:HG22	2:B4:64:ARG:HB3	1.78	0.65
3:A:1995:LEU:HA	3:A:2198:ALA:HB3	1.78	0.65
5:C:696:LYS:O	5:C:700:ASN:ND2	2.28	0.65
6:D:418:GLN:HB2	6:D:427:GLN:HB2	1.78	0.65
7:E:321:GLU:HG2	7:E:370:ARG:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:68:VAL:HG23	13:M:57:HIS:HB3	1.78	0.65
18:Y:205:ALA:O	18:Y:209:MET:HG2	1.96	0.65
5:C:2325:THR:O	5:C:2329:GLY:N	2.29	0.65
9:G:15:LEU:N	9:G:19:GLU:OE2	2.29	0.65
1:A1:36:TYR:HB2	1:A1:59:TYR:HE2	1.60	0.65
6:D:349:ASN:ND2	6:D:352:HIS:O	2.29	0.65
7:E:454:LEU:HB3	7:E:468:VAL:HG11	1.78	0.65
1:A1:77:ARG:NH1	1:A1:87:PRO:HG3	2.11	0.65
2:B6:222:PRO:O	1:B7:322:SER:OG	2.14	0.65
4:B:392:ASN:HA	4:B:395:PHE:HD2	1.60	0.65
2:A2:71:GLU:HG3	1:A3:2:ARG:HH12	1.62	0.65
2:A4:76:ASP:OD1	2:A4:79:ARG:NH2	2.29	0.65
3:A:1489:ARG:O	3:A:1504:LEU:N	2.30	0.65
3:A:1966:LEU:O	3:A:1970:LEU:N	2.29	0.65
3:A:2719:LEU:HA	3:A:2875:ASP:O	1.97	0.65
6:D:195:THR:HG22	15:P:81:THR:HG22	1.78	0.65
18:Y:179:ARG:O	18:Y:183:LYS:HG3	1.97	0.65
1:B3:213:ARG:HH12	1:B3:297:LYS:HD2	1.61	0.65
2:B6:271:SER:OG	2:B6:301:MET:SD	2.55	0.65
7:E:399:ILE:HG12	7:E:400:LEU:HD12	1.79	0.65
1:A3:49:VAL:HG11	1:A3:241:ARG:HG2	1.79	0.65
4:B:2561:SER:HA	4:B:2602:PRO:HA	1.79	0.65
5:C:1902:GLN:HA	5:C:1906:GLY:HA2	1.79	0.65
1:B7:135:VAL:HG21	1:B7:152:ILE:HD11	1.77	0.65
3:A:2070:SER:HA	3:A:2458:LEU:HA	1.79	0.65
4:B:4020:ALA:O	4:B:4024:GLY:N	2.30	0.65
13:K:60:VAL:HG22	13:K:85:ILE:HG12	1.79	0.65
3:A:1920:ILE:O	3:A:1924:LEU:N	2.26	0.64
3:A:3481:GLU:O	3:A:3577:ALA:HB1	1.97	0.64
4:B:3865:SER:O	4:B:3869:TRP:N	2.30	0.64
11:I:72:LEU:HB3	11:I:83:ILE:HB	1.78	0.64
1:A1:67:ASP:OD2	1:A1:72:THR:OG1	2.15	0.64
5:C:586:ARG:HH21	6:D:520:HIS:CG	2.15	0.64
1:B5:91:VAL:HG11	1:B5:116:VAL:HG12	1.79	0.64
3:A:1289:LEU:O	3:A:1293:TRP:CB	2.45	0.64
9:G:99:THR:O	9:G:103:PHE:CB	2.45	0.64
1:B1:282:ARG:NH2	1:B1:292:GLN:OE1	2.31	0.64
3:A:1878:GLU:HA	3:A:1889:ALA:HB1	1.79	0.64
16:X:244:MET:HG3	18:Y:199:PHE:HE1	1.62	0.64
1:A3:268:VAL:HG23	1:A3:300:MET:HB3	1.79	0.64
4:B:1499:THR:HA	4:B:1506:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2726:GLY:O	3:A:2730:LEU:N	2.25	0.64
4:B:1701:ILE:HA	4:B:1720:SER:HA	1.80	0.64
7:E:452:LEU:HB3	7:E:471:SER:HB3	1.80	0.64
2:B2:259:LEU:HD11	2:B2:316:CYS:HB2	1.79	0.64
2:B4:180:ALA:O	1:B5:347:ASN:ND2	2.30	0.64
3:A:2900:GLU:O	3:A:2904:ARG:N	2.30	0.64
9:G:99:THR:O	9:G:103:PHE:HB2	1.97	0.64
1:B7:211:CYS:HA	1:B7:215:LEU:HB2	1.78	0.64
1:A1:215:LEU:HD11	1:A1:228:LEU:HD21	1.79	0.63
2:A6:56:THR:HA	2:B6:285:GLN:HB2	1.79	0.63
2:A6:120:ASP:OD1	2:A6:121:ARG:N	2.31	0.63
1:A7:200:MET:HE1	1:A7:368:ILE:HD12	1.80	0.63
1:B7:183:TYR:HB3	1:B7:398:TYR:HE2	1.63	0.63
3:A:1343:GLU:O	3:A:1347:TRP:N	2.29	0.63
9:G:44:ARG:NH1	9:G:54:PRO:O	2.30	0.63
18:Y:181:LEU:O	18:Y:185:LYS:HG2	1.98	0.63
3:A:4150:LEU:O	3:A:4158:ALA:N	2.30	0.63
6:D:203:TRP:HB2	12:J:59:ARG:HE	1.63	0.63
11:I:76:SER:HB3	11:I:79:HIS:H	1.63	0.63
13:K:45:LYS:HG3	13:K:56:TRP:HB2	1.81	0.63
1:A5:373:ALA:O	1:A5:376:GLU:HG3	1.98	0.63
3:A:2714:SER:H	3:A:2843:THR:HA	1.63	0.63
1:A1:235:GLY:HA3	1:A1:366:THR:HG21	1.79	0.63
2:A2:14:ILE:HD11	2:A2:74:VAL:HG13	1.79	0.63
2:A4:7:ILE:HG13	2:A4:66:ILE:HG13	1.80	0.63
2:B2:174:SER:OG	2:B2:177:VAL:O	2.16	0.63
2:B4:279:GLU:OE1	2:B4:279:GLU:N	2.31	0.63
4:B:2106:MET:O	4:B:2110:ALA:N	2.31	0.63
1:B3:211:CYS:HA	1:B3:215:LEU:HB2	1.78	0.63
3:A:4016:THR:O	3:A:4020:CYS:N	2.31	0.63
4:B:418:PHE:O	4:B:422:ASP:HB2	1.98	0.63
4:B:4351:LYS:O	4:B:4355:LEU:N	2.29	0.63
5:C:2196:THR:HA	5:C:2200:GLY:HA2	1.81	0.63
9:G:136:ARG:HA	9:G:139:LYS:HE2	1.81	0.63
2:A6:172:TYR:HE2	2:A6:203:MET:HG3	1.62	0.63
1:B3:139:LEU:HD12	1:B3:170:VAL:HG22	1.81	0.63
3:A:2369:PRO:HA	3:A:2484:TYR:O	1.98	0.63
3:A:3617:GLY:HA2	3:A:3695:MET:HA	1.80	0.63
5:C:573:PRO:O	5:C:577:ASN:ND2	2.31	0.63
13:N:10:ILE:HA	13:N:78:PHE:HA	1.80	0.63
1:A1:165:LEU:HD11	1:A1:250:LEU:HD23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:816:LEU:HD23	7:E:205:ASN:HD21	1.62	0.63
1:B7:167:PHE:CE2	1:B7:233:MET:HG2	2.33	0.63
3:A:4261:LEU:O	3:A:4265:THR:N	2.22	0.63
3:A:2806:PRO:O	3:A:2810:ARG:N	2.24	0.63
20:Z:14:ASN:O	20:Z:17:ASN:ND2	2.32	0.63
2:A2:210:TYR:HH	2:A2:224:TYR:HE1	1.47	0.62
1:B5:99:ASN:ND2	2:B6:254:GLU:OE1	2.32	0.62
5:C:1514:ASN:O	5:C:1518:THR:N	2.32	0.62
6:D:583:VAL:HG22	6:D:589:VAL:HG22	1.79	0.62
1:A5:375:GLN:NE2	1:A5:423:GLN:OE1	2.30	0.62
3:A:3611:GLY:HA2	3:A:3615:ALA:HB2	1.79	0.62
1:A1:374:ILE:HD11	1:A1:422:TYR:CZ	2.34	0.62
1:A5:173:PRO:HD2	1:A5:380:ARG:NH1	2.14	0.62
3:A:1392:PHE:O	3:A:1395:ILE:N	2.32	0.62
3:A:3615:ALA:HB3	3:A:3618:GLY:H	1.63	0.62
1:A7:345:ILE:O	1:A7:348:ASN:ND2	2.30	0.62
1:B5:253:LEU:HD11	1:B5:316:LEU:HD21	1.81	0.62
3:A:3391:LEU:O	3:A:3395:GLU:N	2.31	0.62
4:B:1611:ASN:H	4:B:1615:ALA:HB2	1.63	0.62
5:C:1029:GLY:O	9:G:65:GLN:NE2	2.32	0.62
4:B:2755:ARG:HA	4:B:2798:ALA:HB2	1.81	0.62
5:C:417:PHE:O	5:C:421:ASP:HB2	1.99	0.62
5:C:2338:PRO:O	5:C:2342:GLN:N	2.28	0.62
13:K:78:PHE:HB2	13:K:85:ILE:HB	1.81	0.62
20:Z:75:PHE:HE1	20:Z:98:VAL:HG11	1.64	0.62
2:A2:188:VAL:HG13	2:A2:425:LEU:HD12	1.80	0.62
1:A7:204:ASN:ND2	23:A7:502:GDP:O2'	2.33	0.62
1:B1:156:ARG:HD2	1:B1:195:ASN:O	1.99	0.62
3:A:1672:CYS:O	3:A:1683:TYR:N	2.32	0.62
3:A:2437:TYR:N	3:A:2484:TYR:HA	2.14	0.62
2:A2:383:ALA:O	2:A2:386:GLU:HG2	2.00	0.62
1:A5:379:LYS:HG2	1:A5:419:VAL:HG21	1.82	0.62
4:B:4021:HIS:O	4:B:4055:HIS:N	2.26	0.62
6:D:408:LEU:O	6:D:409:ASN:ND2	2.32	0.62
1:B7:139:LEU:HD12	1:B7:170:VAL:HG12	1.82	0.62
1:B1:175:VAL:HG13	2:B2:329:ASN:ND2	2.15	0.62
4:B:743:GLN:OE1	7:E:263:ARG:NH2	2.33	0.62
5:C:469:LYS:NZ	5:C:484:ASP:OD2	2.33	0.62
20:Z:132:GLN:O	20:Z:151:THR:OG1	2.17	0.62
1:A1:73:MET:O	1:A1:76:VAL:HG22	2.00	0.61
1:A5:49:VAL:HG11	1:A5:241:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:319:TYR:HB3	2:B2:323:VAL:HG11	1.81	0.61
4:B:2199:PHE:N	4:B:2334:GLY:O	2.30	0.61
5:C:226:ASP:H	5:C:230:ARG:HH12	1.48	0.61
2:A6:20:CYS:HB3	2:A6:24:TYR:HE1	1.65	0.61
3:A:1381:VAL:O	3:A:1385:LEU:N	2.32	0.61
3:A:3417:LEU:O	3:A:3421:ILE:N	2.33	0.61
3:A:3720:ARG:HA	3:A:3723:LEU:CB	2.30	0.61
4:B:506:ARG:HH22	4:B:540:VAL:HG12	1.64	0.61
20:Z:85:ASP:OD2	20:Z:90:GLU:HB2	2.00	0.61
1:B3:175:VAL:HG12	2:B4:329:ASN:ND2	2.13	0.61
3:A:3868:ALA:HA	3:A:3872:ASP:CB	2.31	0.61
4:B:1498:SER:O	4:B:1507:ALA:N	2.33	0.61
13:L:67:TYR:HD2	13:M:45:LYS:HD3	1.65	0.61
1:A3:64:ILE:HD11	1:A3:123:GLU:HG3	1.82	0.61
2:A6:145:THR:OG1	21:A7:501:GTP:O1B	2.19	0.61
3:A:1558:ARG:O	3:A:1562:LEU:CB	2.48	0.61
4:B:147:GLU:OE2	5:C:154:LYS:NZ	2.34	0.61
5:C:476:TYR:O	5:C:479:ASN:ND2	2.33	0.61
5:C:2160:ARG:O	5:C:2164:ASN:N	2.33	0.61
6:D:283:ASP:OD1	6:D:644:ARG:NH1	2.31	0.61
3:A:3788:LEU:O	3:A:3792:ALA:N	2.33	0.61
5:C:2414:SER:O	5:C:2418:ASP:N	2.33	0.61
5:C:3049:ALA:O	5:C:3053:MET:CB	2.49	0.61
3:A:2605:GLU:O	3:A:2609:ALA:N	2.32	0.61
5:C:789:LEU:H	5:C:875:LEU:HD21	1.65	0.61
6:D:451:CYS:SG	6:D:454:LYS:NZ	2.73	0.61
1:B1:131:GLN:HE21	1:B1:250:LEU:HB3	1.66	0.61
2:B4:267:PHE:HB2	2:B4:384:ILE:HD12	1.83	0.61
4:B:2169:ALA:O	4:B:2173:LEU:N	2.32	0.61
4:B:2273:GLN:O	4:B:2314:ARG:N	2.33	0.61
1:A5:220:PRO:HD2	2:A6:326:LYS:HD3	1.82	0.61
1:A7:156:ARG:NE	1:A7:195:ASN:O	2.33	0.61
3:A:1762:GLY:O	3:A:1766:SER:CB	2.49	0.61
20:Z:119:ILE:HD12	20:Z:123:ARG:HE	1.66	0.61
1:B1:211:CYS:HA	1:B1:215:LEU:HB2	1.83	0.61
2:B6:189:LEU:HD11	2:B6:418:PHE:HE1	1.66	0.61
3:A:1996:GLY:O	3:A:2189:ARG:N	2.34	0.61
2:A2:379:SER:OG	2:A2:380:ASN:N	2.34	0.61
1:A3:272:PRO:HD3	1:A3:364:SER:HA	1.82	0.61
1:B1:140:GLY:O	1:B1:184:ASN:ND2	2.34	0.61
2:B2:107:HIS:O	2:B2:112:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:172:SER:OG	1:B5:380:ARG:NH1	2.34	0.61
5:C:669:ARG:NH2	5:C:692:GLU:OE2	2.34	0.60
1:A3:222:PHE:O	1:A3:226:ASN:ND2	2.33	0.60
1:A5:222:PHE:O	1:A5:226:ASN:ND2	2.33	0.60
3:A:274:ASP:O	3:A:278:GLN:N	2.33	0.60
4:B:2592:MET:O	4:B:2640:GLN:N	2.27	0.60
5:C:4327:LYS:O	5:C:4331:LEU:N	2.32	0.60
2:B4:172:TYR:CD2	2:B4:203:MET:HG3	2.37	0.60
1:B5:309:ARG:H	1:B5:372:THR:HG22	1.67	0.60
3:A:2795:LEU:HA	3:A:2799:GLY:HA2	1.83	0.60
4:B:627:LEU:HG	4:B:631:MET:CE	2.31	0.60
5:C:838:TYR:HD1	5:C:839:PRO:HD2	1.65	0.60
2:A4:98:ASP:OD1	2:A4:99:ALA:N	2.34	0.60
1:B1:175:VAL:HG13	2:B2:329:ASN:HD21	1.65	0.60
1:A1:232:VAL:HG22	1:A1:270:PHE:HB2	1.82	0.60
2:B4:14:ILE:HD11	2:B4:74:VAL:HG13	1.83	0.60
1:B5:186:THR:HG22	1:B5:411:ALA:HB1	1.84	0.60
4:B:526:PHE:HB2	4:B:603:ARG:HH21	1.67	0.60
4:B:1875:CYS:O	4:B:1877:ALA:N	2.34	0.60
13:M:55:THR:OG1	13:M:89:LYS:NZ	2.35	0.60
18:Y:232:THR:HA	18:Y:235:GLU:HG2	1.83	0.60
3:A:1628:MET:HA	3:A:1883:ALA:CB	2.31	0.60
3:A:2544:ILE:HA	3:A:2547:ALA:HB3	1.83	0.60
7:E:418:ARG:HD3	7:E:484:LEU:HD13	1.83	0.60
2:A4:417:GLU:HA	2:A4:420:GLU:HG3	1.83	0.60
2:A6:403:ALA:HB2	1:A7:344:TRP:HZ3	1.65	0.60
1:A7:376:GLU:O	1:A7:380:ARG:HG3	2.00	0.60
2:B2:88:HIS:CE1	2:B2:90:GLU:HG2	2.36	0.60
2:B2:387:ILE:HG12	2:B2:390:ARG:HH22	1.67	0.60
1:B5:125:GLU:OE1	1:B5:159:TYR:OH	2.18	0.60
1:B7:282:ARG:NH1	1:B7:288:GLU:OE1	2.35	0.60
4:B:235:THR:O	4:B:239:PHE:HB2	2.01	0.60
1:A1:102:ALA:HB2	1:A1:403:MET:HE3	1.84	0.60
1:A1:152:ILE:HG22	1:A1:195:ASN:HB3	1.84	0.60
3:A:3628:THR:H	3:A:3676:GLY:HA2	1.67	0.60
4:B:321:PHE:HB3	4:B:324:ILE:HD12	1.84	0.60
4:B:2204:ALA:HB1	4:B:2660:ARG:HA	1.84	0.60
5:C:2412:ASN:O	5:C:2416:ASN:N	2.33	0.60
6:D:654:LYS:HG3	6:D:657:ASP:HB2	1.83	0.60
7:E:262:HIS:HB2	7:E:290:LEU:HD13	1.82	0.60
16:X:254:GLU:O	16:X:257:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:103:LYS:NZ	1:A1:397:TRP:O	2.34	0.60
2:A2:224:TYR:O	2:A2:228:ASN:ND2	2.34	0.60
18:Y1:145:LYS:HA	18:Y1:145:LYS:HE3	1.83	0.60
2:A2:413:MET:HB3	2:A2:417:GLU:OE2	2.02	0.60
1:B3:49:VAL:HG11	1:B3:241:ARG:HG2	1.82	0.60
1:B7:113:ILE:HA	1:B7:116:VAL:HG22	1.83	0.60
7:E:385:THR:OG1	7:E:387:ARG:NE	2.35	0.60
3:A:1411:ASN:O	3:A:1414:SER:N	2.35	0.59
3:A:1772:PHE:O	3:A:1843:ILE:HA	2.02	0.59
3:A:3956:LEU:O	3:A:3961:GLU:N	2.28	0.59
10:H:99:LYS:HA	10:H:104:HIS:HA	1.84	0.59
1:A3:121:ARG:NH2	1:A3:158:GLU:OE2	2.34	0.59
2:A6:251:ASP:H	2:A6:254:GLU:HG2	1.67	0.59
2:B4:398:MET:HE2	1:B5:345:ILE:HD12	1.84	0.59
5:C:1833:GLY:O	5:C:1837:GLY:N	2.35	0.59
3:A:4137:GLY:HA2	3:A:4162:VAL:HA	1.84	0.59
4:B:155:PHE:HZ	5:C:152:THR:HG22	1.67	0.59
4:B:1918:ALA:HA	4:B:2021:MET:H	1.67	0.59
7:E:185:LEU:O	7:E:189:GLN:NE2	2.35	0.59
1:A1:345:ILE:O	1:A1:348:ASN:ND2	2.36	0.59
1:A3:121:ARG:HH11	18:Y1:141:LYS:NZ	2.01	0.59
2:A6:384:ILE:O	2:A6:387:ILE:HG22	2.02	0.59
1:A7:173:PRO:HB3	1:A7:384:GLN:HE22	1.66	0.59
1:B3:257:LEU:HD21	1:B3:314:SER:HB3	1.85	0.59
1:B7:165:LEU:HD23	1:B7:167:PHE:CZ	2.37	0.59
3:A:3610:ARG:O	3:A:3614:LEU:N	2.34	0.59
5:C:574:VAL:HG11	5:C:631:TRP:HB2	1.84	0.59
5:C:3930:ARG:O	5:C:3934:ALA:N	2.33	0.59
1:A3:391:ARG:NH2	2:A4:262:TYR:OH	2.35	0.59
3:A:1621:LYS:HA	3:A:1624:ARG:CB	2.32	0.59
3:A:3319:ASP:O	3:A:3323:VAL:N	2.25	0.59
1:A1:208:TYR:HE2	2:A2:329:ASN:HD22	1.49	0.59
1:A3:392:LYS:HD2	1:A3:395:LEU:HD22	1.85	0.59
2:A4:222:PRO:HD2	1:A5:324:LYS:HE3	1.83	0.59
2:A4:339:ARG:HG2	2:A4:339:ARG:HH11	1.67	0.59
2:B2:167:LEU:HD13	2:B2:200:VAL:HB	1.84	0.59
4:B:2273:GLN:N	4:B:2312:SER:O	2.34	0.59
1:A3:128:ASP:OD1	1:A3:129:CYS:N	2.34	0.59
1:B3:5:VAL:HG12	1:B3:133:PHE:HD1	1.67	0.59
3:A:1505:GLY:HA2	3:A:1517:PHE:H	1.67	0.59
4:B:1818:THR:O	4:B:1822:ARG:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2595:VAL:HA	5:C:2598:ALA:HB3	1.84	0.59
2:A4:14:ILE:HD11	2:A4:74:VAL:HG13	1.83	0.59
2:A4:286:LEU:O	2:A4:373:ARG:NH1	2.35	0.59
1:B1:139:LEU:HD22	1:B1:188:SER:HB3	1.85	0.59
1:B5:256:ASN:ND2	1:B5:350:LYS:HD2	2.16	0.59
4:B:2178:ASP:O	4:B:2181:PHE:N	2.30	0.59
5:C:869:GLN:OE1	5:C:956:ARG:NH1	2.34	0.59
3:A:1677:CYS:CB	3:A:1679:ALA:H	2.16	0.59
5:C:129:PRO:HD2	5:C:130:ILE:H	1.67	0.59
7:E:481:SER:OG	7:E:482:THR:N	2.33	0.59
1:A1:153:SER:OG	1:A1:195:ASN:OD1	2.14	0.59
2:A4:31:GLN:HE22	2:A4:37:PRO:HG3	1.68	0.59
6:D:575:LEU:HD11	6:D:644:ARG:HB2	1.85	0.59
20:Z:154:LEU:O	20:Z:158:HIS:ND1	2.36	0.59
2:A2:286:LEU:O	2:A2:373:ARG:NH1	2.35	0.58
1:A3:102:ALA:HB2	1:A3:403:MET:HE2	1.84	0.58
1:A5:286:VAL:HG12	1:A5:329:GLN:HG3	1.84	0.58
2:B2:358:GLN:OE1	2:B2:359:PRO:HD2	2.03	0.58
4:B:3980:VAL:O	4:B:3984:VAL:N	2.25	0.58
1:A1:361:LEU:HG	1:A1:363:MET:H	1.68	0.58
1:A7:113:ILE:HG21	1:A7:150:LEU:HD22	1.85	0.58
4:B:2762:GLU:O	4:B:2766:ARG:N	2.27	0.58
4:B:2885:LYS:O	4:B:2889:ALA:CB	2.48	0.58
20:Z:143:ASN:OD1	20:Z:144:SER:N	2.36	0.58
1:A5:337:ASN:HB3	1:A5:340:TYR:HD2	1.68	0.58
2:B2:165:SER:HB3	2:B2:256:GLN:HE21	1.67	0.58
1:B5:102:ALA:HB2	1:B5:403:MET:HE3	1.85	0.58
3:A:1785:VAL:HA	3:A:3916:GLY:O	2.03	0.58
3:A:4104:GLY:O	3:A:4109:GLY:N	2.33	0.58
4:B:424:PHE:HA	4:B:427:ARG:HD3	1.85	0.58
5:C:2666:GLY:O	5:C:2670:GLY:N	2.28	0.58
6:D:639:LEU:O	6:D:644:ARG:NH2	2.37	0.58
1:B3:388:MET:HE2	2:B4:348:PRO:HD2	1.85	0.58
3:A:1667:ARG:HA	3:A:1670:SER:HA	1.84	0.58
3:A:2689:ALA:H	3:A:3426:PHE:N	2.02	0.58
13:L:57:HIS:HB2	13:L:88:PHE:CE1	2.38	0.58
1:A3:289:LEU:HD11	1:A3:365:ALA:HB2	1.85	0.58
2:A4:120:ASP:OD1	2:A4:123:ARG:NH1	2.34	0.58
3:A:2399:SER:CA	3:A:2438:PHE:O	2.43	0.58
3:A:3525:LEU:HA	3:A:3528:ALA:HB3	1.85	0.58
9:G:44:ARG:NH1	9:G:56:GLU:OE2	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:153:PHE:O	20:Z:157:LEU:HD13	2.04	0.58
2:A2:155:GLU:HG2	2:A2:197:HIS:CD2	2.38	0.58
1:A3:374:ILE:HD11	1:A3:422:TYR:CZ	2.39	0.58
3:A:1791:LYS:O	3:A:1825:PHE:HA	2.03	0.58
4:B:729:SER:OG	4:B:730:ALA:N	2.37	0.58
4:B:3554:CYS:O	4:B:3558:GLY:N	2.37	0.58
5:C:823:GLU:O	5:C:827:ALA:N	2.36	0.58
6:D:366:VAL:HB	6:D:376:LEU:HD11	1.85	0.58
1:A3:5:VAL:HG12	1:A3:62:ARG:HD3	1.85	0.58
1:A3:200:MET:SD	1:A3:268:VAL:HG11	2.43	0.58
1:B7:238:CYS:SG	1:B7:318:ARG:NE	2.77	0.58
3:A:3727:ASP:HA	3:A:3730:ILE:CB	2.34	0.58
6:D:342:ILE:HG23	6:D:357:PHE:HB2	1.85	0.58
12:J:47:VAL:HG11	12:J:90:LEU:HD11	1.86	0.58
2:A2:394:LYS:HB2	1:A3:346:PRO:HG3	1.83	0.58
2:A6:405:VAL:HG13	2:A6:418:PHE:HE2	1.69	0.58
1:B3:388:MET:HE1	2:B4:347:CYS:HA	1.85	0.58
3:A:3625:LEU:O	3:A:3677:GLY:HA2	2.04	0.58
1:A1:77:ARG:HH12	1:A1:87:PRO:HG3	1.66	0.58
2:A6:278:ALA:HA	2:A6:369:ALA:HB2	1.84	0.58
1:A7:309:ARG:H	1:A7:372:THR:HG22	1.68	0.58
1:B1:61:PRO:HD3	1:B1:84:ILE:HG13	1.86	0.58
2:B2:323:VAL:HG13	2:B2:355:ILE:HG23	1.86	0.58
4:B:591:ARG:HH21	4:B:693:LEU:HD21	1.68	0.58
5:C:3891:LEU:CB	5:C:3974:LEU:O	2.51	0.58
13:L:61:GLY:HA3	13:M:64:PHE:HA	1.86	0.58
2:A2:288:VAL:HG21	2:A2:323:VAL:HG13	1.86	0.58
1:A3:252:LYS:O	1:A3:256:ASN:ND2	2.37	0.58
4:B:319:ASP:O	4:B:322:LYS:NZ	2.37	0.58
4:B:4245:ILE:HA	4:B:4248:VAL:H	1.69	0.58
7:E:164:ALA:HB3	7:E:469:GLY:HA3	1.85	0.58
7:E:418:ARG:HD3	7:E:484:LEU:HA	1.84	0.58
1:A1:254:ALA:O	1:A1:258:ILE:HG22	2.04	0.57
1:A3:113:ILE:HD12	1:A3:150:LEU:HD22	1.86	0.57
1:B1:330:MET:SD	1:B1:349:VAL:HG11	2.44	0.57
1:B7:105:HIS:HA	1:B7:150:LEU:HD23	1.86	0.57
3:A:2537:ILE:O	3:A:2541:GLY:N	2.37	0.57
3:A:3866:SER:O	3:A:3870:MET:N	2.32	0.57
3:A:4260:ALA:HB1	3:A:4343:THR:O	2.04	0.57
4:B:348:MET:HA	4:B:351:ILE:HD12	1.84	0.57
5:C:781:LEU:HD21	5:C:824:VAL:HG21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:379:LEU:HB2	7:E:414:TRP:CZ3	2.39	0.57
1:A1:39:ASP:OD1	1:A1:40:SER:N	2.35	0.57
1:B1:191:GLN:HG3	1:B1:195:ASN:HD22	1.69	0.57
2:A2:116:ASP:OD1	2:A2:117:LEU:N	2.37	0.57
2:B4:129:CYS:SG	2:B4:130:THR:N	2.76	0.57
1:B3:135:VAL:HG21	1:B3:152:ILE:HD11	1.86	0.57
2:A4:328:VAL:HG21	2:A4:355:ILE:HD11	1.86	0.57
1:B5:100:ASN:ND2	1:B5:103:LYS:HG3	2.19	0.57
1:B7:152:ILE:HG22	1:B7:195:ASN:HB3	1.86	0.57
4:B:324:ILE:O	4:B:327:THR:HB	2.04	0.57
5:C:116:LEU:HD12	5:C:163:VAL:HB	1.87	0.57
5:C:394:ARG:NH1	5:C:413:GLU:OE1	2.38	0.57
20:Z:154:LEU:HB3	20:Z:158:HIS:CE1	2.38	0.57
1:B7:8:GLN:NE2	1:B7:17:GLY:HA3	2.18	0.57
1:B7:248:ALA:HA	1:B7:252:LYS:HD2	1.86	0.57
6:D:503:ARG:HB3	6:D:514:SER:HB2	1.86	0.57
1:A7:253:LEU:HD11	1:A7:316:LEU:HD21	1.87	0.57
2:B4:28:HIS:CE1	2:B4:49:PHE:HA	2.40	0.57
2:B4:288:VAL:HG13	2:B4:319:TYR:HE2	1.69	0.57
2:B4:384:ILE:HD11	2:B4:432:PHE:CZ	2.40	0.57
3:A:3360:MET:N	3:A:3451:LEU:O	2.37	0.57
4:B:251:HIS:NE2	4:B:285:GLU:OE1	2.38	0.57
1:B1:262:ARG:NE	1:B1:421:GLU:OE2	2.36	0.57
9:G:71:SER:OG	9:G:73:CYS:O	2.21	0.57
2:A4:237:SER:HA	2:A4:320:ARG:HD2	1.86	0.57
4:B:2260:THR:O	4:B:2264:MET:CB	2.53	0.57
4:B:3646:VAL:O	4:B:3650:ARG:N	2.35	0.57
4:B:4556:TRP:O	4:B:4560:GLY:N	2.33	0.57
5:C:569:ARG:NH1	6:D:614:THR:HG1	2.02	0.57
5:C:1030:VAL:HA	9:G:65:GLN:HE22	1.69	0.57
5:C:4047:GLY:HA2	5:C:4050:GLY:H	1.69	0.57
2:A2:422:ARG:O	2:A2:422:ARG:NE	2.37	0.57
1:B5:45:GLU:HG2	1:B5:46:ARG:HG2	1.86	0.57
7:E:379:LEU:HB2	7:E:414:TRP:CH2	2.40	0.57
1:A1:376:GLU:HG3	1:A1:380:ARG:HH12	1.70	0.56
1:B3:303:ALA:HA	1:B3:376:GLU:OE2	2.05	0.56
1:B7:36:TYR:O	1:B7:37:HIS:ND1	2.38	0.56
1:B7:334:GLN:HE22	1:B7:347:ASN:H	1.52	0.56
4:B:2056:MET:O	4:B:2060:GLU:N	2.38	0.56
5:C:120:LYS:HB3	5:C:159:LEU:HD21	1.86	0.56
6:D:212:ASP:CG	15:P:20:LEU:HG	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:85:ASP:O	20:Z:88:GLY:N	2.38	0.56
2:B6:172:TYR:CE1	2:B6:203:MET:HG3	2.39	0.56
3:A:4152:LEU:N	3:A:4156:PHE:O	2.38	0.56
1:A1:274:THR:OG1	1:A1:279:GLN:OE1	2.22	0.56
1:A5:203:ASP:OD1	1:A5:204:ASN:N	2.38	0.56
1:A7:135:VAL:HB	1:A7:166:THR:HG22	1.87	0.56
2:B2:298:PRO:HB3	2:B2:307:PRO:HD2	1.88	0.56
2:B6:167:LEU:HD13	2:B6:200:VAL:HB	1.87	0.56
3:A:2403:ASN:H	3:A:2406:THR:CB	2.19	0.56
4:B:147:GLU:OE2	4:B:151:ASN:ND2	2.38	0.56
4:B:624:TYR:O	4:B:628:TRP:HB2	2.04	0.56
7:E:289:VAL:HB	7:E:306:LEU:HD13	1.87	0.56
2:A6:60:LYS:HD2	2:B6:282:TYR:CZ	2.40	0.56
2:A6:206:ASN:ND2	21:A7:501:GTP:O2'	2.38	0.56
1:B3:309:ARG:H	1:B3:372:THR:HG22	1.69	0.56
2:B4:417:GLU:HA	2:B4:420:GLU:HG2	1.87	0.56
4:B:526:PHE:HB2	4:B:603:ARG:NH2	2.20	0.56
4:B:2937:THR:O	4:B:2941:ILE:N	2.35	0.56
5:C:131:MET:O	5:C:135:GLN:N	2.37	0.56
5:C:1041:HIS:O	5:C:1045:ASN:N	2.31	0.56
7:E:180:VAL:HG21	7:E:201:TRP:HE1	1.71	0.56
2:A6:403:ALA:HB2	1:A7:344:TRP:CZ3	2.40	0.56
2:B2:72:PRO:HG2	1:B3:1:MET:SD	2.46	0.56
1:B5:31:ASP:OD1	1:B5:35:THR:N	2.38	0.56
4:B:768:LEU:O	4:B:772:LYS:N	2.38	0.56
5:C:225:LYS:HB2	5:C:344:ARG:HH22	1.71	0.56
6:D:619:ASN:ND2	6:D:622:HIS:O	2.39	0.56
1:A1:52:ASN:OD1	1:A1:62:ARG:NH2	2.38	0.56
5:C:341:HIS:O	5:C:345:LEU:HB2	2.06	0.56
1:B5:211:CYS:HA	1:B5:215:LEU:HB2	1.86	0.56
5:C:1872:GLU:H	5:C:1921:MET:HA	1.70	0.56
2:B2:90:GLU:OE2	2:B2:121:ARG:NH1	2.39	0.56
2:B2:401:LYS:HD3	1:B3:344:TRP:CG	2.41	0.56
1:B7:11:GLN:N	23:B7:502:GDP:O2B	2.35	0.56
1:B7:183:TYR:HA	1:B7:385:PHE:HE1	1.71	0.56
3:A:4269:ALA:O	3:A:4272:SER:CB	2.54	0.56
4:B:2967:ASP:O	4:B:2971:PHE:CB	2.53	0.56
5:C:3506:ASP:O	5:C:3510:GLU:N	2.34	0.56
7:E:107:ILE:HG21	11:I:3:ASP:HB3	1.88	0.56
7:E:374:ASN:HD21	7:E:489:PRO:HB2	1.71	0.56
7:E:384:TRP:HB3	7:E:408:TYR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X1:251:ALA:O	16:X1:255:LEU:HG	2.06	0.56
1:A1:164:MET:HB3	1:A1:197:ASP:HB2	1.88	0.56
2:A2:403:ALA:HB2	1:A3:344:TRP:HZ3	1.70	0.56
2:B4:346:TRP:CH2	2:B4:435:VAL:HG13	2.41	0.56
2:B6:9:ILE:HD13	2:B6:150:GLY:HA2	1.88	0.56
3:A:1805:GLY:HA2	3:A:1827:ALA:CA	2.36	0.56
5:C:230:ARG:HG3	5:C:348:LYS:HE3	1.88	0.56
1:A3:193:VAL:HG11	1:A3:418:LEU:HD21	1.88	0.56
2:A4:72:PRO:HG3	1:A5:1:MET:HE3	1.88	0.56
1:A5:161:ASP:OD1	1:A5:162:ARG:HD2	2.06	0.56
2:A4:398:MET:HE2	1:A5:346:PRO:HD2	1.87	0.55
1:A5:293:MET:HG3	1:A5:367:PHE:HB2	1.88	0.55
2:A6:381:SER:OG	2:A6:382:THR:N	2.39	0.55
1:A7:285:THR:O	1:A7:289:LEU:HD12	2.06	0.55
1:B5:423:GLN:O	1:B5:426:GLN:HG3	2.05	0.55
1:B7:394:PHE:HA	1:B7:397:TRP:CZ3	2.41	0.55
3:A:2670:TYR:O	3:A:2674:TYR:CB	2.54	0.55
3:A:2720:VAL:O	3:A:2877:PHE:N	2.40	0.55
3:A:4248:LEU:HA	3:A:4258:VAL:HA	1.88	0.55
3:A:4261:LEU:O	3:A:4264:ALA:HB3	2.06	0.55
1:A5:145:SER:O	1:A5:149:THR:OG1	2.18	0.55
1:A5:179:VAL:HG23	2:A6:349:THR:O	2.06	0.55
4:B:3879:ASP:CB	5:C:1534:GLU:CB	2.84	0.55
5:C:676:ARG:HG3	5:C:689:LEU:HD21	1.87	0.55
5:C:784:ILE:HG23	5:C:817:LEU:HD22	1.87	0.55
7:E:120:LEU:HD11	11:I:73:ARG:HH11	1.71	0.55
2:A2:70:LEU:HD21	2:A2:114:ILE:HG21	1.87	0.55
1:A3:262:ARG:NH1	1:A3:421:GLU:OE1	2.39	0.55
1:B3:114:ASP:OD1	1:B3:115:SER:N	2.40	0.55
1:B5:209:ASP:OD2	1:B5:213:ARG:NH1	2.34	0.55
7:E:112:GLN:O	7:E:115:SER:OG	2.22	0.55
1:A1:139:LEU:HD12	1:A1:170:VAL:HG22	1.88	0.55
2:A4:221:ARG:NH1	1:A5:325:GLU:OE2	2.39	0.55
1:B1:177:ASP:N	1:B1:181:GLU:OE2	2.36	0.55
1:B1:293:MET:HG3	1:B1:367:PHE:HB2	1.88	0.55
2:B4:66:ILE:HG13	2:B4:121:ARG:HH21	1.71	0.55
3:A:1967:LEU:O	3:A:1970:LEU:N	2.37	0.55
3:A:3879:PRO:O	3:A:3994:ILE:N	2.32	0.55
4:B:2594:TYR:O	4:B:2642:ALA:N	2.39	0.55
4:B:2807:ALA:H	4:B:2824:ALA:HA	1.72	0.55
7:E:72:LYS:HA	13:K:69:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:168:ASN:OD1	7:E:179:VAL:HB	2.06	0.55
2:A4:383:ALA:O	2:A4:386:GLU:HG2	2.06	0.55
1:B5:144:GLY:N	23:B5:502:GDP:O1B	2.34	0.55
3:A:2714:SER:N	3:A:2843:THR:HA	2.22	0.55
3:A:3319:ASP:O	3:A:3322:LYS:N	2.40	0.55
2:A6:9:ILE:HG22	2:A6:68:LEU:HD11	1.88	0.55
1:B1:309:ARG:H	1:B1:372:THR:HG22	1.71	0.55
2:B4:277:SER:OG	2:B4:278:ALA:N	2.39	0.55
7:E:243:TYR:HD2	7:E:254:GLU:HB2	1.69	0.55
7:E:345:ARG:HA	7:E:353:ARG:HE	1.72	0.55
1:A3:3:GLU:OE2	1:A3:127:CYS:HB2	2.07	0.55
1:B3:226:ASN:OD1	23:B3:502:GDP:N1	2.38	0.55
5:C:296:TYR:HE2	5:C:332:ILE:HG21	1.72	0.55
6:D:428:PHE:HB2	6:D:440:TRP:HB2	1.89	0.55
1:A1:218:THR:O	2:A2:326:LYS:NZ	2.39	0.55
2:A2:317:LEU:HB3	2:A2:319:TYR:HE1	1.71	0.55
1:A3:3:GLU:CD	1:A3:127:CYS:HB2	2.26	0.55
1:A5:401:GLU:OE1	1:A5:401:GLU:N	2.39	0.55
1:B1:3:GLU:HG3	1:B1:127:CYS:HB2	1.89	0.55
2:B2:91:GLN:CG	2:B2:121:ARG:HH21	2.18	0.55
1:B7:5:VAL:HG23	1:B7:62:ARG:HG2	1.87	0.55
4:B:649:THR:HG22	4:B:653:LYS:HE2	1.89	0.55
4:B:1918:ALA:O	4:B:2044:MET:N	2.30	0.55
1:A1:382:SER:OG	1:A1:415:MET:HG2	2.07	0.55
1:A3:102:ALA:HB2	1:A3:403:MET:CE	2.36	0.55
1:B1:175:VAL:HG11	1:B1:204:ASN:HB2	1.88	0.55
3:A:3724:PHE:H	3:A:3727:ASP:CB	2.19	0.55
5:C:3934:ALA:O	5:C:3938:LEU:N	2.37	0.55
7:E:366:TYR:H	7:E:382:GLY:HA3	1.71	0.55
2:A6:223:THR:HG23	2:A6:225:THR:H	1.72	0.55
2:B2:124:LYS:HA	2:B2:127:ASP:HB2	1.88	0.55
3:A:1666:ASP:O	3:A:1670:SER:HA	2.06	0.55
5:C:2123:HIS:HA	5:C:2169:THR:HA	1.89	0.55
2:A2:415:GLU:CD	20:Z:168:ARG:HH12	2.10	0.54
1:A5:27:GLU:HA	1:A5:359:LYS:HE3	1.89	0.54
13:L:76:ILE:O	13:L:86:LEU:HA	2.07	0.54
16:X1:125:ILE:HD13	18:Y1:72:LEU:HD23	1.89	0.54
1:A3:11:GLN:N	23:A3:502:GDP:O2B	2.35	0.54
2:A4:7:ILE:HD13	2:A4:153:LEU:HD21	1.88	0.54
1:A7:135:VAL:HG21	1:A7:152:ILE:HD11	1.89	0.54
3:A:3395:GLU:O	3:A:3399:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2584:TYR:N	4:B:2635:GLU:O	2.40	0.54
4:B:4530:PRO:HA	4:B:4544:GLU:HA	1.89	0.54
18:Y1:188:MET:O	18:Y1:192:ILE:HG12	2.07	0.54
2:A4:174:SER:HB3	2:A4:177:VAL:O	2.07	0.54
2:A6:14:ILE:HD11	2:A6:74:VAL:HG22	1.90	0.54
2:B2:265:ILE:HG22	2:B2:380:ASN:HD21	1.72	0.54
3:A:1589:MET:HA	3:A:1651:GLN:CB	2.37	0.54
4:B:211:GLN:OE1	4:B:253:GLN:NE2	2.40	0.54
6:D:503:ARG:HD2	6:D:550:LEU:HD11	1.89	0.54
7:E:168:ASN:HD22	7:E:223:LYS:HA	1.72	0.54
16:X1:160:THR:HG22	18:Y1:108:LEU:HD13	1.88	0.54
1:A1:35:THR:HA	1:A1:57:GLY:O	2.07	0.54
1:A5:289:LEU:HD23	1:A5:365:ALA:HB2	1.89	0.54
1:A7:189:VAL:HA	1:A7:192:LEU:HG	1.89	0.54
2:B4:102:ASN:HD21	2:B4:411:GLU:HG3	1.72	0.54
2:B6:9:ILE:HG12	2:B6:68:LEU:HD11	1.89	0.54
3:A:2442:LEU:CB	3:A:2486:ALA:HB1	2.38	0.54
3:A:4181:VAL:HA	3:A:4185:MET:O	2.08	0.54
4:B:3841:TYR:O	4:B:3845:GLU:CB	2.56	0.54
15:P:42:VAL:HG21	15:P:92:VAL:HG11	1.88	0.54
1:A7:293:MET:SD	1:A7:367:PHE:HB2	2.48	0.54
1:B5:203:ASP:OD1	1:B5:204:ASN:N	2.41	0.54
3:A:1718:ALA:N	3:A:1864:ARG:O	2.25	0.54
3:A:4378:LEU:O	3:A:4381:ASP:N	2.40	0.54
7:E:361:HIS:HE1	7:E:383:ASP:H	1.55	0.54
1:A1:215:LEU:HB3	1:A1:217:LEU:CD1	2.34	0.54
1:A1:232:VAL:O	1:A1:236:ILE:HD12	2.07	0.54
1:A3:397:TRP:CH2	2:A4:260:VAL:HG23	2.37	0.54
2:B4:11:GLN:NE2	1:B5:247:ASN:OD1	2.40	0.54
2:B6:408:TYR:HD2	2:B6:418:PHE:HZ	1.56	0.54
4:B:2577:GLU:N	4:B:2585:GLY:O	2.40	0.54
1:B3:7:ILE:HG21	1:B3:151:LEU:HD21	1.89	0.54
3:A:1662:ARG:O	3:A:1674:ILE:HA	2.07	0.54
4:B:443:ARG:NH2	4:B:533:GLU:O	2.41	0.54
6:D:329:TYR:HD2	6:D:341:LEU:HD23	1.72	0.54
1:B5:101:TRP:HE1	1:B5:145:SER:HG	1.55	0.54
1:B7:43:GLN:O	1:B7:47:ILE:HG23	2.08	0.54
3:A:1359:GLN:O	3:A:1362:ALA:HB3	2.07	0.54
5:C:500:GLN:NE2	5:C:504:ASN:OD1	2.41	0.54
15:P:21:VAL:HG12	15:P:90:ILE:HG22	1.89	0.54
1:A3:373:ALA:O	1:A3:376:GLU:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:317:PHE:HB3	1:A5:321:MET:SD	2.48	0.54
1:A7:404:ASP:HB2	1:A7:406:MET:SD	2.47	0.54
2:B4:298:PRO:HB3	2:B4:307:PRO:HD2	1.89	0.54
1:B5:69:GLU:HG2	2:B6:2:ARG:HH22	1.73	0.54
1:B7:173:PRO:HB3	1:B7:384:GLN:OE1	2.08	0.54
3:A:4451:ASN:O	3:A:4454:GLY:N	2.41	0.54
4:B:630:GLU:O	4:B:633:GLU:HB2	2.08	0.54
5:C:132:GLN:O	5:C:135:GLN:HB2	2.07	0.54
5:C:792:LEU:HD21	5:C:882:LEU:HD13	1.88	0.54
6:D:504:CYS:SG	6:D:505:SER:N	2.80	0.54
11:I:69:LEU:HA	12:J:74:SER:HA	1.89	0.54
16:X1:248:LYS:HZ3	18:Y1:201:ALA:C	2.10	0.54
4:B:2564:GLU:O	4:B:2568:LEU:N	2.39	0.54
5:C:4033:VAL:O	5:C:4037:LEU:N	2.37	0.54
11:I:85:PRO:HA	11:I:94:TYR:HA	1.90	0.54
1:A3:215:LEU:HB3	1:A3:217:LEU:CD1	2.33	0.53
2:A4:183:GLU:HA	2:A4:186:ASN:HD22	1.72	0.53
1:A7:319:GLY:N	1:A7:354:CYS:O	2.37	0.53
3:A:3852:GLU:O	3:A:3856:GLY:N	2.40	0.53
4:B:2623:HIS:O	4:B:2636:ILE:N	2.42	0.53
13:M:76:ILE:HB	13:M:87:LEU:HB2	1.89	0.53
1:A1:330:MET:HE2	1:A1:349:VAL:HG21	1.89	0.53
2:B6:417:GLU:HA	2:B6:420:GLU:HG2	1.90	0.53
3:A:4257:VAL:O	3:A:4260:ALA:HB3	2.08	0.53
4:B:1916:ALA:O	4:B:2042:VAL:N	2.31	0.53
6:D:369:HIS:HE1	6:D:371:GLU:HB3	1.73	0.53
1:A1:258:ILE:HD12	1:A1:264:HIS:HB3	1.91	0.53
1:B5:39:ASP:OD1	1:B5:40:SER:N	2.42	0.53
3:A:4373:ALA:HB1	3:A:4379:PRO:HA	1.89	0.53
2:A4:318:MET:HB2	2:A4:376:CYS:HB3	1.90	0.53
3:A:3291:THR:O	3:A:3295:ARG:N	2.33	0.53
2:A2:119:LEU:HD21	2:A2:156:ARG:HB3	1.91	0.53
2:A2:145:THR:OG1	21:A3:501:GTP:O1B	2.27	0.53
2:A4:407:TRP:CG	1:A5:255:VAL:HG23	2.44	0.53
1:A5:7:ILE:HD13	1:A5:151:LEU:HD21	1.91	0.53
2:B4:66:ILE:CG1	2:B4:121:ARG:HH21	2.22	0.53
4:B:682:ARG:HH11	7:E:188:GLN:HG2	1.73	0.53
6:D:382:ASP:OD1	6:D:382:ASP:N	2.36	0.53
7:E:450:SER:OG	7:E:452:LEU:N	2.40	0.53
9:G:37:THR:HB	9:G:73:CYS:HB3	1.89	0.53
18:Y1:183:LYS:O	18:Y1:186:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:69:ASP:OD1	2:A2:70:LEU:N	2.42	0.53
2:A2:206:ASN:O	2:A2:210:TYR:HD2	1.91	0.53
1:B7:373:ALA:O	1:B7:376:GLU:HG2	2.08	0.53
3:A:2290:TYR:O	3:A:2294:PHE:N	2.25	0.53
4:B:134:PRO:HA	4:B:137:GLN:HG3	1.89	0.53
4:B:330:LEU:HA	4:B:333:LYS:HB2	1.89	0.53
4:B:1915:GLY:N	4:B:2017:ALA:O	2.29	0.53
1:A1:217:LEU:HD21	1:A1:224:ASP:OD2	2.09	0.53
1:A5:345:ILE:O	1:A5:348:ASN:ND2	2.42	0.53
2:B4:319:TYR:HB3	2:B4:323:VAL:HG21	1.90	0.53
2:B6:407:TRP:O	2:B6:411:GLU:HG2	2.09	0.53
1:B7:52:ASN:OD1	1:B7:62:ARG:NH2	2.41	0.53
5:C:1843:PHE:N	5:C:1869:CYS:O	2.41	0.53
5:C:3384:GLU:O	5:C:3388:ASN:N	2.40	0.53
1:A1:114:ASP:OD1	1:A1:114:ASP:N	2.39	0.53
1:A5:2:ARG:HE	1:A5:240:LEU:HD22	1.74	0.53
1:A5:36:TYR:HB2	1:A5:59:TYR:HE2	1.74	0.53
2:B6:51:THR:HG21	2:B6:243:ARG:HG2	1.91	0.53
2:B6:102:ASN:HD22	2:B6:105:ARG:HG3	1.73	0.53
1:B7:2:ARG:HE	1:B7:240:LEU:HD22	1.74	0.53
3:A:2439:VAL:N	3:A:2486:ALA:HA	2.21	0.53
4:B:381:ARG:HH12	4:B:431:MET:HG3	1.74	0.53
4:B:2595:PHE:HA	4:B:2642:ALA:HB3	1.90	0.53
5:C:328:MET:O	5:C:331:THR:OG1	2.26	0.53
5:C:675:GLN:HB2	5:C:689:LEU:HD23	1.91	0.53
5:C:864:TYR:HA	5:C:867:ILE:HD12	1.91	0.53
1:A5:274:THR:HG21	1:A5:282:ARG:NE	2.24	0.53
4:B:4025:GLY:O	4:B:4059:ARG:N	2.35	0.53
5:C:2065:LYS:O	5:C:2069:GLU:CB	2.57	0.53
5:C:2937:LYS:O	5:C:2941:ARG:N	2.30	0.53
2:A2:381:SER:OG	2:A2:382:THR:N	2.42	0.53
1:A3:210:ILE:O	1:A3:214:THR:OG1	2.24	0.53
1:B3:289:LEU:HD11	1:B3:363:MET:HG2	1.91	0.53
1:B3:309:ARG:H	1:B3:372:THR:CG2	2.22	0.53
2:B4:431:ASP:O	2:B4:434:GLU:HG2	2.09	0.53
4:B:685:ARG:HH12	7:E:265:PRO:HG3	1.73	0.53
4:B:743:GLN:HA	4:B:746:ALA:HB3	1.90	0.53
5:C:1846:SER:HA	5:C:1876:ILE:HA	1.90	0.53
11:I:7:VAL:O	11:I:10:THR:OG1	2.23	0.53
1:A1:314:SER:HB3	1:A1:368:ILE:HG23	1.92	0.52
1:A3:177:ASP:O	2:A4:352:LYS:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:238:CYS:SG	1:B3:318:ARG:NE	2.82	0.52
3:A:1349:LYS:O	3:A:1353:ASP:N	2.23	0.52
3:A:3876:SER:CB	3:A:3965:PRO:HA	2.38	0.52
6:D:510:SER:HB3	6:D:513:LEU:HD23	1.91	0.52
15:P:13:LEU:HD21	15:P:95:ARG:HH11	1.72	0.52
1:A3:8:GLN:O	1:A3:66:MET:HG3	2.08	0.52
2:A6:291:ILE:HD12	2:A6:375:VAL:HG13	1.90	0.52
1:A7:186:THR:HG23	1:A7:187:LEU:HD12	1.90	0.52
2:B2:317:LEU:HB3	2:B2:319:TYR:HE1	1.74	0.52
1:B5:117:LEU:HA	1:B5:120:VAL:HG12	1.90	0.52
1:B7:8:GLN:HB2	1:B7:65:LEU:HA	1.91	0.52
3:A:1946:ALA:O	3:A:1950:PHE:CB	2.57	0.52
3:A:2786:GLU:O	3:A:2788:MET:N	2.42	0.52
3:A:4135:PRO:HA	3:A:4148:PRO:CA	2.39	0.52
11:I:76:SER:OG	12:J:65:ASN:OD1	2.27	0.52
16:X:263:GLU:O	16:X:267:VAL:HG23	2.09	0.52
20:Z:33:LYS:HB3	20:Z:69:CYS:SG	2.49	0.52
2:A2:88:HIS:CE1	2:A2:90:GLU:HB2	2.45	0.52
2:A2:93:ILE:HD12	2:A2:117:LEU:HD21	1.90	0.52
1:B1:198:GLU:HA	1:B1:264:HIS:HB2	1.90	0.52
2:B2:264:ARG:NH1	2:B2:431:ASP:OD2	2.41	0.52
2:B4:91:GLN:HA	2:B4:121:ARG:HH22	1.73	0.52
2:B4:221:ARG:HG2	1:B5:322:SER:HB3	1.90	0.52
1:B5:178:THR:HG22	2:B6:352:LYS:HZ3	1.74	0.52
2:B6:203:MET:HE3	2:B6:267:PHE:HB3	1.92	0.52
3:A:2410:SER:HA	3:A:2803:ASP:CB	2.39	0.52
4:B:1861:TYR:HA	4:B:1872:VAL:HA	1.90	0.52
4:B:2057:LEU:O	4:B:2062:PHE:N	2.42	0.52
5:C:503:VAL:HG21	5:C:536:LEU:HD11	1.90	0.52
5:C:1404:GLU:HA	5:C:1411:VAL:HA	1.90	0.52
5:C:4032:PHE:O	5:C:4036:PHE:N	2.34	0.52
1:A7:4:ILE:HB	1:A7:50:TYR:HE1	1.74	0.52
1:A7:5:VAL:HG23	1:A7:62:ARG:HG2	1.91	0.52
2:B4:172:TYR:CE2	2:B4:203:MET:HG3	2.44	0.52
4:B:3772:THR:O	4:B:3775:GLY:N	2.42	0.52
5:C:3931:LYS:O	5:C:3934:ALA:HB3	2.08	0.52
1:A7:114:ASP:OD1	1:A7:114:ASP:N	2.43	0.52
1:B1:417:ASP:O	1:B1:421:GLU:HG2	2.10	0.52
2:B2:223:THR:HG23	2:B2:225:THR:H	1.75	0.52
1:B3:222:PHE:HE2	2:B4:248:LEU:HD11	1.74	0.52
1:B5:173:PRO:HB3	1:B5:384:GLN:NE2	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:39:ASP:OD1	9:G:40:THR:N	2.39	0.52
11:I:11:PHE:CE2	11:I:34:ARG:HD2	2.44	0.52
13:K:71:GLU:HG2	13:K:89:LYS:HB3	1.92	0.52
18:Y:199:PHE:O	18:Y:202:ARG:HG3	2.10	0.52
2:A6:102:ASN:OD1	1:A7:255:VAL:HG11	2.10	0.52
1:A7:169:VAL:HG23	1:A7:203:ASP:HA	1.91	0.52
3:A:4261:LEU:HA	3:A:4264:ALA:HB3	1.90	0.52
4:B:560:LEU:HD22	4:B:624:TYR:HE1	1.75	0.52
4:B:2106:MET:HA	4:B:2109:ALA:HB3	1.91	0.52
5:C:2465:MET:O	5:C:2469:GLY:N	2.34	0.52
7:E:80:GLY:HA2	13:K:79:TYR:CE2	2.45	0.52
13:L:67:TYR:CD2	13:M:45:LYS:HD3	2.45	0.52
2:B4:99:ALA:O	2:B4:105:ARG:HD3	2.09	0.52
18:Y1:79:GLU:O	18:Y1:82:MET:HG3	2.10	0.52
2:A4:306:ASP:HB3	2:A4:309:HIS:ND1	2.24	0.52
2:B2:402:ARG:NH2	2:B2:415:GLU:OE2	2.42	0.52
2:B4:317:LEU:HB3	2:B4:319:TYR:HE1	1.74	0.52
2:B6:222:PRO:HD2	1:B7:324:LYS:HE3	1.92	0.52
3:A:1612:ILE:HA	3:A:1882:MET:O	2.09	0.52
3:A:2372:PHE:O	3:A:2487:CYS:HA	2.10	0.52
4:B:64:LEU:CB	4:B:75:THR:O	2.58	0.52
4:B:1771:VAL:O	4:B:1775:PHE:CB	2.58	0.52
5:C:204:GLU:HG2	5:C:205:GLU:N	2.25	0.52
2:A2:102:ASN:HB3	2:A2:105:ARG:HB2	1.92	0.52
2:A6:326:LYS:HG3	2:A6:327:ASP:N	2.25	0.52
1:B3:27:GLU:OE1	1:B3:241:ARG:NH1	2.26	0.52
1:B3:124:ALA:HB1	1:B3:130:LEU:HD11	1.91	0.52
3:A:219:ASP:O	3:A:223:MET:HA	2.10	0.52
3:A:1576:ILE:HA	3:A:1663:SER:O	2.10	0.52
3:A:1771:CYS:HA	3:A:1842:PHE:CB	2.40	0.52
3:A:2689:ALA:HB1	3:A:3423:ARG:HA	1.90	0.52
4:B:380:LEU:HD12	4:B:381:ARG:HG3	1.92	0.52
4:B:2472:ASP:O	4:B:2485:TRP:N	2.34	0.52
4:B:2892:ALA:O	4:B:2896:CYS:N	2.42	0.52
5:C:4404:LEU:HA	5:C:4408:GLU:O	2.09	0.52
2:A4:139:ASN:OD1	2:A4:170:THR:HG22	2.09	0.52
2:A6:317:LEU:HB3	2:A6:319:TYR:HE1	1.75	0.52
1:B7:100:ASN:ND2	1:B7:103:LYS:HG3	2.19	0.52
4:B:4476:GLY:HA3	4:B:4513:VAL:O	2.09	0.52
7:E:386:ALA:O	7:E:402:THR:OG1	2.27	0.52
16:X1:256:ALA:O	16:X1:261:ARG:NE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A4:105:ARG:HB2	2:A4:411:GLU:OE1	2.09	0.51
1:A7:334:GLN:OE1	1:A7:348:ASN:N	2.43	0.51
1:B5:66:MET:SD	1:B5:116:VAL:HG11	2.51	0.51
2:B6:53:PHE:HB3	2:B6:61:HIS:HB3	1.91	0.51
4:B:1895:THR:O	4:B:1899:ASP:N	2.32	0.51
4:B:3565:ASN:N	4:B:3609:GLN:O	2.33	0.51
4:B:4531:VAL:O	4:B:4542:VAL:N	2.35	0.51
6:D:334:PHE:O	6:D:337:GLN:NE2	2.43	0.51
1:A1:7:ILE:HD13	1:A1:64:ILE:HB	1.92	0.51
2:A2:387:ILE:HG12	2:A2:390:ARG:HH22	1.74	0.51
1:A3:72:THR:O	1:A3:76:VAL:HG23	2.09	0.51
1:A3:191:GLN:HG3	1:A3:195:ASN:ND2	2.24	0.51
2:B6:102:ASN:HD21	2:B6:411:GLU:HG3	1.74	0.51
3:A:4260:ALA:HA	3:A:4342:TRP:O	2.11	0.51
4:B:2605:ASP:H	4:B:2609:THR:H	1.58	0.51
5:C:1353:HIS:O	5:C:1357:GLN:N	2.44	0.51
1:B3:326:VAL:O	1:B3:330:MET:HG2	2.10	0.51
1:B5:49:VAL:HG11	1:B5:241:ARG:HG2	1.91	0.51
1:B5:212:PHE:HZ	2:B6:326:LYS:HG3	1.76	0.51
3:A:2438:PHE:HA	3:A:2485:VAL:C	2.31	0.51
5:C:803:PHE:O	5:C:806:GLN:HB2	2.10	0.51
5:C:823:GLU:O	5:C:826:ARG:HB2	2.09	0.51
5:C:830:ASP:O	5:C:833:THR:OG1	2.22	0.51
2:A2:402:ARG:HH11	20:Z:168:ARG:NH2	2.03	0.51
1:A3:133:PHE:HZ	1:A3:159:TYR:HD2	1.57	0.51
1:B1:153:SER:O	1:B1:157:GLU:HG2	2.10	0.51
2:B2:15:GLN:NE2	21:B2:501:GTP:O6	2.44	0.51
1:B5:345:ILE:HG23	1:B5:348:ASN:OD1	2.11	0.51
3:A:3724:PHE:O	3:A:3727:ASP:N	2.43	0.51
3:A:4101:TYR:O	3:A:4105:GLU:N	2.44	0.51
3:A:4284:GLY:O	3:A:4290:ASN:N	2.43	0.51
4:B:3876:LYS:HA	4:B:3882:GLN:HA	1.92	0.51
5:C:781:LEU:HB3	5:C:867:ILE:HD11	1.92	0.51
5:C:4398:LEU:O	5:C:4423:LEU:CB	2.59	0.51
13:L:31:LEU:HD12	13:L:40:ILE:HD13	1.93	0.51
1:A1:8:GLN:CD	1:A1:17:GLY:HA3	2.30	0.51
1:B1:236:ILE:HG23	1:B1:237:THR:HG23	1.92	0.51
1:B7:199:CYS:HB3	1:B7:265:PHE:HD1	1.75	0.51
1:B7:292:GLN:HG2	1:B7:298:ASN:ND2	2.25	0.51
1:B7:334:GLN:HE22	1:B7:347:ASN:N	2.08	0.51
3:A:2319:ASN:N	3:A:2324:LYS:O	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4484:LEU:N	4:B:4506:CYS:O	2.44	0.51
1:B1:328:GLU:HA	1:B1:331:LEU:HG	1.91	0.51
1:B3:186:THR:HG23	1:B3:415:MET:HG3	1.91	0.51
2:B4:383:ALA:O	2:B4:386:GLU:HG2	2.11	0.51
3:A:2426:ASN:HA	3:A:2478:ASN:N	2.25	0.51
3:A:3739:ILE:O	3:A:3742:ARG:N	2.39	0.51
3:A:4017:PRO:HA	3:A:4021:ASP:H	1.75	0.51
1:A3:5:VAL:HG22	1:A3:133:PHE:HD1	1.75	0.51
3:A:1992:ILE:O	3:A:1997:LEU:N	2.44	0.51
3:A:3769:ASP:O	3:A:3772:ARG:N	2.32	0.51
4:B:327:THR:HG23	7:E:542:LEU:HD11	1.93	0.51
5:C:316:THR:OG1	5:C:317:GLU:OE1	2.28	0.51
5:C:785:SER:HB2	5:C:867:ILE:HA	1.93	0.51
16:X1:220:VAL:HG13	18:Y1:174:GLN:OE1	2.11	0.51
20:Z:82:CYS:HA	20:Z:85:ASP:HB2	1.93	0.51
2:A2:224:TYR:CE2	1:A3:246:LEU:HD11	2.45	0.51
1:A3:317:PHE:HE2	1:A3:326:VAL:HG13	1.76	0.51
2:A4:274:PRO:HB2	2:A4:276:ILE:HG23	1.93	0.51
2:A4:384:ILE:HD11	2:A4:432:PHE:CE1	2.45	0.51
1:B1:67:ASP:OD2	1:B1:72:THR:OG1	2.28	0.51
2:B2:11:GLN:NE2	2:B2:15:GLN:OE1	2.44	0.51
3:A:3350:ILE:O	3:A:3354:SER:N	2.44	0.51
3:A:3363:PRO:CB	3:A:3456:SER:HA	2.40	0.51
5:C:1507:SER:O	5:C:1510:LEU:N	2.43	0.51
1:A1:272:PRO:HD3	1:A1:364:SER:HA	1.92	0.51
1:A5:118:ASP:OD1	1:A5:122:LYS:NZ	2.44	0.51
2:B4:266:HIS:ND1	2:B4:266:HIS:O	2.43	0.51
1:B5:177:ASP:O	2:B6:352:LYS:HA	2.10	0.51
3:A:2040:ALA:O	3:A:2044:GLY:N	2.44	0.51
3:A:2696:PHE:N	3:A:2699:ALA:HB3	2.24	0.51
5:C:826:ARG:O	5:C:829:GLU:HB3	2.10	0.51
2:A2:398:MET:SD	1:A3:346:PRO:HD2	2.51	0.51
1:A3:409:THR:O	1:A3:412:GLU:HG3	2.11	0.51
1:A5:77:ARG:HE	1:A5:90:PHE:HE2	1.57	0.51
2:A6:240:ALA:O	2:A6:356:ASN:ND2	2.43	0.51
2:B2:381:SER:OG	2:B2:382:THR:N	2.43	0.51
2:B2:407:TRP:CG	1:B3:255:VAL:HG23	2.46	0.51
3:A:1908:SER:O	3:A:1910:GLN:N	2.42	0.51
3:A:2210:LEU:O	3:A:2214:PHE:N	2.44	0.51
3:A:2467:HIS:HA	3:A:2478:ASN:HA	1.93	0.51
4:B:4146:ALA:N	4:B:4266:GLY:HA3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:785:SER:O	5:C:785:SER:OG	2.28	0.51
2:A6:151:SER:O	2:A6:155:GLU:HG3	2.12	0.50
1:A7:236:ILE:HD11	1:A7:368:ILE:HD11	1.91	0.50
1:A7:272:PRO:HD3	1:A7:364:SER:HA	1.93	0.50
2:B6:317:LEU:HB3	2:B6:319:TYR:HE1	1.75	0.50
4:B:2042:VAL:HA	4:B:4196:GLY:HA3	1.92	0.50
5:C:1588:SER:O	5:C:1608:GLN:N	2.37	0.50
5:C:1679:GLU:O	5:C:1683:ALA:N	2.42	0.50
7:E:81:TRP:HE1	7:E:88:THR:HG1	1.58	0.50
12:J:48:PRO:HG3	12:J:88:VAL:HG11	1.93	0.50
1:A1:65:LEU:HD12	1:A1:90:PHE:CE1	2.45	0.50
2:A2:286:LEU:HD12	2:A2:371:VAL:HG23	1.94	0.50
2:A4:266:HIS:O	2:A4:266:HIS:ND1	2.43	0.50
2:B6:116:ASP:OD1	2:B6:117:LEU:N	2.44	0.50
4:B:813:ASN:O	4:B:816:LYS:HG2	2.11	0.50
4:B:2261:PHE:O	4:B:2265:ALA:HB3	2.10	0.50
5:C:791:GLU:OE2	5:C:813:GLN:NE2	2.45	0.50
20:Z:62:VAL:HG11	20:Z:94:LEU:HB3	1.93	0.50
1:B1:144:GLY:N	23:B1:501:GDP:O1B	2.38	0.50
2:B2:66:ILE:O	2:B2:66:ILE:HG13	2.11	0.50
1:B3:212:PHE:CZ	2:B4:326:LYS:HE2	2.47	0.50
2:B4:167:LEU:HD22	2:B4:200:VAL:HB	1.94	0.50
3:A:3922:PRO:O	3:A:3925:ALA:HB3	2.11	0.50
4:B:2583:ARG:HA	4:B:2635:GLU:N	2.26	0.50
6:D:544:ASP:N	6:D:544:ASP:OD1	2.43	0.50
7:E:272:LEU:HD11	7:E:291:TRP:HZ3	1.75	0.50
1:A1:91:VAL:HG11	1:A1:116:VAL:HB	1.93	0.50
1:A3:2:ARG:HB3	1:A3:131:GLN:HB2	1.92	0.50
1:A3:8:GLN:CD	1:A3:17:GLY:HA3	2.31	0.50
2:A6:76:ASP:OD1	2:A6:79:ARG:NH2	2.44	0.50
1:A7:3:GLU:OE1	1:A7:127:CYS:HB2	2.11	0.50
1:A7:27:GLU:OE2	1:A7:318:ARG:NH2	2.44	0.50
1:B1:36:TYR:CZ	1:B1:44:LEU:HD21	2.47	0.50
1:B3:121:ARG:NH1	1:B3:158:GLU:OE2	2.44	0.50
1:B3:128:ASP:OD1	1:B3:129:CYS:N	2.41	0.50
3:A:1938:VAL:O	3:A:1942:VAL:N	2.40	0.50
3:A:2555:VAL:HA	3:A:2558:THR:CB	2.41	0.50
3:A:2585:SER:HA	3:A:2664:TYR:CB	2.41	0.50
4:B:4093:LEU:O	4:B:4097:LEU:CB	2.59	0.50
6:D:499:GLY:HA2	6:D:521:LEU:O	2.11	0.50
7:E:245:ASP:OD1	7:E:246:VAL:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:313:ALA:O	1:A1:349:VAL:HA	2.12	0.50
2:A2:339:ARG:NH1	2:A2:339:ARG:HB2	2.26	0.50
1:A3:189:VAL:HG11	1:A3:378:PHE:HE1	1.76	0.50
3:A:1568:GLN:N	3:A:1689:GLY:O	2.45	0.50
3:A:2020:VAL:O	3:A:2151:ILE:HA	2.12	0.50
5:C:239:TRP:HZ3	5:C:290:SER:HA	1.77	0.50
5:C:580:TRP:HZ3	5:C:623:PHE:HE2	1.58	0.50
6:D:539:ALA:HB1	6:D:567:ILE:HG21	1.92	0.50
11:I:55:LYS:NZ	13:K:32:GLU:O	2.45	0.50
16:X1:178:ILE:HD12	18:Y1:131:ARG:HG2	1.94	0.50
20:Z:104:ASP:O	20:Z:105:LYS:HD3	2.11	0.50
1:A1:334:GLN:HA	1:A1:341:PHE:CE2	2.47	0.50
1:A5:337:ASN:HB3	1:A5:340:TYR:CD2	2.47	0.50
2:A6:21:TRP:HZ2	2:A6:65:CYS:HB3	1.77	0.50
2:A6:137:VAL:HG22	2:A6:168:GLY:HA2	1.94	0.50
1:A7:215:LEU:HB3	1:A7:217:LEU:HG	1.93	0.50
2:B4:98:ASP:OD1	2:B4:99:ALA:N	2.44	0.50
1:B5:342:VAL:HG12	1:B5:345:ILE:HG22	1.94	0.50
2:B6:129:CYS:SG	2:B6:132:LEU:HB2	2.52	0.50
4:B:3768:GLY:HA3	4:B:3804:THR:HA	1.92	0.50
5:C:1592:VAL:HA	5:C:1605:MET:HA	1.93	0.50
16:X1:191:GLU:O	16:X1:194:GLU:HG3	2.11	0.50
2:A6:60:LYS:HD2	2:B6:282:TYR:CE2	2.47	0.50
1:A7:11:GLN:HG3	1:A7:15:GLN:HE22	1.76	0.50
4:B:3528:ILE:O	4:B:3532:GLU:N	2.39	0.50
13:M:25:ASP:HA	13:M:28:THR:HG22	1.93	0.50
16:X:240:HIS:O	16:X:243:GLU:HG3	2.11	0.50
1:A1:26:ASP:OD1	1:A1:359:LYS:NZ	2.44	0.50
1:A3:156:ARG:NH1	1:A3:195:ASN:O	2.44	0.50
1:A5:246:LEU:HD22	1:A5:352:SER:HA	1.94	0.50
1:B3:3:GLU:HG3	1:B3:127:CYS:HB2	1.94	0.50
3:A:1745:PHE:HA	3:A:2137:PRO:HA	1.93	0.50
4:B:507:ARG:HD3	6:D:509:SER:HB3	1.94	0.50
5:C:669:ARG:HH12	5:C:692:GLU:HG3	1.77	0.50
7:E:169:TRP:NE1	7:E:460:GLN:OE1	2.44	0.50
1:A1:21:TRP:HA	1:A1:24:VAL:HG22	1.93	0.50
2:A2:151:SER:O	2:A2:155:GLU:HG3	2.11	0.50
2:A6:21:TRP:CZ2	2:A6:65:CYS:HB3	2.47	0.50
2:A6:139:ASN:OD1	2:A6:170:THR:HG22	2.12	0.50
2:A6:183:GLU:HG2	2:A6:184:PRO:HD3	1.94	0.50
1:A7:211:CYS:HA	1:A7:215:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:267:PHE:HB2	2:B2:384:ILE:HD12	1.94	0.50
1:B3:179:VAL:H	2:B4:258:ASN:ND2	2.10	0.50
3:A:2316:TYR:HA	3:A:2328:TRP:H	1.77	0.50
3:A:2347:PHE:CB	3:A:2383:LEU:HA	2.42	0.50
3:A:3326:ASP:O	3:A:3330:VAL:N	2.37	0.50
4:B:525:THR:O	4:B:529:LEU:CB	2.60	0.50
4:B:3083:PHE:O	4:B:3087:PHE:N	2.30	0.50
4:B:4138:PHE:C	4:B:4151:GLY:H	2.16	0.50
5:C:578:ILE:HD11	5:C:627:TRP:HB2	1.93	0.50
6:D:542:ARG:NH1	6:D:544:ASP:OD2	2.45	0.50
2:A4:326:LYS:HG3	2:A4:327:ASP:N	2.26	0.49
2:A4:384:ILE:O	2:A4:387:ILE:HG22	2.12	0.49
1:B1:378:PHE:HB3	1:B1:415:MET:HE3	1.94	0.49
2:B4:251:ASP:H	2:B4:254:GLU:HG3	1.77	0.49
2:B6:425:LEU:O	2:B6:429:GLU:HG2	2.13	0.49
3:A:1651:GLN:C	3:A:1653:ASP:H	2.15	0.49
3:A:2036:VAL:O	3:A:2040:ALA:HB3	2.12	0.49
3:A:2561:LYS:HA	3:A:2568:TYR:O	2.12	0.49
3:A:2720:VAL:C	3:A:2877:PHE:H	2.15	0.49
3:A:3536:VAL:O	3:A:3540:GLU:N	2.28	0.49
4:B:2474:TYR:O	4:B:2483:VAL:N	2.44	0.49
2:A4:200:VAL:HG13	2:A4:268:MET:CE	2.42	0.49
2:A4:276:ILE:HD11	2:A4:371:VAL:HG22	1.94	0.49
1:B3:39:ASP:N	1:B3:39:ASP:OD1	2.45	0.49
1:B5:330:MET:SD	1:B5:349:VAL:HG11	2.53	0.49
4:B:380:LEU:O	4:B:383:THR:OG1	2.25	0.49
4:B:520:THR:HG22	4:B:521:THR:HG23	1.93	0.49
6:D:597:ASN:OD1	6:D:598:LYS:N	2.44	0.49
7:E:280:CYS:SG	7:E:292:TRP:HB2	2.51	0.49
18:Y:234:ILE:O	18:Y:238:LYS:HG2	2.12	0.49
1:A1:200:MET:SD	1:A1:268:VAL:HG11	2.52	0.49
1:A3:121:ARG:HH11	18:Y1:141:LYS:HZ2	1.60	0.49
1:A3:211:CYS:HA	1:A3:215:LEU:HB2	1.94	0.49
1:A5:257:LEU:HD21	1:A5:314:SER:HB2	1.93	0.49
1:A7:2:ARG:HH21	1:A7:240:LEU:HA	1.77	0.49
2:B4:21:TRP:CZ2	2:B4:65:CYS:HB3	2.47	0.49
1:B5:31:ASP:OD2	1:B5:35:THR:OG1	2.30	0.49
4:B:264:LYS:HA	4:B:267:GLU:HB2	1.94	0.49
16:X:248:LYS:O	16:X:252:GLU:OE1	2.30	0.49
19:Y0:275:UNK:O	19:Y0:279:UNK:CB	2.61	0.49
18:Y1:96:MET:O	18:Y1:99:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:137:HIS:NE2	1:A1:166:THR:OG1	2.45	0.49
2:A4:223:THR:HG23	2:A4:225:THR:H	1.77	0.49
2:A4:251:ASP:H	2:A4:254:GLU:HG3	1.78	0.49
2:A6:9:ILE:HG13	2:A6:139:ASN:HB3	1.92	0.49
1:B1:285:THR:HG23	1:B1:288:GLU:H	1.76	0.49
2:B4:384:ILE:O	2:B4:387:ILE:HG12	2.12	0.49
1:B5:113:ILE:HA	1:B5:116:VAL:HG22	1.94	0.49
3:A:2518:LEU:O	3:A:2523:GLY:N	2.32	0.49
4:B:499:VAL:O	4:B:503:GLU:HB2	2.12	0.49
4:B:2041:PRO:O	4:B:4196:GLY:HA3	2.12	0.49
5:C:671:ALA:O	5:C:675:GLN:NE2	2.44	0.49
20:Z:157:LEU:O	20:Z:161:GLN:HG2	2.12	0.49
2:A2:11:GLN:HG3	2:A2:74:VAL:HG21	1.93	0.49
1:A3:203:ASP:OD1	1:A3:301:CYS:HA	2.13	0.49
1:A3:337:ASN:HB3	1:A3:340:TYR:HD2	1.77	0.49
1:A3:385:PHE:HZ	1:A3:408:PHE:HD1	1.59	0.49
1:A7:49:VAL:HG11	1:A7:241:ARG:HG2	1.94	0.49
1:B1:121:ARG:NH2	1:B1:158:GLU:OE2	2.43	0.49
1:B1:260:PHE:HB2	1:B1:263:LEU:HD23	1.95	0.49
1:B1:271:THR:OG1	1:B1:365:ALA:HB3	2.13	0.49
1:B5:252:LYS:HG2	1:B5:350:LYS:HE2	1.93	0.49
1:B7:100:ASN:HD21	1:B7:102:ALA:HB3	1.78	0.49
3:A:1718:ALA:O	3:A:1865:PRO:HA	2.12	0.49
4:B:522:ILE:O	4:B:556:TYR:OH	2.25	0.49
4:B:3878:LEU:O	4:B:3882:GLN:N	2.46	0.49
20:Z:49:LYS:H	20:Z:146:LYS:NZ	2.11	0.49
2:A4:371:VAL:HG12	2:A4:373:ARG:H	1.78	0.49
3:A:3375:GLU:O	3:A:3378:ASN:N	2.43	0.49
3:A:3916:GLY:H	3:A:3920:GLU:CB	2.25	0.49
3:A:4153:ALA:HB3	3:A:4156:PHE:CB	2.42	0.49
5:C:1273:TRP:CB	5:C:1352:ASP:H	2.25	0.49
5:C:2518:GLY:O	5:C:2533:ILE:N	2.41	0.49
7:E:287:GLY:O	7:E:289:VAL:N	2.41	0.49
11:I:24:ILE:HD11	11:I:42:THR:HG23	1.94	0.49
15:P:51:LYS:HA	15:P:54:GLN:HB2	1.94	0.49
1:A1:257:LEU:HB3	1:A1:266:PHE:HE2	1.77	0.49
2:A6:362:VAL:HG12	2:A6:368:LEU:HD12	1.93	0.49
1:A7:70:PRO:HD3	1:A7:92:PHE:HZ	1.77	0.49
2:B2:312:TYR:HD1	2:B2:381:SER:HB2	1.78	0.49
1:B3:208:TYR:CD1	2:B4:326:LYS:HD3	2.48	0.49
2:B6:119:LEU:HA	2:B6:122:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2346:VAL:HA	3:A:2386:GLY:CA	2.42	0.49
4:B:166:MET:HG2	4:B:167:LYS:HD3	1.93	0.49
4:B:4139:GLY:N	4:B:4149:GLY:O	2.45	0.49
5:C:959:LYS:HE2	9:G:158:LEU:HA	1.94	0.49
7:E:162:ARG:NH1	7:E:194:MET:SD	2.83	0.49
13:M:40:ILE:HB	13:M:60:VAL:HG11	1.94	0.49
2:A2:88:HIS:CD2	2:A2:89:PRO:HD2	2.48	0.49
1:A5:237:THR:O	1:A5:237:THR:HG22	2.13	0.49
2:B4:91:GLN:HA	2:B4:121:ARG:NH2	2.27	0.49
2:B6:174:SER:HB3	2:B6:177:VAL:O	2.13	0.49
2:B6:183:GLU:HG3	2:B6:184:PRO:HD3	1.94	0.49
3:A:2275:ILE:O	3:A:2279:GLY:N	2.35	0.49
3:A:2448:ASP:H	3:A:2451:GLU:HA	1.77	0.49
4:B:515:ALA:HB1	4:B:528:LEU:HD21	1.94	0.49
4:B:4135:ARG:O	4:B:4151:GLY:HA3	2.13	0.49
5:C:358:LYS:NZ	5:C:475:ASP:OD1	2.40	0.49
5:C:3929:ALA:O	5:C:3933:MET:N	2.31	0.49
20:Z:27:ASP:HA	20:Z:38:GLU:OE1	2.13	0.49
1:A1:103:LYS:HA	1:A1:107:THR:HB	1.94	0.49
2:A6:20:CYS:O	2:A6:24:TYR:HD1	1.95	0.49
1:B1:334:GLN:HA	1:B1:341:PHE:CE2	2.48	0.49
2:B4:407:TRP:CG	1:B5:255:VAL:HG23	2.48	0.49
1:B5:100:ASN:HD22	1:B5:103:LYS:H	1.59	0.49
2:B6:172:TYR:CD1	2:B6:203:MET:HG3	2.48	0.49
2:B6:323:VAL:HG23	2:B6:355:ILE:HG23	1.94	0.49
3:A:1388:ALA:HB2	3:A:1438:ALA:HB3	1.95	0.49
4:B:323:PRO:HA	4:B:326:HIS:ND1	2.28	0.49
4:B:625:ASP:O	4:B:629:GLU:HB2	2.12	0.49
5:C:4400:LEU:O	5:C:4421:ASN:CB	2.60	0.49
11:I:75:ARG:HG2	11:I:80:GLU:HG3	1.95	0.49
18:Y:237:ASP:O	18:Y:240:GLU:HG3	2.13	0.49
1:A1:167:PHE:CZ	1:A1:233:MET:HG3	2.48	0.49
2:A6:234:VAL:HG13	2:A6:376:CYS:SG	2.52	0.49
1:A7:36:TYR:CZ	1:A7:44:LEU:HD21	2.48	0.49
2:B2:327:ASP:N	2:B2:327:ASP:OD1	2.45	0.49
1:B5:141:GLY:O	1:B5:145:SER:HB3	2.13	0.49
1:B7:49:VAL:HG11	1:B7:241:ARG:HG2	1.94	0.49
1:B7:270:PHE:HD2	1:B7:273:LEU:HD21	1.78	0.49
3:A:238:ILE:HA	3:A:261:LYS:HA	1.95	0.49
3:A:1930:LEU:O	3:A:1934:GLU:N	2.46	0.49
4:B:4211:LEU:O	4:B:4215:VAL:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:361:ILE:HG12	5:C:378:ASN:HB3	1.95	0.49
5:C:1580:HIS:O	5:C:1584:GLY:N	2.46	0.49
7:E:236:GLN:OE1	7:E:240:GLN:HB2	2.13	0.49
7:E:384:TRP:HA	7:E:409:LEU:HB2	1.95	0.49
1:A5:7:ILE:HB	1:A5:135:VAL:HG22	1.95	0.48
1:A5:272:PRO:HD3	1:A5:364:SER:HA	1.94	0.48
2:A6:185:TYR:HA	2:A6:395:PHE:CE2	2.48	0.48
3:A:1931:LEU:O	3:A:1935:ALA:HA	2.13	0.48
3:A:2280:GLY:O	3:A:2509:ALA:N	2.34	0.48
3:A:2282:LEU:O	3:A:2509:ALA:HB3	2.13	0.48
3:A:4267:MET:O	3:A:4271:LEU:N	2.27	0.48
4:B:566:LEU:HD11	7:E:407:THR:H	1.77	0.48
4:B:812:LEU:HA	4:B:815:ILE:HG22	1.95	0.48
4:B:2624:GLY:HA3	4:B:2635:GLU:HA	1.95	0.48
5:C:931:THR:HA	5:C:934:LYS:HZ3	1.76	0.48
7:E:272:LEU:HD11	7:E:291:TRP:CZ3	2.47	0.48
18:Y1:82:MET:SD	18:Y1:83:LEU:HD12	2.52	0.48
2:A2:7:ILE:HG13	2:A2:66:ILE:HG13	1.94	0.48
1:A3:22:GLU:HG3	1:A3:81:TYR:CD2	2.48	0.48
1:A3:313:ALA:HB3	1:A3:349:VAL:HG22	1.95	0.48
2:A4:16:VAL:HA	2:A4:228:ASN:HD22	1.78	0.48
2:B2:272:TYR:HB3	2:B2:275:ILE:HD11	1.95	0.48
1:B3:144:GLY:N	23:B3:502:GDP:O1B	2.38	0.48
1:B5:152:ILE:HG22	1:B5:195:ASN:HB3	1.95	0.48
2:B6:298:PRO:HB3	2:B6:307:PRO:HD2	1.96	0.48
1:B7:114:ASP:N	1:B7:114:ASP:OD1	2.45	0.48
3:A:1808:LEU:H	3:A:1824:SER:CB	2.26	0.48
3:A:2610:ASP:CB	3:A:2875:ASP:HA	2.44	0.48
3:A:3935:GLY:H	3:A:3967:PHE:HA	1.77	0.48
4:B:563:VAL:HG13	4:B:593:LEU:HD22	1.95	0.48
4:B:4358:ASP:O	4:B:4362:LYS:N	2.45	0.48
5:C:782:GLY:O	5:C:786:SER:OG	2.31	0.48
5:C:1658:ASP:O	5:C:1662:GLY:N	2.25	0.48
5:C:4052:ASN:O	5:C:4453:ARG:HA	2.12	0.48
1:A5:2:ARG:HH21	1:A5:240:LEU:HA	1.78	0.48
1:A5:3:GLU:OE1	1:A5:127:CYS:HB2	2.14	0.48
1:A5:67:ASP:OD1	1:A5:68:LEU:N	2.43	0.48
1:A5:139:LEU:HD12	1:A5:170:VAL:HG12	1.94	0.48
2:A6:70:LEU:HG	2:A6:145:THR:HG22	1.94	0.48
2:A6:121:ARG:NH1	2:A6:124:LYS:HE2	2.28	0.48
1:B1:117:LEU:HD11	1:B1:154:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:129:CYS:SG	2:B2:130:THR:N	2.85	0.48
4:B:4456:VAL:N	4:B:4516:VAL:O	2.32	0.48
5:C:224:ILE:HD13	5:C:238:TYR:CZ	2.49	0.48
5:C:789:LEU:N	5:C:875:LEU:HD21	2.28	0.48
5:C:1019:ALA:HA	5:C:1022:THR:HG22	1.94	0.48
5:C:3750:LEU:O	5:C:3752:SER:N	2.46	0.48
7:E:381:ILE:HD11	7:E:424:THR:HA	1.94	0.48
9:G:99:THR:O	9:G:103:PHE:HB3	2.14	0.48
13:N:79:TYR:HA	13:N:84:ALA:HA	1.95	0.48
2:A2:132:LEU:HD23	2:A2:164:LYS:HD3	1.95	0.48
2:A6:123:ARG:NH1	2:A6:161:TYR:OH	2.46	0.48
1:B5:166:THR:OG1	1:B5:199:CYS:SG	2.52	0.48
3:A:2425:ILE:O	3:A:2477:LYS:HA	2.13	0.48
3:A:2437:TYR:N	3:A:2483:GLN:O	2.45	0.48
3:A:3395:GLU:HA	3:A:3398:ILE:CB	2.44	0.48
4:B:134:PRO:HA	4:B:137:GLN:HE21	1.77	0.48
4:B:816:LYS:O	4:B:820:LYS:HG2	2.14	0.48
5:C:864:TYR:O	5:C:867:ILE:HB	2.13	0.48
7:E:247:ARG:HH21	7:E:248:LYS:HZ1	1.61	0.48
18:Y:196:ASN:O	18:Y:200:GLU:HG2	2.13	0.48
18:Y1:78:ASP:OD1	18:Y1:79:GLU:N	2.46	0.48
2:A4:9:ILE:HD11	2:A4:139:ASN:HB3	1.96	0.48
1:A5:173:PRO:O	1:A5:176:SER:OG	2.29	0.48
1:B3:317:PHE:HB3	1:B3:321:MET:SD	2.53	0.48
2:B6:345:ASP:N	2:B6:345:ASP:OD1	2.47	0.48
1:B7:8:GLN:O	1:B7:66:MET:HG3	2.12	0.48
1:B7:139:LEU:HD22	1:B7:188:SER:HB3	1.95	0.48
3:A:1636:HIS:CB	3:A:1696:ILE:H	2.27	0.48
3:A:1642:LEU:O	3:A:1646:GLU:N	2.47	0.48
5:C:583:GLN:NE2	6:D:543:LEU:HD13	2.28	0.48
6:D:368:PHE:CD1	6:D:376:LEU:HD13	2.49	0.48
11:I:40:ASP:HA	11:I:43:VAL:HG22	1.96	0.48
16:X1:193:VAL:O	16:X1:196:GLU:HG2	2.12	0.48
1:B1:259:PRO:HG3	1:B1:311:LEU:HD23	1.95	0.48
2:B2:250:VAL:HG23	2:B2:254:GLU:HG3	1.95	0.48
2:B4:91:GLN:HG2	2:B4:121:ARG:HH12	1.79	0.48
4:B:296:LYS:NZ	7:E:549:THR:O	2.44	0.48
4:B:506:ARG:NH2	4:B:540:VAL:HG12	2.27	0.48
5:C:2982:LYS:O	5:C:2985:LYS:N	2.39	0.48
7:E:324:THR:HG22	7:E:376:LYS:HD3	1.95	0.48
11:I:75:ARG:NH1	11:I:76:SER:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:232:THR:O	18:Y:236:GLU:HG2	2.13	0.48
1:A1:54:ALA:HB3	1:A1:58:ARG:HB3	1.96	0.48
2:B6:403:ALA:HB2	1:B7:344:TRP:HZ3	1.79	0.48
3:A:2554:ARG:O	3:A:2558:THR:N	2.44	0.48
4:B:678:PRO:N	7:E:188:GLN:HE22	2.12	0.48
5:C:876:GLN:HG3	5:C:960:ALA:HB1	1.95	0.48
5:C:2594:VAL:HA	5:C:2662:ALA:HA	1.96	0.48
16:X1:156:GLN:O	16:X1:160:THR:HG23	2.14	0.48
2:A2:137:VAL:HG22	2:A2:168:GLY:HA2	1.95	0.48
2:A2:317:LEU:HB3	2:A2:319:TYR:CE1	2.47	0.48
1:A3:414:ASN:O	1:A3:418:LEU:HD23	2.14	0.48
1:A3:421:GLU:O	1:A3:424:GLN:HG2	2.13	0.48
2:A6:287:SER:OG	2:A6:288:VAL:N	2.47	0.48
2:B2:72:PRO:HD2	1:B3:2:ARG:NH1	2.29	0.48
1:B5:8:GLN:OE1	1:B5:17:GLY:HA3	2.13	0.48
4:B:385:ARG:HH12	4:B:428:CYS:HB2	1.77	0.48
4:B:633:GLU:O	4:B:636:THR:OG1	2.29	0.48
4:B:1707:SER:N	4:B:1711:GLU:O	2.39	0.48
4:B:4531:VAL:N	4:B:4543:PHE:O	2.46	0.48
5:C:675:GLN:OE1	5:C:675:GLN:N	2.46	0.48
6:D:509:SER:O	6:D:509:SER:OG	2.31	0.48
13:M:58:CYS:HB2	13:M:87:LEU:HD13	1.95	0.48
16:X1:255:LEU:HD11	18:Y1:205:ALA:HB1	1.95	0.48
1:B1:31:ASP:OD1	1:B1:35:THR:N	2.28	0.48
1:B1:220:PRO:HD2	2:B2:326:LYS:HE2	1.96	0.48
2:B4:388:PHE:HB2	2:B4:429:GLU:OE2	2.14	0.48
1:B5:153:SER:O	1:B5:157:GLU:HG2	2.14	0.48
3:A:75:ALA:HB1	3:A:92:GLY:HA3	1.95	0.48
3:A:3615:ALA:HB3	3:A:3618:GLY:O	2.14	0.48
3:A:3699:ALA:O	3:A:3703:ARG:N	2.40	0.48
4:B:2849:MET:O	4:B:2884:GLY:HA2	2.12	0.48
5:C:696:LYS:HA	5:C:696:LYS:HD2	1.69	0.48
15:P:45:TYR:CD2	15:P:51:LYS:HG3	2.49	0.48
2:A6:237:SER:HA	2:A6:320:ARG:HD2	1.96	0.48
2:B2:170:THR:HG21	2:B2:194:LEU:HD21	1.96	0.48
2:B2:246:GLY:HA2	2:B2:357:TYR:CD2	2.49	0.48
2:B2:288:VAL:HG13	2:B2:319:TYR:CE2	2.45	0.48
2:B2:377:MET:SD	2:B2:379:SER:HB3	2.54	0.48
2:B4:241:SER:OG	2:B4:250:VAL:O	2.20	0.48
3:A:1947:LEU:O	3:A:1951:ASN:N	2.33	0.48
3:A:4335:ARG:HA	3:A:4357:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1916:ALA:HB3	4:B:2041:PRO:HA	1.96	0.48
6:D:428:PHE:O	6:D:439:LEU:HD12	2.14	0.48
6:D:537:LEU:HD23	6:D:572:TRP:CE2	2.49	0.48
9:G:152:ASP:OD1	9:G:153:GLU:N	2.46	0.48
20:Z:4:ALA:O	20:Z:7:ARG:HG2	2.14	0.48
1:A5:8:GLN:CD	1:A5:17:GLY:HA3	2.34	0.47
2:A6:141:VAL:HG22	2:A6:172:TYR:HA	1.95	0.47
1:B5:134:GLN:HE21	1:B5:167:PHE:HE2	1.62	0.47
1:B5:268:VAL:HG23	1:B5:300:MET:HB2	1.96	0.47
1:B7:7:ILE:HG12	1:B7:64:ILE:HD11	1.96	0.47
3:A:3622:GLY:HA2	3:A:3696:ALA:HB2	1.94	0.47
3:A:4260:ALA:O	3:A:4343:THR:HA	2.14	0.47
4:B:254:LEU:HD12	4:B:255:THR:HG23	1.95	0.47
5:C:1060:GLN:HA	5:C:1063:HIS:HB3	1.95	0.47
7:E:154:PHE:CZ	7:E:203:VAL:HG22	2.49	0.47
16:X:244:MET:HG3	18:Y:199:PHE:CE1	2.47	0.47
1:A3:317:PHE:HB3	1:A3:321:MET:SD	2.54	0.47
1:B3:208:TYR:CE1	1:B3:225:LEU:HD11	2.49	0.47
2:B4:307:PRO:HA	2:B4:383:ALA:HB2	1.96	0.47
1:B5:309:ARG:H	1:B5:372:THR:CG2	2.27	0.47
4:B:687:THR:O	4:B:691:LEU:HB3	2.13	0.47
4:B:1970:PHE:N	4:B:2018:PHE:O	2.35	0.47
4:B:4525:ASP:O	4:B:4549:SER:N	2.41	0.47
5:C:226:ASP:O	5:C:230:ARG:NH1	2.47	0.47
5:C:1028:ASN:HD21	5:C:1048:LYS:HE3	1.79	0.47
13:K:57:HIS:HB2	13:K:88:PHE:CE1	2.49	0.47
1:A1:178:THR:OG1	1:A1:181:GLU:HG3	2.14	0.47
1:A3:238:CYS:SG	1:A3:318:ARG:NE	2.87	0.47
1:A3:364:SER:OG	1:A3:365:ALA:N	2.47	0.47
1:A5:179:VAL:HG11	2:A6:258:ASN:HA	1.97	0.47
2:A6:361:THR:HA	2:A6:370:LYS:NZ	2.30	0.47
1:A7:282:ARG:HH12	1:A7:284:LEU:HD13	1.79	0.47
1:A7:309:ARG:H	1:A7:372:THR:CG2	2.27	0.47
2:B4:287:SER:OG	2:B4:288:VAL:N	2.45	0.47
3:A:1677:CYS:CA	3:A:1679:ALA:H	2.27	0.47
4:B:234:LEU:HD13	4:B:237:LEU:HD22	1.95	0.47
4:B:822:THR:HA	4:B:825:ILE:HD12	1.95	0.47
7:E:231:LEU:HA	7:E:244:PHE:O	2.15	0.47
16:X1:230:SER:HB3	18:Y1:184:LEU:HD22	1.96	0.47
1:A7:169:VAL:HG21	1:A7:204:ASN:OD1	2.15	0.47
2:B4:203:MET:HE1	2:B4:267:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:5:VAL:HG22	1:B5:62:ARG:HD3	1.96	0.47
3:A:1375:PHE:CB	3:A:1389:THR:HA	2.45	0.47
3:A:1677:CYS:C	3:A:1679:ALA:H	2.18	0.47
3:A:3697:PRO:CB	3:A:3703:ARG:HA	2.45	0.47
4:B:326:HIS:O	4:B:329:MET:HG2	2.14	0.47
4:B:2610:GLN:O	4:B:2613:ILE:N	2.39	0.47
6:D:615:LYS:O	6:D:627:VAL:HA	2.14	0.47
16:X1:135:LYS:NZ	18:Y1:80:GLY:O	2.35	0.47
1:A1:214:THR:HG23	1:A1:297:LYS:NZ	2.30	0.47
1:B7:8:GLN:OE1	1:B7:14:ASN:HA	2.14	0.47
1:B7:150:LEU:O	1:B7:153:SER:OG	2.29	0.47
3:A:1710:ALA:O	3:A:1714:SER:N	2.48	0.47
3:A:2562:THR:HA	3:A:2566:PHE:HA	1.96	0.47
3:A:4053:GLY:HA2	3:A:4066:PHE:H	1.79	0.47
4:B:632:THR:HA	4:B:635:ARG:HG3	1.95	0.47
5:C:2609:TRP:O	5:C:2613:GLN:N	2.47	0.47
7:E:146:PRO:HB2	7:E:445:LEU:HD22	1.95	0.47
18:Y:228:ARG:HA	18:Y:231:THR:HG22	1.97	0.47
2:A4:176:GLN:HG2	2:A4:177:VAL:N	2.30	0.47
2:B4:213:CYS:HA	2:B4:217:LEU:HB2	1.97	0.47
2:B4:326:LYS:HD2	2:B4:326:LYS:HA	1.51	0.47
1:B5:3:GLU:HB2	1:B5:130:LEU:HA	1.96	0.47
1:B5:67:ASP:N	1:B5:67:ASP:OD1	2.48	0.47
2:B6:79:ARG:O	2:B6:84:ARG:HG3	2.15	0.47
2:B6:194:LEU:O	2:B6:198:THR:HG22	2.15	0.47
1:B7:210:ILE:O	1:B7:214:THR:OG1	2.29	0.47
3:A:189:PRO:HA	3:A:198:ASP:HA	1.97	0.47
3:A:1504:LEU:O	3:A:1517:PHE:N	2.47	0.47
4:B:544:ASP:O	4:B:547:LYS:NZ	2.37	0.47
4:B:2279:GLY:O	4:B:2319:ILE:HA	2.14	0.47
4:B:4051:VAL:HA	4:B:4054:ALA:HB2	1.94	0.47
5:C:1594:PHE:HA	5:C:1602:MET:HA	1.96	0.47
11:I:76:SER:OG	11:I:77:LYS:N	2.47	0.47
1:A1:8:GLN:NE2	1:A1:17:GLY:HA3	2.30	0.47
1:A1:392:LYS:HD2	1:A1:395:LEU:HD22	1.96	0.47
2:A2:296:PHE:HZ	2:A2:351:PHE:HE1	1.60	0.47
2:A6:50:ASN:O	2:A6:64:ARG:NH2	2.47	0.47
2:A6:198:THR:HG21	2:A6:201:ALA:HB2	1.96	0.47
1:A7:105:HIS:CD2	1:A7:150:LEU:HD12	2.49	0.47
2:B2:269:LEU:HD23	2:B2:301:MET:SD	2.55	0.47
1:B3:244:GLY:HA2	1:B3:355:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B3:417:ASP:O	1:B3:421:GLU:HG3	2.14	0.47
2:B4:379:SER:OG	2:B4:380:ASN:N	2.48	0.47
2:B6:9:ILE:HG22	2:B6:146:GLY:HA2	1.97	0.47
2:B6:250:VAL:HG11	2:B6:352:LYS:HE3	1.96	0.47
1:B7:100:ASN:ND2	1:B7:103:LYS:H	2.13	0.47
1:B7:178:THR:HG23	1:B7:181:GLU:HG3	1.95	0.47
3:A:1360:ILE:HA	3:A:1363:GLU:CB	2.45	0.47
3:A:2370:ILE:HA	3:A:2506:MET:O	2.14	0.47
3:A:2467:HIS:HA	3:A:2477:LYS:O	2.15	0.47
3:A:2531:LYS:HA	3:A:2534:SER:O	2.14	0.47
3:A:2666:GLU:H	3:A:2668:ALA:N	2.12	0.47
3:A:3385:MET:H	3:A:3408:ASN:CB	2.27	0.47
6:D:490:SER:OG	6:D:505:SER:OG	2.25	0.47
7:E:241:LEU:HD11	7:E:282:THR:HG21	1.96	0.47
7:E:306:LEU:O	7:E:313:THR:OG1	2.32	0.47
7:E:342:SER:HB3	7:E:356:TYR:HB2	1.97	0.47
13:L:59:ILE:HG22	13:M:66:SER:HB2	1.97	0.47
13:L:77:TYR:HD1	13:L:86:LEU:HD12	1.80	0.47
16:X:226:LEU:HA	16:X:229:ASP:OD2	2.14	0.47
1:A3:175:VAL:HG22	1:A3:205:GLU:HG3	1.97	0.47
1:A5:4:ILE:HD11	1:A5:250:LEU:HD11	1.96	0.47
1:A5:330:MET:SD	1:A5:349:VAL:HG11	2.55	0.47
2:A6:220:GLU:HG2	2:A6:221:ARG:HG3	1.97	0.47
2:B2:72:PRO:HG3	2:B2:95:GLY:O	2.13	0.47
2:B2:319:TYR:CZ	2:B2:328:VAL:HG23	2.50	0.47
1:B3:392:LYS:HD2	1:B3:395:LEU:HD22	1.97	0.47
2:B4:100:ALA:HA	1:B5:252:LYS:HE3	1.97	0.47
2:B6:306:ASP:HB3	2:B6:309:HIS:ND1	2.29	0.47
3:A:3392:GLN:O	3:A:3396:ARG:N	2.25	0.47
3:A:3797:ASP:O	3:A:3801:ASN:N	2.38	0.47
3:A:3956:LEU:CA	3:A:3960:ALA:H	2.28	0.47
1:A1:19:LYS:HD2	1:A1:22:GLU:OE1	2.15	0.47
1:A7:289:LEU:HD11	1:A7:363:MET:CE	2.45	0.47
1:B1:69:GLU:OE2	1:B1:96:GLY:HA3	2.15	0.47
1:B1:220:PRO:HD2	2:B2:326:LYS:CE	2.45	0.47
2:B2:222:PRO:O	1:B3:322:SER:OG	2.33	0.47
2:B6:76:ASP:HA	2:B6:79:ARG:HD2	1.97	0.47
3:A:1878:GLU:CA	3:A:1889:ALA:HB1	2.45	0.47
3:A:2067:ASN:HA	3:A:2114:GLY:HA3	1.97	0.47
3:A:2347:PHE:H	3:A:2386:GLY:HA3	1.79	0.47
5:C:322:LEU:HD21	5:C:349:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:4:ILE:HB	1:A5:50:TYR:HE1	1.80	0.47
1:A5:135:VAL:O	1:A5:166:THR:HA	2.15	0.47
1:B3:69:GLU:C	1:B3:92:PHE:HZ	2.18	0.47
2:B4:9:ILE:HG12	2:B4:68:LEU:HD21	1.96	0.47
3:A:2707:SER:N	3:A:2734:ALA:HB1	2.30	0.47
3:A:3322:LYS:HA	3:A:3325:VAL:O	2.15	0.47
3:A:3899:ASN:HA	3:A:3908:GLY:HA2	1.97	0.47
3:A:4260:ALA:HB1	3:A:4343:THR:C	2.36	0.47
5:C:790:VAL:HG22	5:C:875:LEU:HD22	1.97	0.47
6:D:186:THR:OG1	13:L:65:GLY:HA2	2.15	0.47
6:D:598:LYS:HG3	6:D:599:LEU:HD12	1.96	0.47
7:E:248:LYS:HD3	7:E:250:ASN:HD21	1.80	0.47
7:E:272:LEU:HD21	7:E:291:TRP:CZ3	2.49	0.47
13:L:58:CYS:O	13:M:66:SER:OG	2.25	0.47
16:X1:129:ARG:HG3	18:Y1:76:LEU:HD21	1.97	0.47
2:A2:31:GLN:HG2	2:A2:37:PRO:HD3	1.97	0.46
2:A4:81:GLY:O	2:A4:84:ARG:HG3	2.15	0.46
1:B1:309:ARG:H	1:B1:372:THR:CG2	2.28	0.46
1:B1:388:MET:HG2	2:B2:346:TRP:O	2.16	0.46
2:B6:28:HIS:CE1	2:B6:49:PHE:HA	2.49	0.46
2:B6:431:ASP:O	2:B6:434:GLU:HG3	2.15	0.46
1:B7:183:TYR:HA	1:B7:385:PHE:CE1	2.49	0.46
3:A:1578:TRP:HA	3:A:1600:TYR:CB	2.45	0.46
3:A:3770:LEU:HA	3:A:3771:SER:HA	1.53	0.46
3:A:4341:ALA:O	3:A:4344:ALA:HB3	2.14	0.46
4:B:742:GLN:O	4:B:746:ALA:N	2.47	0.46
4:B:2745:GLU:N	4:B:2822:TYR:O	2.48	0.46
5:C:2718:TYR:O	5:C:2745:SER:HA	2.15	0.46
16:X1:249:GLU:HA	16:X1:252:GLU:OE2	2.15	0.46
20:Z:59:ILE:HG13	20:Z:70:ILE:CD1	2.37	0.46
1:A1:291:GLN:OE1	1:A1:291:GLN:N	2.48	0.46
2:A2:121:ARG:NH1	2:A2:124:LYS:HD2	2.30	0.46
2:A2:402:ARG:NH1	20:Z:168:ARG:HH22	2.06	0.46
1:A5:213:ARG:O	1:A5:216:LYS:NZ	2.41	0.46
1:A7:94:GLN:OE1	1:A7:94:GLN:N	2.48	0.46
1:B1:178:THR:HG22	1:B1:181:GLU:HG3	1.97	0.46
2:B2:398:MET:HE2	1:B3:345:ILE:HG23	1.97	0.46
6:D:584:THR:OG1	6:D:585:ASP:N	2.47	0.46
7:E:294:LEU:O	7:E:296:LYS:N	2.47	0.46
7:E:426:LYS:HE3	7:E:430:ALA:HB3	1.97	0.46
13:L:77:TYR:CD1	13:L:86:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:60:VAL:HA	13:M:84:ALA:O	2.15	0.46
1:A1:102:ALA:HB1	1:A1:401:GLU:OE1	2.15	0.46
1:A3:54:ALA:HB3	1:A3:58:ARG:HB3	1.97	0.46
1:A3:67:ASP:OD2	1:A3:72:THR:OG1	2.30	0.46
1:A3:287:PRO:HG3	1:A3:329:GLN:NE2	2.29	0.46
2:A4:317:LEU:HB3	2:A4:319:TYR:CE1	2.44	0.46
2:A6:107:HIS:HB3	2:A6:108:TYR:CD2	2.50	0.46
2:A6:206:ASN:OD1	21:A7:501:GTP:N2	2.48	0.46
1:A7:242:PHE:CD1	1:A7:356:ILE:HG13	2.51	0.46
1:B1:134:GLN:HE21	1:B1:167:PHE:HE2	1.63	0.46
1:B7:74:ASP:N	1:B7:74:ASP:OD1	2.49	0.46
3:A:2639:ASP:O	3:A:2642:TYR:CB	2.63	0.46
4:B:115:PRO:HG2	4:B:116:LEU:HD12	1.97	0.46
5:C:449:ILE:HD13	5:C:523:PHE:HE1	1.80	0.46
5:C:551:LEU:HD11	5:C:613:TYR:HB2	1.96	0.46
5:C:1041:HIS:NE2	9:G:58:ASP:OD2	2.40	0.46
7:E:77:VAL:HG21	13:K:84:ALA:HB2	1.96	0.46
7:E:105:ASP:OD1	7:E:106:TYR:N	2.48	0.46
12:J:59:ARG:HG3	12:J:65:ASN:O	2.15	0.46
2:A2:98:ASP:OD1	2:A2:99:ALA:N	2.48	0.46
1:A3:186:THR:HG23	1:A3:187:LEU:HD12	1.97	0.46
2:A4:22:GLU:O	2:A4:26:LEU:HD23	2.16	0.46
2:A4:221:ARG:HG3	1:A5:325:GLU:OE2	2.16	0.46
1:A5:219:THR:HG23	2:A6:324:VAL:HG21	1.97	0.46
2:A6:316:CYS:SG	2:A6:352:LYS:HB3	2.55	0.46
2:B2:69:ASP:OD1	2:B2:70:LEU:N	2.44	0.46
3:A:4132:GLU:HA	3:A:4145:TRP:CB	2.45	0.46
3:A:4484:MET:O	3:A:4487:LYS:N	2.49	0.46
4:B:499:VAL:O	4:B:503:GLU:CB	2.64	0.46
4:B:2786:THR:O	4:B:2790:PHE:N	2.48	0.46
5:C:578:ILE:HD12	5:C:624:GLU:HA	1.97	0.46
5:C:3949:HIS:CB	5:C:3979:GLU:H	2.29	0.46
15:P:55:MET:O	15:P:59:GLN:HG2	2.15	0.46
1:A1:371:SER:OG	1:A1:372:THR:N	2.49	0.46
1:A5:208:TYR:HE1	1:A5:225:LEU:HD11	1.79	0.46
2:A6:266:HIS:O	2:A6:266:HIS:ND1	2.48	0.46
2:A6:336:LYS:HZ2	2:A6:343:PHE:HE2	1.64	0.46
1:B1:249:ASP:O	1:B1:253:LEU:HD13	2.15	0.46
1:B3:207:LEU:HB3	1:B3:225:LEU:HD22	1.97	0.46
3:A:36:CYS:HA	3:A:43:ALA:HA	1.98	0.46
3:A:1378:SER:O	3:A:1382:LYS:N	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4063:GLY:HA3	3:A:4189:ALA:HA	1.98	0.46
4:B:128:MET:SD	4:B:129:PRO:HD3	2.55	0.46
4:B:3925:PHE:O	4:B:3929:ARG:N	2.45	0.46
5:C:4446:LYS:HA	5:C:4480:ILE:O	2.15	0.46
7:E:152:THR:HG21	7:E:206:PRO:HG3	1.96	0.46
1:A3:390:ARG:O	1:A3:390:ARG:HD3	2.15	0.46
2:A4:344:VAL:HG23	2:A4:347:CYS:HB2	1.97	0.46
2:A6:213:CYS:HA	2:A6:217:LEU:HB2	1.97	0.46
1:B3:70:PRO:N	1:B3:92:PHE:HZ	2.13	0.46
3:A:1583:GLU:HA	3:A:1586:PHE:CB	2.46	0.46
3:A:4246:VAL:O	3:A:4248:LEU:N	2.48	0.46
4:B:274:TYR:HA	4:B:277:PHE:HD2	1.81	0.46
5:C:324:THR:HG22	5:C:327:ARG:HH22	1.81	0.46
5:C:581:ALA:HB2	5:C:623:PHE:HD2	1.81	0.46
5:C:4181:THR:O	5:C:4184:VAL:N	2.49	0.46
9:G:31:ASP:HB2	9:G:38:ILE:HD13	1.97	0.46
1:A1:100:ASN:OD1	2:A2:257:THR:HG21	2.16	0.46
1:A1:141:GLY:O	1:A1:145:SER:HB3	2.16	0.46
2:A6:5:ILE:HD11	2:A6:135:PHE:CE2	2.50	0.46
1:A7:286:VAL:HG12	1:A7:329:GLN:HG3	1.97	0.46
1:B1:113:ILE:HA	1:B1:116:VAL:HG22	1.96	0.46
2:B4:183:GLU:HG3	2:B4:184:PRO:HD3	1.98	0.46
1:B5:102:ALA:HB2	1:B5:403:MET:CE	2.45	0.46
1:B5:296:ALA:HB1	1:B5:304:ASP:OD1	2.15	0.46
2:B6:69:ASP:OD1	2:B6:69:ASP:N	2.47	0.46
1:B7:117:LEU:HA	1:B7:120:VAL:HG12	1.98	0.46
1:B7:165:LEU:HD23	1:B7:167:PHE:HZ	1.79	0.46
1:B7:317:PHE:HE2	1:B7:326:VAL:HG13	1.81	0.46
3:A:1829:ASP:C	3:A:1831:VAL:H	2.19	0.46
3:A:4324:THR:H	3:A:4327:ALA:HB3	1.80	0.46
3:A:4409:HIS:HA	3:A:4439:VAL:HA	1.98	0.46
4:B:122:ILE:HA	4:B:126:VAL:HG22	1.97	0.46
4:B:592:GLY:O	7:E:362:HIS:NE2	2.45	0.46
4:B:649:THR:O	4:B:652:GLU:HG3	2.15	0.46
5:C:239:TRP:HB3	5:C:294:VAL:HG22	1.97	0.46
2:A2:88:HIS:HD2	2:B2:283:HIS:HB2	1.80	0.46
2:A2:155:GLU:HG2	2:A2:197:HIS:NE2	2.31	0.46
1:A3:144:GLY:N	23:A3:502:GDP:O1B	2.49	0.46
2:A4:243:ARG:HH11	2:A4:243:ARG:HG3	1.80	0.46
2:A6:395:PHE:HD1	2:A6:422:ARG:HH11	1.62	0.46
1:B3:259:PRO:HG3	1:B3:311:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1379:GLU:O	3:A:1383:LYS:N	2.38	0.46
3:A:2375:GLY:O	3:A:2377:GLY:N	2.46	0.46
3:A:2438:PHE:HA	3:A:2485:VAL:H	1.81	0.46
3:A:2719:LEU:N	3:A:2849:PHE:O	2.47	0.46
4:B:517:ASP:OD1	4:B:517:ASP:N	2.48	0.46
4:B:1700:LYS:O	4:B:1721:CYS:N	2.42	0.46
4:B:2244:TYR:O	4:B:2253:LYS:N	2.26	0.46
4:B:4223:MET:O	4:B:4231:MET:N	2.49	0.46
5:C:564:GLU:OE1	5:C:564:GLU:N	2.49	0.46
5:C:1407:ASN:O	5:C:1409:GLY:N	2.49	0.46
7:E:155:LYS:NZ	7:E:159:ASN:O	2.48	0.46
13:L:39:ASP:N	13:L:39:ASP:OD1	2.47	0.46
13:M:24:VAL:HG22	13:M:78:PHE:HE1	1.81	0.46
16:X:255:LEU:HD13	18:Y:209:MET:SD	2.56	0.46
2:A2:223:THR:HG23	2:A2:225:THR:H	1.81	0.46
2:A4:422:ARG:NH2	2:A4:425:LEU:HD23	2.31	0.46
1:A5:114:ASP:N	1:A5:114:ASP:OD1	2.49	0.46
2:A6:27:GLU:HG3	2:A6:361:THR:HG21	1.97	0.46
2:A6:217:LEU:HB3	2:A6:219:ILE:HD12	1.97	0.46
2:A6:413:MET:HB3	2:A6:417:GLU:OE2	2.16	0.46
1:A7:113:ILE:HA	1:A7:116:VAL:HG12	1.98	0.46
1:B1:395:LEU:HD23	1:B1:395:LEU:HA	1.79	0.46
3:A:1991:THR:CB	3:A:2040:ALA:HB2	2.45	0.46
3:A:2651:ILE:H	3:A:2667:VAL:CB	2.29	0.46
13:M:59:ILE:O	13:M:85:ILE:HA	2.15	0.46
13:M:80:LEU:HD12	13:M:80:LEU:HA	1.81	0.46
20:Z:92:ARG:HG3	20:Z:92:ARG:HH21	1.81	0.46
1:A1:100:ASN:HB3	1:A1:103:LYS:HD3	1.97	0.46
1:A3:114:ASP:N	1:A3:114:ASP:OD1	2.48	0.46
2:A6:195:LEU:HD21	2:A6:264:ARG:NH1	2.31	0.46
1:A7:91:VAL:HG11	1:A7:116:VAL:HG23	1.97	0.46
1:B1:242:PHE:CD1	1:B1:356:ILE:HG13	2.50	0.46
2:B2:98:ASP:OD1	2:B2:99:ALA:N	2.48	0.46
2:B4:8:HIS:O	2:B4:68:LEU:HD23	2.16	0.46
3:A:2654:HIS:HA	3:A:2663:ALA:HA	1.97	0.46
3:A:2720:VAL:HA	3:A:2851:ALA:C	2.36	0.46
3:A:3537:ALA:O	3:A:3541:SER:CB	2.64	0.46
4:B:391:LYS:HA	4:B:391:LYS:HD2	1.80	0.46
4:B:570:TYR:OH	7:E:428:ASP:OD2	2.33	0.46
4:B:1596:ASN:O	4:B:1600:GLN:CB	2.64	0.46
4:B:1968:GLY:O	4:B:2017:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:149:LEU:O	5:C:152:THR:OG1	2.30	0.46
5:C:422:LEU:HB3	5:C:476:TYR:CG	2.51	0.46
7:E:414:TRP:HB3	7:E:415:SER:H	1.57	0.46
7:E:418:ARG:NH1	7:E:435:ASP:OD2	2.48	0.46
13:K:56:TRP:HA	13:K:88:PHE:O	2.15	0.46
20:Z:90:GLU:HB3	20:Z:91:PRO:HD2	1.97	0.46
1:A1:292:GLN:HG2	1:A1:298:ASN:ND2	2.30	0.45
1:A5:54:ALA:O	1:B5:283:ALA:HA	2.15	0.45
1:A5:112:LEU:O	1:A5:115:SER:OG	2.27	0.45
2:A6:316:CYS:HB2	2:A6:378:ILE:HG23	1.98	0.45
1:A7:315:ALA:HB1	1:A7:317:PHE:CE1	2.51	0.45
1:A7:377:MET:O	1:A7:381:VAL:HG22	2.16	0.45
1:B1:6:HIS:CD2	1:B1:8:GLN:HG2	2.51	0.45
1:B1:334:GLN:HE22	1:B1:348:ASN:H	1.64	0.45
2:B4:405:VAL:HG23	2:B4:418:PHE:CE2	2.50	0.45
3:A:4145:TRP:O	3:A:4147:ALA:N	2.49	0.45
4:B:525:THR:O	4:B:529:LEU:HB2	2.15	0.45
4:B:2403:LEU:O	4:B:2407:LEU:N	2.49	0.45
4:B:3986:ALA:O	4:B:3990:LYS:N	2.45	0.45
4:B:4409:HIS:O	4:B:4413:VAL:N	2.34	0.45
5:C:1441:SER:O	5:C:1445:ARG:N	2.49	0.45
5:C:1872:GLU:N	5:C:1921:MET:HA	2.30	0.45
6:D:266:MET:HG3	12:J:71:ARG:NH2	2.30	0.45
6:D:315:VAL:HG11	6:D:626:LEU:HD12	1.97	0.45
6:D:528:TRP:CH2	6:D:550:LEU:HD13	2.51	0.45
2:A2:183:GLU:HG3	2:A2:184:PRO:HD3	1.98	0.45
2:A2:265:ILE:HG12	2:A2:432:PHE:CE1	2.51	0.45
1:A3:191:GLN:HE21	1:A3:195:ASN:HD21	1.63	0.45
1:A7:60:VAL:HG11	1:A7:86:ARG:NH2	2.31	0.45
1:B5:11:GLN:HE21	1:B5:15:GLN:HE22	1.64	0.45
3:A:2644:LYS:C	3:A:2646:ASP:H	2.18	0.45
3:A:2878:GLN:O	3:A:2879:PRO:C	2.55	0.45
3:A:3589:SER:CB	3:A:4208:VAL:HA	2.46	0.45
4:B:164:GLY:O	4:B:168:GLY:N	2.49	0.45
4:B:4309:LYS:N	4:B:4417:ALA:O	2.49	0.45
5:C:261:VAL:HA	5:C:264:ILE:HD12	1.98	0.45
5:C:611:LYS:HA	5:C:611:LYS:HD2	1.70	0.45
5:C:789:LEU:HD23	5:C:875:LEU:HD11	1.98	0.45
9:G:104:VAL:HA	9:G:108:GLY:HA3	1.96	0.45
13:K:76:ILE:HB	13:K:87:LEU:HD23	1.98	0.45
2:A4:287:SER:N	2:A4:290:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:103:LYS:HA	1:A7:107:THR:HB	1.98	0.45
1:A7:262:ARG:HH21	1:A7:418:LEU:HB3	1.81	0.45
1:B1:232:VAL:HG11	1:B1:268:VAL:HG11	1.98	0.45
2:B2:88:HIS:ND1	2:B2:90:GLU:HG2	2.30	0.45
2:B4:66:ILE:HD12	2:B4:121:ARG:HE	1.81	0.45
2:B4:70:LEU:HD12	2:B4:99:ALA:HB2	1.97	0.45
2:B6:151:SER:HB2	2:B6:193:SER:OG	2.17	0.45
1:B7:152:ILE:HA	1:B7:155:ILE:HG22	1.98	0.45
3:A:2113:ASP:HA	3:A:2153:GLU:CB	2.47	0.45
4:B:1537:ASN:O	4:B:1539:MET:N	2.42	0.45
5:C:1681:GLN:O	5:C:1685:SER:N	2.48	0.45
5:C:4174:ASN:CB	5:C:4417:LYS:HA	2.46	0.45
6:D:489:GLU:OE1	6:D:506:LYS:NZ	2.45	0.45
6:D:562:ASP:OD1	6:D:563:LEU:N	2.49	0.45
6:D:573:ALA:HB1	6:D:575:LEU:HD23	1.98	0.45
7:E:164:ALA:HA	7:E:182:TYR:HA	1.98	0.45
7:E:241:LEU:HB2	7:E:256:THR:HB	1.99	0.45
7:E:323:ASP:HB3	7:E:327:GLY:HA2	1.97	0.45
2:A4:269:LEU:HD21	2:A4:384:ILE:HG22	1.98	0.45
2:A4:428:LEU:HD11	2:A4:432:PHE:HE2	1.82	0.45
2:A6:306:ASP:HB3	2:A6:309:HIS:ND1	2.32	0.45
1:B1:207:LEU:HB3	1:B1:225:LEU:HD22	1.98	0.45
2:B4:289:ALA:HA	2:B4:331:SER:OG	2.17	0.45
2:B6:246:GLY:HA2	2:B6:357:TYR:CD2	2.52	0.45
2:B6:305:CYS:HB3	2:B6:387:ILE:HD11	1.99	0.45
4:B:4027:VAL:O	4:B:4061:PHE:N	2.43	0.45
6:D:342:ILE:HD11	6:D:376:LEU:HD21	1.99	0.45
6:D:484:LYS:HG2	6:D:492:TYR:HB3	1.98	0.45
7:E:356:TYR:HB3	7:E:358:LEU:HD12	1.98	0.45
7:E:369:ARG:HH21	7:E:413:THR:HG21	1.82	0.45
11:I:63:LEU:HD11	12:J:43:TYR:HE1	1.82	0.45
13:K:79:TYR:OH	13:K:82:GLN:OE1	2.35	0.45
1:A1:95:THR:OG1	1:A1:96:GLY:N	2.50	0.45
1:A1:272:PRO:HD2	1:A1:361:LEU:HD21	1.99	0.45
2:B2:399:TYR:O	2:B2:402:ARG:NH1	2.49	0.45
1:B7:199:CYS:HB3	1:B7:265:PHE:CD1	2.51	0.45
3:A:2438:PHE:HA	3:A:2485:VAL:O	2.16	0.45
4:B:637:ARG:HA	4:B:637:ARG:HD3	1.77	0.45
4:B:687:THR:O	4:B:691:LEU:CB	2.64	0.45
4:B:807:ASP:O	4:B:811:VAL:HG23	2.16	0.45
4:B:3757:SER:N	4:B:4080:GLN:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:3750:LEU:O	5:C:3755:LYS:N	2.50	0.45
7:E:272:LEU:HD13	7:E:322:TYR:CE2	2.51	0.45
13:M:28:THR:O	13:M:32:GLU:HG2	2.16	0.45
13:M:57:HIS:HB2	13:M:88:PHE:CE1	2.51	0.45
1:A1:47:ILE:HG22	1:A1:51:PHE:HB2	1.99	0.45
2:A2:315:CYS:N	2:A2:350:GLY:O	2.48	0.45
1:A3:52:ASN:OD1	1:A3:62:ARG:NH2	2.49	0.45
1:A5:5:VAL:HG22	1:A5:62:ARG:HD3	1.99	0.45
2:A6:417:GLU:HA	2:A6:420:GLU:HG2	1.99	0.45
2:B2:133:GLN:HG3	2:B2:242:LEU:HD11	1.98	0.45
1:B7:342:VAL:HG11	1:B7:345:ILE:HD13	1.99	0.45
5:C:825:ARG:HE	5:C:864:TYR:HE2	1.64	0.45
13:L:24:VAL:HG22	13:L:78:PHE:CE1	2.51	0.45
18:Y1:100:GLN:HA	18:Y1:103:GLU:HG3	1.98	0.45
2:A4:222:PRO:O	1:A5:322:SER:OG	2.34	0.45
2:B2:28:HIS:CE1	2:B2:49:PHE:HA	2.52	0.45
2:B4:4:VAL:HG23	2:B4:134:GLY:O	2.16	0.45
1:B5:128:ASP:OD1	1:B5:128:ASP:N	2.41	0.45
1:B5:417:ASP:O	1:B5:421:GLU:HG3	2.17	0.45
2:B6:319:TYR:CZ	2:B6:328:VAL:HG23	2.52	0.45
4:B:2878:VAL:N	4:B:3033:ASP:O	2.48	0.45
5:C:804:VAL:O	5:C:807:ASN:HB2	2.17	0.45
5:C:2408:GLY:O	5:C:2412:ASN:N	2.37	0.45
5:C:4273:LEU:HA	5:C:4276:ALA:HB3	1.99	0.45
6:D:394:LYS:O	6:D:396:GLU:N	2.48	0.45
6:D:541:CYS:HA	6:D:566:SER:HB2	1.99	0.45
13:M:47:GLU:HG2	13:M:50:ARG:NH1	2.32	0.45
2:A2:335:ILE:HG23	2:A2:341:ILE:HD11	1.98	0.45
1:A3:9:GLY:HA2	1:A3:66:MET:O	2.17	0.45
1:A3:401:GLU:N	1:A3:401:GLU:OE1	2.50	0.45
1:A5:47:ILE:HG22	1:A5:51:PHE:HB2	1.98	0.45
1:A5:388:MET:HB3	1:A5:393:ALA:HB3	1.97	0.45
2:A6:185:TYR:HA	2:A6:395:PHE:HE2	1.81	0.45
1:A7:386:THR:O	1:A7:390:ARG:HG2	2.16	0.45
2:B2:4:VAL:HG13	2:B2:52:PHE:HE1	1.82	0.45
2:B4:234:VAL:HG21	2:B4:302:MET:HE2	1.99	0.45
1:B7:100:ASN:OD1	1:B7:398:TYR:HE1	2.00	0.45
3:A:3289:PRO:HA	3:A:3470:LEU:CB	2.47	0.45
5:C:1434:SER:O	5:C:1438:ASN:N	2.50	0.45
13:K:57:HIS:O	13:K:87:LEU:HA	2.16	0.45
2:A4:145:THR:OG1	21:A5:501:GTP:O1B	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:68:LEU:HD12	1:A5:143:THR:HB	1.98	0.45
2:B2:434:GLU:OE2	2:B2:435:VAL:HG23	2.17	0.45
1:B5:44:LEU:O	1:B5:47:ILE:HG12	2.17	0.45
1:B7:73:MET:O	1:B7:76:VAL:HB	2.17	0.45
1:B7:296:ALA:HB1	1:B7:305:PRO:HD2	1.99	0.45
3:A:2040:ALA:C	3:A:2043:LYS:H	2.20	0.45
3:A:2350:THR:O	3:A:2351:ALA:C	2.55	0.45
3:A:3366:GLN:O	3:A:3370:TRP:CB	2.65	0.45
3:A:3611:GLY:CA	3:A:3615:ALA:HB2	2.46	0.45
4:B:4244:PHE:O	4:B:4248:VAL:N	2.50	0.45
5:C:443:LEU:HD11	5:C:452:LEU:HD22	1.99	0.45
15:P:45:TYR:HB2	15:P:52:CYS:SG	2.57	0.45
1:A5:137:HIS:O	1:A5:168:SER:HA	2.17	0.45
1:A7:102:ALA:HB3	1:A7:401:GLU:OE2	2.17	0.45
1:B1:186:THR:HG22	1:B1:411:ALA:HB1	1.99	0.45
1:B1:204:ASN:OD1	23:B1:501:GDP:O2'	2.35	0.45
1:B1:278:SER:O	1:B1:278:SER:OG	2.35	0.45
1:B7:150:LEU:HD12	1:B7:151:LEU:N	2.32	0.45
3:A:4230:LEU:C	3:A:4232:THR:H	2.20	0.45
4:B:2873:GLY:H	4:B:3004:HIS:HA	1.82	0.45
6:D:413:TRP:CZ3	6:D:433:SER:HB2	2.51	0.45
6:D:558:VAL:HG23	6:D:559:MET:HG3	1.99	0.45
12:J:78:GLU:HB3	12:J:93:GLN:O	2.17	0.45
16:X:230:SER:HB2	18:Y:184:LEU:HD22	1.98	0.45
2:A4:339:ARG:HG2	2:A4:339:ARG:NH1	2.30	0.44
1:A5:8:GLN:O	1:A5:66:MET:HG3	2.17	0.44
2:B4:260:VAL:O	2:B4:260:VAL:HG23	2.18	0.44
2:B6:213:CYS:HA	2:B6:217:LEU:HB2	1.99	0.44
3:A:2882:GLU:O	3:A:2886:PHE:CB	2.65	0.44
3:A:3601:LEU:O	3:A:3605:VAL:CB	2.65	0.44
3:A:4004:MET:H	3:A:4178:GLU:CB	2.31	0.44
3:A:4335:ARG:HA	3:A:4357:GLY:CA	2.47	0.44
4:B:280:LEU:O	4:B:284:VAL:HG23	2.16	0.44
4:B:647:ALA:O	4:B:650:SER:OG	2.27	0.44
4:B:693:LEU:HD23	4:B:693:LEU:HA	1.78	0.44
5:C:811:LYS:O	5:C:814:ALA:HB3	2.17	0.44
6:D:576:GLN:NE2	6:D:578:THR:OG1	2.50	0.44
20:Z:96:ASN:HA	20:Z:99:GLU:HG3	1.99	0.44
1:A1:180:VAL:HG23	1:A1:184:ASN:HD21	1.82	0.44
1:A1:271:THR:HG23	1:A1:292:GLN:OE1	2.16	0.44
1:A7:8:GLN:CD	1:A7:17:GLY:HA3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B1:167:PHE:CZ	1:B1:233:MET:HG2	2.52	0.44
1:B5:2:ARG:NE	1:B5:240:LEU:HD22	2.27	0.44
1:B5:403:MET:HE2	1:B5:403:MET:HB2	1.51	0.44
3:A:3462:PRO:O	3:A:3466:ALA:HB2	2.18	0.44
4:B:266:LEU:HB3	4:B:274:TYR:CZ	2.53	0.44
4:B:2872:ARG:O	4:B:2874:ASN:N	2.49	0.44
5:C:1403:ALA:N	5:C:1412:ILE:O	2.50	0.44
5:C:3388:ASN:HA	5:C:3389:ARG:HA	1.58	0.44
7:E:399:ILE:HG23	7:E:400:LEU:H	1.82	0.44
15:P:31:LYS:O	15:P:35:MET:HB2	2.17	0.44
16:X:260:ARG:N	16:X:260:ARG:HD3	2.32	0.44
20:Z:72:LEU:O	20:Z:76:GLN:OE1	2.35	0.44
20:Z:96:ASN:O	20:Z:99:GLU:HG3	2.17	0.44
2:A4:395:PHE:CE2	2:A4:422:ARG:HD2	2.53	0.44
2:A4:398:MET:CE	1:A5:346:PRO:HD2	2.47	0.44
1:A7:173:PRO:HB3	1:A7:384:GLN:NE2	2.31	0.44
1:B3:232:VAL:HG11	1:B3:268:VAL:HG11	1.99	0.44
2:B4:119:LEU:HD21	2:B4:156:ARG:HD3	1.99	0.44
1:B5:22:GLU:HG3	1:B5:81:TYR:CD2	2.52	0.44
1:B7:105:HIS:CD2	1:B7:150:LEU:HB3	2.52	0.44
3:A:2424:GLY:N	3:A:2425:ILE:HA	2.32	0.44
4:B:510:ALA:HA	4:B:513:ILE:HG22	1.98	0.44
5:C:120:LYS:HG2	5:C:159:LEU:HD11	1.99	0.44
7:E:395:VAL:O	7:E:397:THR:N	2.50	0.44
1:A1:237:THR:O	1:A1:237:THR:HG22	2.18	0.44
2:A2:136:LEU:HA	2:A2:167:LEU:O	2.17	0.44
1:A3:170:VAL:N	1:A3:202:LEU:O	2.49	0.44
1:A3:189:VAL:O	1:A3:193:VAL:HG23	2.18	0.44
1:A7:367:PHE:O	1:A7:368:ILE:HD13	2.18	0.44
1:B1:312:THR:HG22	1:B1:313:ALA:N	2.32	0.44
3:A:1677:CYS:C	3:A:1679:ALA:N	2.68	0.44
3:A:4057:GLY:HA2	3:A:4196:SER:CB	2.48	0.44
3:A:4130:ARG:C	3:A:4132:GLU:H	2.20	0.44
3:A:4385:PHE:HA	3:A:4443:LYS:O	2.18	0.44
4:B:4309:LYS:H	4:B:4417:ALA:HB3	1.80	0.44
5:C:1052:VAL:HA	5:C:1055:LYS:NZ	2.32	0.44
7:E:361:HIS:CE1	7:E:383:ASP:H	2.33	0.44
16:X1:177:TYR:CD2	18:Y1:132:ILE:HD12	2.52	0.44
20:Z:73:LEU:HA	20:Z:76:GLN:OE1	2.17	0.44
1:A1:30:ILE:HD12	1:A1:36:TYR:HA	1.99	0.44
1:A1:40:SER:OG	1:A1:41:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:384:GLN:HB3	2:A2:348:PRO:HG3	1.99	0.44
2:A4:203:MET:SD	2:A4:267:PHE:HB3	2.57	0.44
2:A4:246:GLY:HA3	2:A4:356:ASN:HA	1.99	0.44
2:A6:66:ILE:HD11	2:A6:122:ILE:HD11	1.99	0.44
1:B3:91:VAL:HG11	1:B3:116:VAL:HG22	2.00	0.44
2:B4:246:GLY:HA3	2:B4:356:ASN:HA	2.00	0.44
1:B5:389:PHE:HZ	1:B5:405:GLU:HG3	1.83	0.44
1:B7:263:LEU:HD22	1:B7:422:TYR:CZ	2.53	0.44
3:A:1683:TYR:HA	3:A:1738:LEU:O	2.16	0.44
3:A:3615:ALA:CB	3:A:3618:GLY:H	2.27	0.44
3:A:3791:PHE:HA	3:A:3794:LEU:CB	2.48	0.44
3:A:3935:GLY:O	3:A:3968:ARG:N	2.37	0.44
4:B:266:LEU:HB3	4:B:274:TYR:CE1	2.53	0.44
5:C:3054:PHE:O	5:C:3058:ALA:N	2.31	0.44
7:E:199:TYR:CE2	7:E:209:PRO:HG3	2.53	0.44
13:N:9:VAL:O	13:N:79:TYR:N	2.49	0.44
1:A1:208:TYR:O	1:A1:212:PHE:HD1	2.01	0.44
1:A3:189:VAL:HG11	1:A3:378:PHE:CE1	2.53	0.44
1:B1:201:VAL:HG11	1:B1:377:MET:HE3	2.00	0.44
2:B4:72:PRO:HD2	1:B5:2:ARG:HH12	1.83	0.44
2:B4:72:PRO:HD2	1:B5:2:ARG:NH1	2.33	0.44
2:B6:170:THR:HG21	2:B6:194:LEU:HD11	2.00	0.44
1:B7:128:ASP:N	1:B7:128:ASP:OD1	2.44	0.44
3:A:4248:LEU:CA	3:A:4258:VAL:HA	2.48	0.44
4:B:330:LEU:HB3	7:E:542:LEU:HD22	1.99	0.44
4:B:3489:LYS:O	4:B:3493:GLU:N	2.48	0.44
5:C:224:ILE:HG13	5:C:344:ARG:NH2	2.32	0.44
5:C:399:THR:HB	5:C:403:GLN:HE22	1.83	0.44
7:E:481:SER:HG	7:E:482:THR:H	1.61	0.44
11:I:100:ASP:OD1	11:I:100:ASP:N	2.50	0.44
13:K:14:ASP:OD1	13:K:14:ASP:N	2.48	0.44
15:P:20:LEU:HD13	15:P:20:LEU:HA	1.81	0.44
2:A2:90:GLU:OE1	2:A2:121:ARG:NH2	2.50	0.44
1:A5:113:ILE:HD11	1:A5:151:LEU:HB2	2.00	0.44
1:A5:385:PHE:HZ	1:A5:408:PHE:HD2	1.65	0.44
1:A7:213:ARG:HD3	1:A7:297:LYS:HD2	1.99	0.44
1:B3:91:VAL:CG1	1:B3:116:VAL:HG22	2.47	0.44
1:B5:209:ASP:CG	1:B5:213:ARG:HH12	2.18	0.44
3:A:3827:THR:O	3:A:3831:GLN:N	2.48	0.44
4:B:520:THR:HG21	7:E:402:THR:HA	1.99	0.44
4:B:3103:SER:CB	4:B:3586:GLY:HA3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2160:ARG:O	5:C:2163:LYS:N	2.51	0.44
7:E:366:TYR:H	7:E:382:GLY:CA	2.31	0.44
13:K:40:ILE:HD13	13:K:40:ILE:HA	1.85	0.44
14:O:63:LYS:O	14:O:65:PHE:N	2.51	0.44
16:X:277:ARG:O	17:X0:280:UNK:N	2.41	0.44
2:A2:346:TRP:CZ3	2:A2:347:CYS:HB2	2.53	0.44
2:A4:392:ASP:OD1	2:A4:422:ARG:NH1	2.51	0.44
2:A6:434:GLU:OE1	2:A6:435:VAL:HG23	2.18	0.44
1:B1:114:ASP:N	1:B1:114:ASP:OD1	2.50	0.44
2:B4:402:ARG:HD2	2:B4:405:VAL:HG11	1.99	0.44
1:B7:267:MET:CE	1:B7:299:MET:HG3	2.48	0.44
3:A:3598:GLN:O	3:A:3991:GLN:HA	2.17	0.44
3:A:3926:VAL:HA	3:A:3929:LYS:CB	2.48	0.44
4:B:464:ILE:HD13	4:B:508:LEU:HD12	1.99	0.44
4:B:622:ARG:O	4:B:625:ASP:HB2	2.18	0.44
4:B:1966:ALA:O	4:B:2015:VAL:HA	2.17	0.44
4:B:2176:GLN:O	4:B:2178:ASP:N	2.46	0.44
4:B:4529:CYS:N	4:B:4545:ALA:O	2.51	0.44
6:D:318:ASN:HA	6:D:368:PHE:HD2	1.83	0.44
6:D:516:TYR:CZ	6:D:548:VAL:HG11	2.52	0.44
7:E:545:GLU:HA	7:E:548:LYS:HD2	2.00	0.44
2:A4:387:ILE:HG23	2:A4:388:PHE:HD1	1.83	0.44
2:A6:70:LEU:CD2	2:A6:114:ILE:HD12	2.48	0.44
2:A6:304:LYS:HA	2:A6:304:LYS:HD3	1.74	0.44
1:B5:274:THR:HG21	1:B5:282:ARG:HD2	2.00	0.44
2:B6:405:VAL:HG13	2:B6:418:PHE:CE2	2.44	0.44
5:C:225:LYS:HA	5:C:344:ARG:HH12	1.82	0.44
5:C:3438:MET:O	5:C:3442:ALA:N	2.23	0.44
6:D:408:LEU:HD23	6:D:408:LEU:HA	1.87	0.44
18:Y:241:ARG:HD2	18:Y:245:ARG:NH2	2.32	0.44
2:A2:81:GLY:O	2:A2:84:ARG:HG3	2.18	0.43
2:A2:150:GLY:O	2:A2:154:LEU:HD23	2.18	0.43
1:A3:103:LYS:HA	1:A3:107:THR:HB	1.99	0.43
2:A6:179:THR:O	1:A7:350:LYS:HD2	2.18	0.43
2:A6:407:TRP:O	2:A6:411:GLU:HG3	2.18	0.43
2:B4:287:SER:HB3	2:B4:290:GLU:OE2	2.18	0.43
1:B5:70:PRO:HD2	2:B6:2:ARG:NH2	2.32	0.43
1:B5:236:ILE:HD13	1:B5:368:ILE:HD11	1.99	0.43
3:A:2397:SER:O	3:A:2835:ALA:HB2	2.18	0.43
3:A:4461:TYR:O	3:A:4497:LEU:N	2.28	0.43
4:B:239:PHE:HD2	4:B:240:TRP:HD1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4113:ALA:HB2	4:B:4236:ALA:HB2	2.00	0.43
4:B:4222:ASN:HA	4:B:4231:MET:O	2.18	0.43
5:C:129:PRO:HD2	5:C:130:ILE:N	2.31	0.43
5:C:203:MET:HE3	5:C:266:SER:HB2	2.00	0.43
5:C:1024:VAL:HG13	5:C:1044:LYS:NZ	2.33	0.43
5:C:3471:THR:O	5:C:3494:ILE:HA	2.18	0.43
11:I:55:LYS:HD3	11:I:55:LYS:HA	1.80	0.43
2:A2:189:LEU:HD11	2:A2:418:PHE:HE1	1.82	0.43
1:B1:91:VAL:CG1	1:B1:116:VAL:HG12	2.47	0.43
1:B3:152:ILE:HG22	1:B3:195:ASN:HB3	2.00	0.43
2:B4:102:ASN:HB3	2:B4:105:ARG:HB3	2.00	0.43
2:B6:179:THR:HG22	1:B7:327:ASP:OD1	2.18	0.43
1:B7:130:LEU:HD21	1:B7:133:PHE:CE1	2.52	0.43
1:B7:224:ASP:OD1	1:B7:225:LEU:N	2.50	0.43
3:A:1782:VAL:HA	3:A:1785:VAL:CB	2.48	0.43
3:A:2102:MET:HA	3:A:2103:PRO:C	2.38	0.43
3:A:3883:ILE:HA	3:A:3973:ALA:O	2.17	0.43
4:B:293:ASP:O	4:B:296:LYS:HG2	2.18	0.43
4:B:453:LYS:O	4:B:455:LYS:N	2.51	0.43
4:B:583:TYR:HB3	4:B:642:TRP:CZ3	2.53	0.43
4:B:4092:GLY:O	4:B:4096:ASN:N	2.38	0.43
5:C:211:CYS:SG	5:C:276:TRP:NE1	2.90	0.43
5:C:500:GLN:HG2	5:C:535:ASP:OD2	2.18	0.43
7:E:247:ARG:HG3	7:E:248:LYS:NZ	2.34	0.43
20:Z:70:ILE:HG22	20:Z:71:SER:N	2.33	0.43
2:A2:326:LYS:HB3	2:A2:326:LYS:HE2	1.70	0.43
2:A6:72:PRO:HA	2:A6:94:SER:HB2	1.99	0.43
1:A7:122:LYS:HA	1:A7:125:GLU:HG3	1.99	0.43
2:B2:21:TRP:CZ2	2:B2:65:CYS:HB3	2.54	0.43
3:A:1300:PHE:HA	3:A:1312:LYS:H	1.83	0.43
4:B:603:ARG:HH11	4:B:603:ARG:HD3	1.60	0.43
4:B:820:LYS:HA	4:B:823:GLN:HG3	2.00	0.43
4:B:2933:THR:HA	4:B:3003:LEU:O	2.18	0.43
5:C:2823:PHE:HA	5:C:2853:TYR:O	2.18	0.43
6:D:352:HIS:CD2	6:D:353:PRO:HD2	2.53	0.43
7:E:236:GLN:HB3	7:E:237:TYR:H	1.63	0.43
13:N:15:MET:HA	13:N:74:HIS:HA	2.00	0.43
1:A1:362:LYS:HB2	1:A1:362:LYS:HE3	1.62	0.43
1:A3:8:GLN:NE2	1:A3:17:GLY:HA3	2.34	0.43
1:A3:135:VAL:HG21	1:A3:152:ILE:HD11	2.00	0.43
2:A4:178:SER:HB2	2:A4:183:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A6:283:HIS:CG	2:A6:283:HIS:O	2.70	0.43
1:A7:200:MET:CE	1:A7:368:ILE:HD12	2.47	0.43
1:B1:5:VAL:HG22	1:B1:62:ARG:HD3	2.01	0.43
1:B1:40:SER:O	1:B1:43:GLN:HG2	2.19	0.43
1:B1:91:VAL:HG11	1:B1:116:VAL:HG12	1.99	0.43
2:B4:66:ILE:CB	2:B4:121:ARG:HH21	2.32	0.43
1:B5:205:GLU:OE1	1:B5:205:GLU:N	2.52	0.43
3:A:1558:ARG:CB	3:A:1607:GLN:HA	2.47	0.43
3:A:3623:LYS:CB	3:A:3680:SER:HA	2.48	0.43
3:A:4410:GLY:N	3:A:4438:PRO:O	2.32	0.43
4:B:3484:ASP:O	4:B:3488:ALA:HB2	2.19	0.43
5:C:2043:ILE:O	5:C:2047:PHE:N	2.48	0.43
5:C:2310:ALA:HB3	5:C:2369:THR:O	2.18	0.43
1:A1:204:ASN:HA	1:A1:207:LEU:HD12	2.00	0.43
2:A2:265:ILE:HG23	2:A2:432:PHE:HE1	1.82	0.43
2:A4:21:TRP:CZ3	2:A4:63:PRO:HB3	2.53	0.43
2:A6:52:PHE:HE2	2:A6:239:THR:HG21	1.83	0.43
2:B2:196:GLU:OE2	2:B2:197:HIS:NE2	2.51	0.43
1:B5:113:ILE:HD12	1:B5:116:VAL:HG21	2.00	0.43
3:A:3392:GLN:HA	3:A:3395:GLU:CB	2.48	0.43
5:C:669:ARG:O	5:C:673:TYR:N	2.51	0.43
13:K:21:ALA:HA	13:K:24:VAL:HG22	2.00	0.43
16:X:237:LEU:HB3	18:Y:191:MET:CE	2.48	0.43
1:A1:258:ILE:O	1:A1:258:ILE:HG23	2.18	0.43
1:A3:309:ARG:H	1:A3:372:THR:HG22	1.84	0.43
2:A4:413:MET:HB3	2:A4:417:GLU:OE2	2.18	0.43
1:A5:21:TRP:CZ2	1:A5:63:ALA:HB2	2.53	0.43
1:A5:271:THR:CG2	1:A5:365:ALA:HB3	2.49	0.43
1:A7:113:ILE:HD13	1:A7:150:LEU:HD21	1.99	0.43
1:A7:192:LEU:HD13	1:A7:199:CYS:SG	2.58	0.43
2:B2:47:ASP:OD1	2:B2:48:ALA:N	2.51	0.43
1:B3:249:ASP:OD1	1:B3:252:LYS:HB2	2.18	0.43
1:B5:271:THR:OG1	1:B5:365:ALA:HB3	2.19	0.43
2:B6:155:GLU:HG2	2:B6:197:HIS:CD2	2.53	0.43
3:A:2051:ASP:C	3:A:2106:ASP:HA	2.39	0.43
3:A:3732:LEU:O	3:A:3736:THR:CB	2.67	0.43
4:B:1949:MET:HA	4:B:1953:ALA:HB3	1.99	0.43
5:C:2520:MET:O	5:C:2531:LYS:N	2.51	0.43
7:E:71:ASN:O	13:K:70:HIS:N	2.52	0.43
2:A2:425:LEU:HD23	2:A2:425:LEU:HA	1.85	0.43
1:A3:253:LEU:HD11	1:A3:316:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A5:215:LEU:HB3	1:A5:217:LEU:HG	2.01	0.43
2:A6:200:VAL:HG13	2:A6:268:MET:CE	2.48	0.43
2:A6:345:ASP:OD1	2:A6:346:TRP:N	2.51	0.43
2:B4:121:ARG:HD2	2:B4:121:ARG:C	2.39	0.43
1:B5:3:GLU:HB2	1:B5:130:LEU:HD12	2.01	0.43
3:A:2040:ALA:O	3:A:2043:LYS:N	2.46	0.43
3:A:2764:TYR:O	3:A:2768:GLY:N	2.35	0.43
3:A:3882:PHE:HA	3:A:3996:ILE:O	2.19	0.43
3:A:3936:TRP:HA	3:A:3968:ARG:O	2.19	0.43
4:B:583:TYR:HB3	4:B:642:TRP:CH2	2.54	0.43
5:C:296:TYR:O	5:C:299:THR:OG1	2.33	0.43
5:C:784:ILE:HD13	5:C:784:ILE:HG21	1.81	0.43
5:C:872:LEU:O	5:C:876:GLN:HG2	2.19	0.43
5:C:1399:ASN:HA	5:C:1513:GLN:O	2.18	0.43
6:D:406:GLY:HA3	6:D:449:PRO:HG3	2.01	0.43
9:G:43:LEU:HD12	9:G:43:LEU:HA	1.84	0.43
16:X1:123:ASN:HA	16:X1:126:LYS:HG2	1.99	0.43
16:X1:200:ARG:HA	16:X1:200:ARG:HD2	1.86	0.43
18:Y1:200:GLU:O	18:Y1:203:GLU:HG3	2.18	0.43
1:A1:309:ARG:H	1:A1:372:THR:HG22	1.83	0.43
2:A2:353:CYS:SG	2:A2:354:GLY:N	2.91	0.43
2:A2:387:ILE:HG12	2:A2:390:ARG:NH2	2.32	0.43
1:A3:296:ALA:HB1	1:A3:304:ASP:OD1	2.18	0.43
2:A6:52:PHE:CE2	2:A6:239:THR:HG21	2.54	0.43
1:B1:220:PRO:HD2	2:B2:326:LYS:HD3	2.00	0.43
2:B2:372:GLN:OE1	2:B2:372:GLN:HA	2.19	0.43
2:B4:143:GLY:O	2:B4:147:SER:HB3	2.19	0.43
1:B5:3:GLU:HG3	1:B5:127:CYS:HB2	1.99	0.43
2:B6:70:LEU:HB3	2:B6:97:GLU:O	2.19	0.43
1:B7:367:PHE:O	1:B7:368:ILE:HD13	2.18	0.43
3:A:3306:LEU:O	3:A:3311:MET:N	2.51	0.43
3:A:3339:PRO:CB	3:A:3483:GLN:HA	2.49	0.43
4:B:1495:LEU:N	4:B:1610:THR:O	2.50	0.43
4:B:2551:THR:O	4:B:2553:SER:N	2.51	0.43
4:B:3565:ASN:HA	4:B:3610:THR:HA	2.00	0.43
5:C:446:HIS:HD2	5:C:526:ILE:HG12	1.84	0.43
5:C:589:GLU:OE1	5:C:613:TYR:OH	2.24	0.43
5:C:728:ASP:OD1	5:C:732:ARG:NH1	2.51	0.43
7:E:272:LEU:CG	7:E:291:TRP:HZ3	2.32	0.43
7:E:377:TYR:CD1	7:E:390:VAL:HG22	2.53	0.43
7:E:502:GLU:O	7:E:506:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:44:ILE:HG22	13:M:87:LEU:HD11	2.00	0.43
1:A3:191:GLN:HG3	1:A3:195:ASN:HD22	1.84	0.43
2:A6:12:ALA:HB2	21:A7:501:GTP:C8	2.54	0.43
1:A7:289:LEU:HD11	1:A7:363:MET:HE3	2.00	0.43
1:B1:170:VAL:HG22	1:B1:202:LEU:O	2.18	0.43
1:B3:242:PHE:CD1	1:B3:356:ILE:HG13	2.54	0.43
3:A:1716:GLY:O	3:A:1864:ARG:N	2.29	0.43
3:A:1747:CYS:H	3:A:1773:ASP:H	1.66	0.43
3:A:3381:GLN:N	3:A:3404:VAL:HA	2.34	0.43
5:C:859:TYR:O	5:C:863:MET:HG2	2.19	0.43
6:D:490:SER:HA	6:D:506:LYS:HD3	1.99	0.43
12:J:87:PHE:HE1	12:J:89:LEU:HB2	1.84	0.43
13:M:55:THR:O	13:M:89:LYS:NZ	2.52	0.43
20:Z:86:LYS:HB2	20:Z:86:LYS:HE2	1.81	0.43
2:A2:9:ILE:HG12	2:A2:68:LEU:HD21	2.00	0.43
1:A5:107:THR:OG1	1:A5:108:GLU:OE1	2.28	0.43
1:A5:421:GLU:HA	1:A5:424:GLN:HG3	2.01	0.43
2:A6:311:LYS:HG2	2:A6:342:GLN:HG3	2.00	0.43
2:B2:102:ASN:OD1	1:B3:255:VAL:HG21	2.19	0.43
2:B4:258:ASN:CG	2:B4:352:LYS:HD3	2.39	0.43
1:B5:385:PHE:HZ	1:B5:408:PHE:HD1	1.67	0.43
1:B5:397:TRP:CH2	2:B6:256:GLN:HB3	2.54	0.43
1:B7:167:PHE:CD2	1:B7:233:MET:HG2	2.54	0.43
3:A:2345:THR:HA	3:A:2385:LYS:CB	2.48	0.43
3:A:4130:ARG:C	3:A:4132:GLU:N	2.72	0.43
3:A:4352:SER:HA	3:A:4409:HIS:CB	2.49	0.43
4:B:2230:ALA:HA	4:B:2276:VAL:O	2.19	0.43
5:C:394:ARG:HH12	5:C:416:ILE:HG21	1.84	0.43
5:C:1013:GLU:HA	5:C:1016:LYS:HE3	2.01	0.43
7:E:77:VAL:HG13	13:K:63:ASN:H	1.84	0.43
7:E:184:ILE:HD12	7:E:191:PRO:HG3	2.00	0.43
7:E:199:TYR:CZ	7:E:209:PRO:HG3	2.54	0.43
9:G:130:LEU:HD11	9:G:133:ASN:ND2	2.34	0.43
11:I:22:GLY:HA2	11:I:36:THR:HG21	2.01	0.43
2:A4:377:MET:SD	2:A4:379:SER:HB3	2.59	0.42
1:A5:149:THR:HG22	1:A5:191:GLN:HG2	2.01	0.42
2:B2:9:ILE:HD13	2:B2:150:GLY:HA2	2.01	0.42
1:B5:264:HIS:ND1	1:B5:264:HIS:O	2.48	0.42
1:B7:190:HIS:ND1	1:B7:414:ASN:OD1	2.51	0.42
1:B7:293:MET:SD	1:B7:367:PHE:HB2	2.59	0.42
3:A:219:ASP:O	3:A:223:MET:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1861:ALA:HA	3:A:4073:ASN:CB	2.48	0.42
3:A:2371:MET:HA	3:A:2486:ALA:HB3	2.01	0.42
3:A:2538:GLN:C	3:A:2541:GLY:H	2.23	0.42
4:B:68:ASP:O	4:B:70:LYS:N	2.51	0.42
4:B:434:LEU:HD12	4:B:434:LEU:HA	1.77	0.42
4:B:457:LEU:HD22	4:B:511:ILE:HG23	2.00	0.42
4:B:2564:GLU:H	4:B:2567:ALA:HB3	1.83	0.42
4:B:2596:VAL:N	4:B:2642:ALA:O	2.43	0.42
4:B:3563:ILE:O	4:B:3609:GLN:N	2.52	0.42
5:C:789:LEU:HA	5:C:813:GLN:OE1	2.19	0.42
5:C:1819:GLY:HA3	5:C:1944:MET:CB	2.49	0.42
6:D:209:TYR:CZ	15:P:94:GLY:HA2	2.54	0.42
7:E:269:PHE:HE2	7:E:271:TRP:CZ2	2.37	0.42
11:I:71:PHE:CD1	12:J:73:ARG:HB2	2.54	0.42
16:X:266:ARG:HH12	18:Y:220:GLN:HA	1.84	0.42
18:Y1:146:TYR:O	18:Y1:150:ILE:HG12	2.19	0.42
20:Z:99:GLU:HA	20:Z:102:MET:HG2	2.00	0.42
1:A1:146:GLY:O	1:A1:149:THR:HG22	2.20	0.42
1:A1:378:PHE:HA	1:A1:381:VAL:HG22	2.00	0.42
2:A2:4:VAL:HG23	2:A2:134:GLY:O	2.19	0.42
1:A3:133:PHE:HD2	1:A3:164:MET:HE3	1.84	0.42
2:A4:171:VAL:HA	2:A4:204:LEU:O	2.18	0.42
1:B1:213:ARG:NH1	1:B1:297:LYS:HE2	2.34	0.42
1:B3:8:GLN:CD	1:B3:17:GLY:HA3	2.40	0.42
1:B5:175:VAL:HG23	1:B5:205:GLU:CD	2.39	0.42
2:B6:66:ILE:HG13	2:B6:66:ILE:O	2.19	0.42
3:A:2404:TYR:HA	3:A:2444:MET:O	2.19	0.42
3:A:2559:PHE:HA	3:A:2563:ALA:HB2	1.99	0.42
3:A:3574:ARG:O	3:A:3577:ALA:HB3	2.20	0.42
4:B:210:LYS:HA	4:B:210:LYS:HD3	1.77	0.42
4:B:4255:LEU:C	4:B:4258:GLY:H	2.22	0.42
5:C:764:GLU:O	5:C:767:ARG:HG3	2.19	0.42
7:E:228:ASP:OD1	7:E:229:ASN:N	2.52	0.42
10:H:97:HIS:HA	10:H:106:ILE:HA	2.02	0.42
13:L:60:VAL:HG12	13:L:85:ILE:HG23	2.01	0.42
16:X1:248:LYS:HD3	18:Y1:202:ARG:HG2	2.01	0.42
18:Y:234:ILE:HB	18:Y:238:LYS:NZ	2.34	0.42
2:A2:8:HIS:CD2	2:A2:138:PHE:HD2	2.37	0.42
2:A4:291:ILE:HD12	2:A4:375:VAL:HG23	2.01	0.42
1:A5:271:THR:OG1	1:A5:272:PRO:HA	2.20	0.42
1:B1:395:LEU:O	1:B1:399:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:8:HIS:O	2:B2:68:LEU:HD23	2.19	0.42
2:B2:402:ARG:O	2:B2:405:VAL:HG12	2.19	0.42
1:B3:392:LYS:HE3	1:B3:405:GLU:OE1	2.19	0.42
1:B5:69:GLU:HG2	2:B6:2:ARG:NH2	2.34	0.42
1:B5:257:LEU:HD21	1:B5:314:SER:HB2	2.01	0.42
2:B6:278:ALA:HA	2:B6:369:ALA:HB2	2.00	0.42
5:C:53:GLN:HA	5:C:83:HIS:HA	2.01	0.42
5:C:549:LYS:O	5:C:552:ASP:HB3	2.19	0.42
6:D:357:PHE:O	6:D:358:HIS:ND1	2.52	0.42
7:E:392:ASP:O	7:E:396:LYS:NZ	2.33	0.42
16:X1:169:GLY:O	16:X1:171:LEU:HD12	2.20	0.42
1:A3:245:GLN:C	1:A3:246:LEU:HD12	2.39	0.42
1:A3:406:MET:O	1:A3:410:GLU:HG3	2.18	0.42
2:A4:431:ASP:O	2:A4:434:GLU:HG3	2.19	0.42
2:A6:155:GLU:HG2	2:A6:197:HIS:CD2	2.54	0.42
1:A7:11:GLN:N	23:A7:502:GDP:O2B	2.45	0.42
1:A7:314:SER:OG	1:A7:368:ILE:HB	2.18	0.42
1:B1:226:ASN:OD1	23:B1:501:GDP:N1	2.39	0.42
1:B3:208:TYR:CG	2:B4:326:LYS:HD3	2.55	0.42
2:B4:121:ARG:O	2:B4:124:LYS:HG2	2.19	0.42
1:B5:68:LEU:HB3	1:B5:96:GLY:HA2	2.02	0.42
1:B5:175:VAL:N	1:B5:205:GLU:OE2	2.51	0.42
2:B6:394:LYS:HB2	1:B7:346:PRO:HG3	2.01	0.42
3:A:1553:TYR:HA	3:A:1555:SER:N	2.33	0.42
5:C:1015:LYS:HD3	5:C:1015:LYS:HA	1.78	0.42
6:D:212:ASP:OD2	15:P:20:LEU:HG	2.18	0.42
6:D:276:ALA:O	6:D:279:PHE:HB3	2.18	0.42
16:X:272:LYS:O	16:X:275:GLU:HG2	2.19	0.42
18:Y1:177:LEU:HD23	18:Y1:177:LEU:HA	1.83	0.42
2:A2:198:THR:HG21	2:A2:201:ALA:HB2	2.01	0.42
2:A2:328:VAL:O	2:A2:332:VAL:HG23	2.19	0.42
1:A3:232:VAL:O	1:A3:236:ILE:HG12	2.20	0.42
1:A3:391:ARG:NH2	2:A4:262:TYR:CZ	2.87	0.42
2:A4:241:SER:OG	2:A4:250:VAL:O	2.24	0.42
2:A6:67:PHE:HB2	2:A6:92:LEU:HD23	2.01	0.42
2:A6:102:ASN:ND2	2:A6:411:GLU:OE2	2.51	0.42
2:A6:209:ILE:HG23	2:A6:230:LEU:HD11	2.01	0.42
1:A7:232:VAL:HG11	1:A7:268:VAL:HG11	2.01	0.42
1:A7:383:GLU:HA	1:A7:386:THR:HG22	2.01	0.42
1:B1:3:GLU:HG3	1:B1:127:CYS:CB	2.49	0.42
2:B4:3:GLU:HA	2:B4:51:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B4:53:PHE:C	2:B4:64:ARG:HH22	2.22	0.42
3:A:2407:ASP:H	3:A:2410:SER:CB	2.32	0.42
3:A:3930:TYR:O	3:A:3934:GLY:N	2.46	0.42
3:A:4094:ILE:O	3:A:4096:TRP:N	2.45	0.42
4:B:2878:VAL:O	4:B:3035:PHE:N	2.35	0.42
5:C:528:GLN:HE22	5:C:533:GLN:HG3	1.84	0.42
5:C:2182:ILE:O	5:C:2185:LEU:N	2.42	0.42
6:D:615:LYS:HB2	6:D:615:LYS:HE2	1.78	0.42
9:G:101:ASP:OD1	9:G:102:ALA:N	2.52	0.42
13:M:37:GLU:OE1	13:M:60:VAL:HG13	2.19	0.42
13:N:8:ALA:HA	13:N:80:LEU:HA	2.01	0.42
16:X1:190:GLU:O	16:X1:193:VAL:HG12	2.20	0.42
1:A1:173:PRO:HG3	1:A1:380:ARG:HD2	2.02	0.42
2:A2:104:ALA:HB2	2:A2:413:MET:SD	2.59	0.42
2:A4:100:ALA:HB1	1:A5:252:LYS:HA	2.00	0.42
1:A7:109:GLY:O	1:A7:113:ILE:HG12	2.19	0.42
1:A7:267:MET:SD	1:A7:303:ALA:HB3	2.59	0.42
2:B2:171:VAL:HA	2:B2:204:LEU:O	2.19	0.42
1:B3:67:ASP:CG	1:B3:68:LEU:H	2.22	0.42
2:B4:192:HIS:ND1	2:B4:424:ASP:OD2	2.41	0.42
3:A:2274:MET:O	3:A:2278:PHE:CB	2.67	0.42
3:A:2408:VAL:H	3:A:2454:MET:CB	2.32	0.42
4:B:4359:LEU:O	4:B:4363:GLY:N	2.53	0.42
5:C:632:ILE:O	5:C:635:ILE:HG22	2.19	0.42
6:D:516:TYR:CE2	6:D:548:VAL:HG11	2.55	0.42
7:E:371:ASN:HB3	7:E:414:TRP:CH2	2.55	0.42
7:E:547:PHE:HA	7:E:550:THR:HG23	2.00	0.42
16:X1:188:ILE:HG13	18:Y1:143:TYR:CE1	2.55	0.42
18:Y1:182:ALA:HA	18:Y1:185:LYS:HG2	2.01	0.42
1:A1:4:ILE:HB	1:A1:50:TYR:HE1	1.83	0.42
1:A1:109:GLY:O	1:A1:113:ILE:HG12	2.20	0.42
2:A2:210:TYR:OH	2:A2:224:TYR:HE1	2.01	0.42
2:A2:213:CYS:HA	2:A2:217:LEU:HB2	2.01	0.42
2:A4:267:PHE:HB2	2:A4:384:ILE:CD1	2.50	0.42
1:A5:35:THR:HA	1:A5:57:GLY:O	2.19	0.42
2:B2:80:THR:O	2:B2:80:THR:HG22	2.20	0.42
2:B4:26:LEU:HD21	2:B4:364:PRO:HD2	2.01	0.42
1:B5:69:GLU:CG	2:B6:2:ARG:HH22	2.32	0.42
1:B7:203:ASP:O	1:B7:207:LEU:HG	2.20	0.42
3:A:2594:THR:HA	3:A:2638:ILE:CB	2.50	0.42
3:A:4416:ALA:HA	3:A:4425:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3833:LEU:O	4:B:3837:GLY:N	2.52	0.42
5:C:783:ALA:HA	5:C:786:SER:HG	1.83	0.42
5:C:1687:ALA:HB2	5:C:1749:ASP:N	2.34	0.42
5:C:2248:TRP:O	5:C:2252:ARG:N	2.49	0.42
6:D:313:THR:HG23	6:D:363:VAL:O	2.19	0.42
18:Y1:205:ALA:O	18:Y1:208:GLU:HG3	2.19	0.42
2:A6:422:ARG:HA	2:A6:422:ARG:HD2	1.88	0.42
1:B3:3:GLU:HG3	1:B3:127:CYS:SG	2.59	0.42
2:B4:91:GLN:CA	2:B4:121:ARG:HH22	2.32	0.42
2:B4:215:ARG:HG2	2:B4:215:ARG:HH11	1.84	0.42
2:B4:327:ASP:OD1	2:B4:327:ASP:N	2.51	0.42
2:B6:7:ILE:HD12	2:B6:153:LEU:HD23	2.00	0.42
1:B7:64:ILE:O	1:B7:64:ILE:HG13	2.20	0.42
3:A:2466:GLY:O	3:A:2478:ASN:HA	2.18	0.42
4:B:475:PHE:HE1	4:B:493:ASP:HB3	1.85	0.42
5:C:1286:GLN:O	5:C:1290:TYR:CB	2.67	0.42
5:C:1354:PHE:HA	5:C:1357:GLN:CB	2.49	0.42
5:C:4397:GLY:HA2	5:C:4423:LEU:O	2.20	0.42
7:E:161:LYS:O	7:E:184:ILE:HD11	2.20	0.42
7:E:169:TRP:HZ3	7:E:467:ALA:HB2	1.85	0.42
7:E:414:TRP:HD1	7:E:420:GLY:HA2	1.82	0.42
15:P:59:GLN:HB3	15:P:63:LYS:HZ1	1.83	0.42
18:Y1:78:ASP:OD1	18:Y1:79:GLU:HG2	2.20	0.42
1:A1:317:PHE:CE2	1:A1:326:VAL:HG13	2.54	0.42
1:A3:149:THR:HG23	1:A3:191:GLN:HG2	2.02	0.42
2:A6:9:ILE:HG22	2:A6:68:LEU:CD1	2.49	0.42
2:A6:104:ALA:HB3	2:A6:411:GLU:OE1	2.20	0.42
1:B1:145:SER:OG	1:B1:146:GLY:N	2.52	0.42
1:B5:392:LYS:HD2	1:B5:395:LEU:HD22	2.01	0.42
1:B7:170:VAL:HG22	1:B7:202:LEU:O	2.19	0.42
3:A:1829:ASP:O	3:A:1831:VAL:N	2.53	0.42
3:A:2793:ASN:O	3:A:2797:SER:CB	2.68	0.42
3:A:3443:TYR:CB	3:A:3447:PHE:H	2.33	0.42
4:B:273:TYR:HB3	4:B:277:PHE:CE2	2.55	0.42
5:C:2409:ALA:O	5:C:2413:LEU:N	2.33	0.42
6:D:480:MET:SD	6:D:524:TYR:HA	2.60	0.42
6:D:493:LEU:HD21	6:D:550:LEU:HD11	2.01	0.42
16:X:230:SER:OG	18:Y:184:LEU:HD13	2.19	0.42
1:A1:64:ILE:HA	1:A1:89:ASN:HB3	2.02	0.42
1:A1:334:GLN:HA	1:A1:341:PHE:HE2	1.83	0.42
1:A3:163:MET:HE2	1:A3:251:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:317:PHE:CE2	1:A3:326:VAL:HG13	2.54	0.42
2:A4:422:ARG:HH22	2:A4:425:LEU:HD23	1.85	0.42
1:A5:103:LYS:HD2	1:A5:107:THR:OG1	2.20	0.42
1:A5:325:GLU:O	1:A5:329:GLN:HG2	2.20	0.42
1:A7:60:VAL:HG23	1:A7:84:ILE:O	2.20	0.42
1:A7:203:ASP:OD1	1:A7:204:ASN:N	2.53	0.42
1:A7:293:MET:CG	1:A7:367:PHE:HB2	2.50	0.42
2:B2:326:LYS:HB2	2:B2:326:LYS:HE3	1.81	0.42
1:B3:172:SER:HB3	1:B3:175:VAL:HG22	2.02	0.42
1:B3:421:GLU:HA	1:B3:424:GLN:HB3	2.02	0.42
2:B4:174:SER:HB3	2:B4:177:VAL:O	2.19	0.42
2:B6:223:THR:OG1	2:B6:224:TYR:N	2.53	0.42
1:B7:292:GLN:HG2	1:B7:298:ASN:HD22	1.85	0.42
1:B7:310:TYR:CD1	1:B7:371:SER:HB2	2.55	0.42
3:A:3593:ILE:O	3:A:3595:ALA:HA	2.20	0.42
3:A:3598:GLN:C	3:A:3991:GLN:HA	2.40	0.42
3:A:4229:ALA:HB1	3:A:4272:SER:O	2.19	0.42
4:B:271:SER:OG	4:B:272:THR:N	2.52	0.42
4:B:389:THR:O	4:B:393:TYR:HB2	2.20	0.42
4:B:2228:TYR:HA	4:B:2274:TRP:O	2.20	0.42
11:I:66:ASP:OD1	11:I:66:ASP:N	2.53	0.42
15:P:92:VAL:HG13	15:P:96:THR:OG1	2.20	0.42
16:X:256:ALA:O	16:X:260:ARG:HG2	2.19	0.42
20:Z:7:ARG:HD3	20:Z:120:MET:HA	2.00	0.42
1:A1:175:VAL:HG13	2:A2:329:ASN:ND2	2.29	0.41
1:A3:137:HIS:O	1:A3:168:SER:HA	2.20	0.41
2:A4:119:LEU:HA	2:A4:122:ILE:HG22	2.01	0.41
2:A4:141:VAL:O	2:A4:147:SER:OG	2.31	0.41
1:A5:26:ASP:O	1:A5:359:LYS:NZ	2.38	0.41
2:A6:71:GLU:HB2	2:A6:98:ASP:OD1	2.19	0.41
2:A6:267:PHE:HB2	2:A6:384:ILE:HD12	2.02	0.41
1:B1:138:SER:O	1:B1:139:LEU:HD23	2.20	0.41
2:B2:330:ALA:O	2:B2:334:THR:HG23	2.20	0.41
1:B3:103:LYS:HA	1:B3:107:THR:OG1	2.20	0.41
1:B3:391:ARG:NH2	2:B4:346:TRP:HE1	2.14	0.41
2:B4:344:VAL:HG13	2:B4:346:TRP:H	1.84	0.41
3:A:2903:VAL:O	3:A:2906:ALA:HB3	2.20	0.41
3:A:4095:PRO:O	3:A:4098:ASP:N	2.52	0.41
4:B:3913:TRP:O	4:B:3917:GLN:N	2.53	0.41
4:B:4376:LYS:O	4:B:4380:THR:N	2.26	0.41
6:D:268:ASN:O	6:D:268:ASN:ND2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:234:ALA:HB3	7:E:242:ALA:HB3	2.02	0.41
7:E:506:GLU:HA	7:E:509:LEU:HG	2.02	0.41
9:G:118:VAL:O	9:G:122:ARG:HG3	2.20	0.41
13:L:44:ILE:O	13:L:48:PHE:HB2	2.20	0.41
20:Z:31:ASP:OD1	20:Z:32:LYS:N	2.43	0.41
2:A2:63:PRO:HB2	2:A2:65:CYS:SG	2.61	0.41
1:A5:186:THR:HG23	1:A5:415:MET:SD	2.60	0.41
2:B2:189:LEU:HD11	2:B2:418:PHE:CE1	2.56	0.41
1:B7:305:PRO:HA	1:B7:373:ALA:CB	2.51	0.41
3:A:1523:LEU:O	3:A:1525:ASN:N	2.53	0.41
3:A:2571:THR:O	3:A:2574:HIS:N	2.53	0.41
3:A:2717:ALA:O	3:A:2848:VAL:HA	2.20	0.41
3:A:2867:ALA:HA	3:A:2871:SER:H	1.84	0.41
4:B:729:SER:N	4:B:732:ASP:OD2	2.52	0.41
5:C:129:PRO:O	5:C:133:GLU:N	2.42	0.41
7:E:273:GLN:HE21	7:E:273:GLN:HB3	1.53	0.41
13:L:12:ASN:HB2	13:L:75:PHE:HE2	1.84	0.41
1:A1:289:LEU:HD11	1:A1:365:ALA:HB2	2.03	0.41
2:A2:274:PRO:HB2	2:A2:276:ILE:HG12	2.02	0.41
1:A5:376:GLU:O	1:A5:380:ARG:HB2	2.19	0.41
2:B6:150:GLY:O	2:B6:154:LEU:HD23	2.20	0.41
1:B7:145:SER:OG	1:B7:146:GLY:N	2.53	0.41
1:B7:253:LEU:HD11	1:B7:316:LEU:HD21	2.02	0.41
3:A:1505:GLY:CA	3:A:1517:PHE:H	2.31	0.41
3:A:1804:PRO:HA	3:A:1834:PRO:CA	2.47	0.41
3:A:2666:GLU:H	3:A:2667:VAL:C	2.22	0.41
3:A:3956:LEU:HA	3:A:3960:ALA:H	1.83	0.41
4:B:583:TYR:CE2	4:B:682:ARG:HD3	2.55	0.41
5:C:562:LYS:HA	5:C:623:PHE:HZ	1.86	0.41
5:C:1015:LYS:HA	5:C:1018:MET:HB2	2.03	0.41
5:C:1957:LEU:HA	5:C:1960:ALA:HB3	2.02	0.41
5:C:2045:ASP:O	5:C:4365:ALA:HA	2.20	0.41
7:E:342:SER:OG	7:E:343:CYS:N	2.53	0.41
1:A1:135:VAL:HG12	1:A1:137:HIS:HD2	1.86	0.41
2:A2:428:LEU:HD21	2:A2:432:PHE:HE2	1.84	0.41
2:A4:91:GLN:NE2	2:A4:121:ARG:HH21	2.19	0.41
1:A5:117:LEU:HD23	1:A5:117:LEU:HA	1.82	0.41
2:A6:313:MET:HE3	2:A6:382:THR:HG22	2.02	0.41
2:B2:425:LEU:O	2:B2:429:GLU:HG2	2.20	0.41
1:B3:50:TYR:OH	1:B3:237:THR:HG21	2.21	0.41
3:A:1399:VAL:O	3:A:1400:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1734:LEU:O	3:A:1738:LEU:CB	2.69	0.41
4:B:385:ARG:HH22	4:B:428:CYS:HB3	1.84	0.41
4:B:543:HIS:HA	4:B:546:GLU:OE1	2.20	0.41
5:C:975:VAL:O	5:C:979:ILE:HD12	2.20	0.41
5:C:1025:THR:HA	5:C:1028:ASN:ND2	2.35	0.41
5:C:1028:ASN:ND2	5:C:1048:LYS:HE3	2.36	0.41
6:D:408:LEU:HD22	6:D:432:SER:HB3	2.02	0.41
9:G:63:ILE:O	9:G:67:ASP:N	2.39	0.41
2:A2:370:LYS:H	2:A2:370:LYS:HG2	1.61	0.41
2:A4:331:SER:O	2:A4:334:THR:OG1	2.36	0.41
1:A7:21:TRP:CZ2	1:A7:63:ALA:HB2	2.55	0.41
1:B3:3:GLU:HB2	1:B3:130:LEU:HD23	2.03	0.41
2:B4:165:SER:HA	2:B4:199:ASP:OD2	2.21	0.41
6:D:296:LEU:HA	6:D:638:LYS:O	2.20	0.41
6:D:316:CYS:SG	6:D:317:TRP:N	2.93	0.41
6:D:520:HIS:CE1	6:D:542:ARG:HH21	2.39	0.41
7:E:154:PHE:HZ	7:E:203:VAL:HG22	1.85	0.41
18:Y:184:LEU:O	18:Y:188:MET:HG2	2.20	0.41
18:Y1:189:ALA:O	18:Y1:193:GLN:HG2	2.21	0.41
2:A2:264:ARG:NH1	2:A2:431:ASP:OD2	2.54	0.41
1:A5:235:GLY:HA2	1:A5:318:ARG:HH11	1.85	0.41
1:A7:48:ASN:OD1	1:A7:48:ASN:N	2.54	0.41
1:B1:244:GLY:HA2	1:B1:355:ASP:OD2	2.20	0.41
2:B2:317:LEU:HB3	2:B2:319:TYR:CE1	2.55	0.41
1:B3:113:ILE:HD12	1:B3:113:ILE:HA	1.85	0.41
1:B5:172:SER:HB3	1:B5:205:GLU:OE2	2.21	0.41
2:B6:288:VAL:HG21	2:B6:327:ASP:CG	2.41	0.41
1:B7:267:MET:HE1	1:B7:299:MET:HG3	2.01	0.41
3:A:1688:LEU:O	3:A:1690:ASN:N	2.54	0.41
3:A:3610:ARG:O	3:A:3615:ALA:N	2.53	0.41
4:B:2691:ASP:O	4:B:2695:ALA:N	2.53	0.41
5:C:759:LEU:HD12	5:C:759:LEU:HA	1.83	0.41
2:A2:66:ILE:HG13	2:A2:66:ILE:O	2.21	0.41
2:A4:179:THR:O	1:A5:350:LYS:HA	2.20	0.41
2:A4:272:TYR:HD2	2:A4:275:ILE:HD11	1.85	0.41
1:A5:224:ASP:O	1:A5:228:LEU:HG	2.20	0.41
1:A5:273:LEU:HD23	1:A5:273:LEU:HA	1.93	0.41
2:A6:167:LEU:HB3	2:A6:169:PHE:CE1	2.55	0.41
2:B4:91:GLN:CG	2:B4:121:ARG:HH12	2.33	0.41
3:A:1747:CYS:O	3:A:1775:PHE:HA	2.20	0.41
3:A:2372:PHE:HA	3:A:2508:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:762:LEU:O	4:B:766:LYS:N	2.53	0.41
4:B:3766:LYS:O	4:B:3770:ASP:CB	2.69	0.41
5:C:390:ARG:HH22	5:C:421:ASP:N	2.19	0.41
5:C:927:LYS:O	5:C:931:THR:HG23	2.20	0.41
5:C:2447:THR:HA	5:C:2487:MET:HA	2.03	0.41
5:C:4025:GLN:O	5:C:4029:GLN:N	2.36	0.41
6:D:590:HIS:HB3	6:D:604:SER:HA	2.02	0.41
13:L:20:GLN:O	13:L:24:VAL:HG23	2.20	0.41
16:X:271:LYS:HA	16:X:271:LYS:HD3	1.84	0.41
1:A1:140:GLY:O	1:A1:184:ASN:ND2	2.54	0.41
2:A4:80:THR:HA	2:A4:84:ARG:HG2	2.02	0.41
1:A5:135:VAL:HG12	1:A5:137:HIS:HD2	1.86	0.41
1:A5:320:ARG:NH1	1:A5:355:ASP:HB3	2.36	0.41
2:A6:66:ILE:HG21	2:A6:121:ARG:HG3	2.02	0.41
2:B2:387:ILE:HG12	2:B2:390:ARG:NH2	2.33	0.41
1:B3:156:ARG:NH2	1:B3:197:ASP:OD1	2.52	0.41
1:B5:233:MET:O	1:B5:236:ILE:HG22	2.20	0.41
2:B6:2:ARG:HE	2:B6:2:ARG:HB3	1.68	0.41
2:B6:255:PHE:N	2:B6:255:PHE:CD1	2.88	0.41
3:A:1967:LEU:HA	3:A:1971:PHE:H	1.86	0.41
3:A:1996:GLY:HA3	3:A:2189:ARG:HA	2.01	0.41
3:A:3397:ALA:HA	3:A:3401:GLY:H	1.86	0.41
4:B:2056:MET:HA	4:B:2059:ALA:HB3	2.03	0.41
4:B:2528:PHE:O	4:B:2644:CYS:HA	2.21	0.41
5:C:752:LEU:HD23	5:C:752:LEU:HA	1.68	0.41
5:C:1772:ILE:O	5:C:1778:ASP:HA	2.21	0.41
7:E:495:ILE:HA	7:E:498:MET:HG2	2.03	0.41
18:Y1:202:ARG:HE	18:Y1:206:ILE:HD11	1.86	0.41
20:Z:155:HIS:CG	20:Z:156:CYS:N	2.89	0.41
2:A2:8:HIS:O	2:A2:68:LEU:HD23	2.21	0.41
2:A2:55:GLU:OE1	2:A2:61:HIS:ND1	2.53	0.41
2:A2:392:ASP:OD1	2:A2:422:ARG:NH1	2.53	0.41
2:A2:405:VAL:HG21	20:Z:168:ARG:NH2	2.36	0.41
1:A3:23:VAL:HG11	1:A3:230:SER:HB2	2.03	0.41
1:A3:135:VAL:HG12	1:A3:137:HIS:HD2	1.86	0.41
1:A3:257:LEU:HD13	1:A3:314:SER:OG	2.20	0.41
2:A4:381:SER:OG	2:A4:382:THR:N	2.54	0.41
1:A5:91:VAL:CG1	1:A5:116:VAL:HG22	2.51	0.41
1:A5:112:LEU:HD12	1:A5:112:LEU:HA	1.93	0.41
1:A5:313:ALA:HB3	1:A5:349:VAL:HG22	2.02	0.41
1:A5:404:ASP:CG	1:A5:405:GLU:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A7:6:HIS:CE1	1:A7:8:GLN:HG2	2.56	0.41
1:B1:322:SER:OG	1:B1:325:GLU:HG3	2.21	0.41
2:B2:155:GLU:HG2	2:B2:197:HIS:NE2	2.35	0.41
2:B2:304:LYS:HD3	2:B2:304:LYS:HA	1.89	0.41
1:B3:139:LEU:HD22	1:B3:188:SER:HB2	2.03	0.41
1:B5:73:MET:HA	1:B5:73:MET:CE	2.50	0.41
1:B5:91:VAL:CG1	1:B5:116:VAL:HG12	2.49	0.41
2:B6:21:TRP:CZ2	2:B6:65:CYS:HB3	2.55	0.41
1:B7:359:LYS:HD2	1:B7:359:LYS:HA	1.88	0.41
3:A:1572:VAL:O	3:A:1576:ILE:CB	2.69	0.41
3:A:1780:PRO:O	3:A:3944:LEU:O	2.39	0.41
3:A:2706:ILE:O	3:A:2710:VAL:CB	2.69	0.41
3:A:4379:PRO:HA	3:A:4380:LEU:HA	1.54	0.41
4:B:738:ASP:HA	4:B:741:ARG:HH11	1.86	0.41
4:B:2807:ALA:HB3	4:B:2823:ASN:O	2.20	0.41
5:C:931:THR:HG22	5:C:934:LYS:HZ1	1.85	0.41
6:D:302:PHE:CZ	6:D:325:PHE:HE2	2.39	0.41
7:E:243:TYR:CD2	7:E:254:GLU:HB2	2.53	0.41
7:E:272:LEU:HD13	7:E:322:TYR:HE2	1.86	0.41
7:E:371:ASN:N	7:E:377:TYR:O	2.53	0.41
7:E:417:SER:O	7:E:417:SER:OG	2.29	0.41
12:J:23:VAL:O	12:J:87:PHE:HB2	2.21	0.41
16:X1:132:LEU:HD12	18:Y1:83:LEU:HD22	2.03	0.41
2:A2:155:GLU:HA	2:A2:197:HIS:CE1	2.56	0.41
2:A2:222:PRO:HD2	1:A3:324:LYS:HD3	2.01	0.41
1:A3:199:CYS:HB3	1:A3:265:PHE:CD1	2.56	0.41
2:A4:7:ILE:CG2	2:A4:137:VAL:HG12	2.51	0.41
1:A5:9:GLY:HA2	1:A5:66:MET:O	2.21	0.41
1:A5:67:ASP:CG	1:A5:68:LEU:H	2.22	0.41
1:A5:183:TYR:HD2	1:A5:398:TYR:CE2	2.39	0.41
1:A7:416:ASN:O	1:A7:419:VAL:HG22	2.21	0.41
1:B7:150:LEU:HD12	1:B7:150:LEU:C	2.41	0.41
3:A:1490:LEU:HA	3:A:1503:ALA:HA	2.02	0.41
3:A:2066:ILE:O	3:A:2113:ASP:N	2.53	0.41
3:A:2560:ARG:C	3:A:2569:GLU:HA	2.42	0.41
4:B:155:PHE:HE1	5:C:155:PHE:HE2	1.68	0.41
4:B:3988:GLY:C	4:B:3998:GLY:HA2	2.40	0.41
5:C:672:LYS:NZ	5:C:687:MET:O	2.44	0.41
5:C:732:ARG:NH1	5:C:732:ARG:HB2	2.35	0.41
5:C:2493:ASP:HA	5:C:2542:MET:HA	2.03	0.41
6:D:318:ASN:HB3	6:D:368:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:432:SER:OG	6:D:433:SER:N	2.53	0.41
7:E:339:GLN:HB3	7:E:357:VAL:HG23	2.02	0.41
13:K:40:ILE:HG22	13:K:60:VAL:HG21	2.02	0.41
20:Z:152:GLU:HA	20:Z:155:HIS:ND1	2.36	0.41
1:A1:240:LEU:HD11	1:A1:250:LEU:HD13	2.03	0.40
1:A1:285:THR:HG22	1:A1:288:GLU:OE1	2.20	0.40
1:A1:391:ARG:O	1:A1:391:ARG:HG2	2.21	0.40
2:A2:434:GLU:HG3	2:A2:435:VAL:N	2.36	0.40
1:A3:14:ASN:OD1	1:A3:65:LEU:HD22	2.22	0.40
1:A3:178:THR:HG22	1:A3:179:VAL:H	1.86	0.40
2:A4:73:THR:CG2	1:A5:2:ARG:HH22	2.34	0.40
1:A7:105:HIS:CD2	1:A7:150:LEU:HB2	2.55	0.40
1:B3:145:SER:OG	1:B3:146:GLY:N	2.53	0.40
1:B3:391:ARG:HE	2:B4:346:TRP:HE1	1.69	0.40
2:B4:11:GLN:HB3	21:B5:501:GTP:PA	2.61	0.40
2:B4:114:ILE:HG23	2:B4:149:LEU:HD11	2.03	0.40
1:B7:314:SER:OG	1:B7:368:ILE:HB	2.21	0.40
3:A:1282:MET:HA	3:A:1285:ALA:HB3	2.02	0.40
3:A:2544:ILE:HA	3:A:2547:ALA:CB	2.50	0.40
3:A:3280:ALA:HA	3:A:3320:PRO:CB	2.51	0.40
3:A:3616:PRO:HA	3:A:3623:LYS:CA	2.39	0.40
4:B:756:LYS:HA	4:B:759:ARG:HG2	2.03	0.40
16:X1:121:GLN:OE1	18:Y1:69:ALA:HB3	2.21	0.40
16:X1:147:ARG:O	16:X1:150:GLU:HG2	2.21	0.40
20:Z:148:LEU:HD12	20:Z:148:LEU:HA	1.88	0.40
1:A1:409:THR:O	1:A1:412:GLU:HG3	2.22	0.40
1:A3:283:ALA:HB3	1:A3:288:GLU:OE2	2.21	0.40
2:A4:157:LEU:HD23	2:A4:157:LEU:HA	1.91	0.40
2:A4:407:TRP:CD1	1:A5:255:VAL:HG23	2.57	0.40
2:A6:123:ARG:NE	2:A6:123:ARG:HA	2.37	0.40
1:A7:304:ASP:OD2	1:A7:306:ARG:HG2	2.22	0.40
2:B2:276:ILE:HG23	2:B2:281:ALA:HB2	2.01	0.40
2:B2:322:ASP:HB2	2:B2:373:ARG:HH21	1.86	0.40
1:B3:167:PHE:CE2	1:B3:200:MET:HE2	2.55	0.40
1:B3:167:PHE:CZ	1:B3:233:MET:HG2	2.56	0.40
2:B4:221:ARG:HG2	1:B5:322:SER:CB	2.52	0.40
2:B6:273:ALA:HA	2:B6:274:PRO:HA	1.80	0.40
1:B7:3:GLU:HG3	1:B7:127:CYS:HB2	2.04	0.40
1:B7:399:THR:HA	1:B7:403:MET:O	2.21	0.40
3:A:4406:VAL:O	3:A:4442:VAL:CB	2.69	0.40
4:B:597:ILE:HG23	4:B:628:TRP:NE1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:681:CYS:SG	5:C:682:SER:N	2.95	0.40
5:C:850:LYS:O	5:C:853:SER:OG	2.31	0.40
13:L:78:PHE:N	13:L:85:ILE:O	2.53	0.40
15:P:57:LYS:HB3	15:P:70:VAL:HG23	2.03	0.40
16:X:249:GLU:OE1	16:X:253:ARG:NH2	2.48	0.40
20:Z:73:LEU:O	20:Z:77:THR:HG23	2.21	0.40
1:A1:303:ALA:HB2	1:A1:377:MET:HE2	2.03	0.40
2:A2:167:LEU:HB3	2:A2:169:PHE:CE1	2.57	0.40
1:A3:35:THR:HA	1:A3:57:GLY:O	2.20	0.40
1:A3:170:VAL:HG22	1:A3:202:LEU:O	2.21	0.40
2:A4:151:SER:HB2	2:A4:193:SER:OG	2.21	0.40
1:A5:407:GLU:O	1:A5:410:GLU:HG2	2.22	0.40
2:A6:210:TYR:CG	1:A7:324:LYS:HG3	2.55	0.40
2:A6:312:TYR:HD1	2:A6:381:SER:HB2	1.86	0.40
1:A7:157:GLU:HA	1:A7:157:GLU:OE1	2.21	0.40
1:A7:260:PHE:HB2	1:A7:263:LEU:HD23	2.02	0.40
1:A7:415:MET:O	1:A7:418:LEU:HG	2.21	0.40
1:B1:350:LYS:HD2	1:B1:351:SER:H	1.86	0.40
2:B2:335:ILE:HD13	2:B2:335:ILE:HA	1.93	0.40
2:B4:75:VAL:HG11	2:B4:94:SER:CB	2.47	0.40
2:B6:62:VAL:HA	2:B6:63:PRO:HD3	1.93	0.40
2:B6:100:ALA:HA	1:B7:252:LYS:HE3	2.03	0.40
1:B7:167:PHE:CD1	1:B7:167:PHE:N	2.88	0.40
1:B7:267:MET:HG2	1:B7:369:GLY:O	2.21	0.40
3:A:1897:ALA:O	3:A:1901:TYR:N	2.46	0.40
3:A:2223:LEU:O	3:A:2227:LYS:N	2.54	0.40
3:A:2501:LEU:O	3:A:2503:ARG:N	2.54	0.40
3:A:2688:ASN:HA	3:A:3426:PHE:HA	2.02	0.40
4:B:3415:ARG:HA	4:B:3418:ALA:HB3	2.03	0.40
7:E:202:ASP:OD1	7:E:203:VAL:N	2.54	0.40
7:E:248:LYS:HE3	7:E:248:LYS:HB3	1.96	0.40
7:E:374:ASN:ND2	7:E:489:PRO:HB2	2.36	0.40
2:A2:306:ASP:OD2	2:A2:308:ARG:HB2	2.22	0.40
1:A3:421:GLU:HA	1:A3:424:GLN:HG2	2.02	0.40
2:A6:327:ASP:N	2:A6:327:ASP:OD1	2.55	0.40
1:A7:140:GLY:O	1:A7:184:ASN:ND2	2.48	0.40
1:B1:139:LEU:HD22	1:B1:188:SER:CB	2.51	0.40
1:B5:86:ARG:HB3	1:B5:89:ASN:ND2	2.37	0.40
3:A:2713:PRO:HA	3:A:2843:THR:O	2.20	0.40
3:A:3898:ALA:HB2	3:A:3936:TRP:CB	2.51	0.40
3:A:4096:TRP:O	3:A:4100:GLN:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:4482:LEU:HA	4:B:4564:PHE:O	2.21	0.40
5:C:151:SER:O	5:C:154:LYS:HG3	2.20	0.40
7:E:166:TYR:HE1	7:E:168:ASN:HB3	1.85	0.40
7:E:286:ASP:O	7:E:314:THR:HA	2.21	0.40
11:I:79:HIS:O	11:I:79:HIS:ND1	2.54	0.40
13:L:36:ILE:HG12	13:L:37:GLU:H	1.87	0.40
13:M:40:ILE:HG21	13:M:60:VAL:HG21	2.04	0.40
20:Z:172:LYS:HA	20:Z:172:LYS:HD3	1.84	0.40
2:A2:219:ILE:HG13	2:A2:219:ILE:O	2.21	0.40
2:A2:312:TYR:O	2:A2:344:VAL:HG23	2.21	0.40
1:A3:185:ALA:HB3	1:A3:381:VAL:HG21	2.04	0.40
1:A3:256:ASN:HD22	1:A3:350:LYS:HE2	1.86	0.40
1:A3:330:MET:SD	1:A3:349:VAL:HG11	2.62	0.40
2:A4:55:GLU:HG3	2:A4:57:GLY:H	1.87	0.40
1:A5:70:PRO:HG2	2:A6:2:ARG:NH2	2.36	0.40
2:A6:66:ILE:HG23	2:A6:125:LEU:HD11	2.04	0.40
2:A6:124:LYS:HA	2:A6:127:ASP:HB2	2.04	0.40
2:A6:175:PRO:HG2	2:A6:176:GLN:OE1	2.21	0.40
2:A6:205:ASP:CB	2:A6:303:VAL:HA	2.52	0.40
1:B1:21:TRP:O	1:B1:25:SER:OG	2.32	0.40
1:B1:256:ASN:O	1:B1:312:THR:HG21	2.22	0.40
2:B2:5:ILE:HG22	2:B2:64:ARG:HD3	2.02	0.40
1:B3:396:HIS:CD2	2:B4:263:PRO:HG3	2.56	0.40
1:B5:8:GLN:CD	1:B5:17:GLY:HA3	2.42	0.40
1:B5:117:LEU:HA	1:B5:117:LEU:HD23	1.91	0.40
3:A:1399:VAL:O	3:A:1402:VAL:N	2.54	0.40
3:A:4057:GLY:O	3:A:4322:VAL:HA	2.22	0.40
4:B:566:LEU:HD11	7:E:406:PRO:HA	2.03	0.40
4:B:2143:LEU:O	4:B:2147:PHE:N	2.39	0.40
4:B:3103:SER:HA	4:B:3585:LYS:O	2.22	0.40
5:C:2104:GLY:O	5:C:2107:ALA:N	2.54	0.40
7:E:304:MET:O	7:E:306:LEU:HD12	2.21	0.40
9:G:62:MET:O	9:G:65:GLN:HG2	2.22	0.40
9:G:127:GLU:H	9:G:127:GLU:HG2	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
1	A3	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	A5	424/443 (96%)	407 (96%)	17 (4%)	0	100	100
1	A7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	B1	415/443 (94%)	396 (95%)	19 (5%)	0	100	100
1	B3	404/443 (91%)	392 (97%)	12 (3%)	0	100	100
1	B5	424/443 (96%)	403 (95%)	21 (5%)	0	100	100
1	B7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
2	A2	426/451 (94%)	402 (94%)	24 (6%)	0	100	100
2	A4	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
2	A6	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	B2	405/451 (90%)	391 (96%)	14 (4%)	0	100	100
2	B4	403/451 (89%)	385 (96%)	18 (4%)	0	100	100
2	B6	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	A	3266/4503 (72%)	2704 (83%)	550 (17%)	12 (0%)	34	72
4	B	3500/4568 (77%)	3121 (89%)	377 (11%)	2 (0%)	51	86
5	C	3840/4485 (86%)	3484 (91%)	353 (9%)	3 (0%)	51	86
6	D	450/683 (66%)	387 (86%)	63 (14%)	0	100	100
7	E	470/567 (83%)	371 (79%)	94 (20%)	5 (1%)	14	52
8	F	98/136 (72%)	94 (96%)	4 (4%)	0	100	100
9	G	134/159 (84%)	125 (93%)	9 (7%)	0	100	100
10	H	89/120 (74%)	77 (86%)	12 (14%)	0	100	100
11	I	101/105 (96%)	89 (88%)	11 (11%)	1 (1%)	15	54
12	J	92/100 (92%)	81 (88%)	11 (12%)	0	100	100
13	K	80/91 (88%)	73 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	L	80/91 (88%)	72 (90%)	8 (10%)	0	100	100
13	M	80/91 (88%)	73 (91%)	7 (9%)	0	100	100
13	N	80/91 (88%)	68 (85%)	12 (15%)	0	100	100
14	O	95/117 (81%)	92 (97%)	3 (3%)	0	100	100
15	P	96/103 (93%)	89 (93%)	7 (7%)	0	100	100
16	X	54/749 (7%)	54 (100%)	0	0	100	100
16	X1	140/749 (19%)	140 (100%)	0	0	100	100
18	Y	71/552 (13%)	71 (100%)	0	0	100	100
18	Y1	145/552 (26%)	145 (100%)	0	0	100	100
20	Z	168/184 (91%)	155 (92%)	11 (6%)	2 (1%)	13	50
All	All	18997/25046 (76%)	17179 (90%)	1793 (9%)	25 (0%)	54	86

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1677	CYS
4	B	625	ASP
4	B	1876	ASP
5	C	4432	LEU
7	E	298	ASN
11	I	85	PRO
20	Z	86	LYS
20	Z	141	ASP
3	A	1793	VAL
7	E	295	ARG
3	A	1678	ASP
3	A	4231	GLU
5	C	114	TRP
7	E	269	PHE
3	A	4139	PRO
3	A	4247	GLU
7	E	231	LEU
3	A	4147	ALA
3	A	4148	PRO
3	A	1830	GLY
3	A	4138	ASN
7	E	209	PRO
3	A	1805	GLY

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Mol	Chain	Res	Type
3	A	4438	PRO
5	C	839	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	367/379 (97%)	367 (100%)	0	100	100
1	A3	367/379 (97%)	366 (100%)	1 (0%)	92	95
1	A5	367/379 (97%)	367 (100%)	0	100	100
1	A7	367/379 (97%)	367 (100%)	0	100	100
1	B1	363/379 (96%)	363 (100%)	0	100	100
1	B3	356/379 (94%)	356 (100%)	0	100	100
1	B5	367/379 (97%)	367 (100%)	0	100	100
1	B7	367/379 (97%)	366 (100%)	1 (0%)	92	95
2	A2	361/374 (96%)	360 (100%)	1 (0%)	92	95
2	A4	359/374 (96%)	354 (99%)	5 (1%)	67	80
2	A6	361/374 (96%)	361 (100%)	0	100	100
2	B2	347/374 (93%)	347 (100%)	0	100	100
2	B4	346/374 (92%)	346 (100%)	0	100	100
2	B6	359/374 (96%)	359 (100%)	0	100	100
4	B	463/3998 (12%)	455 (98%)	8 (2%)	60	78
5	C	702/3945 (18%)	696 (99%)	6 (1%)	78	87
6	D	401/584 (69%)	396 (99%)	5 (1%)	71	83
7	E	400/489 (82%)	396 (99%)	4 (1%)	76	86
9	G	121/136 (89%)	121 (100%)	0	100	100
11	I	90/91 (99%)	89 (99%)	1 (1%)	73	84
12	J	83/87 (95%)	83 (100%)	0	100	100
13	K	70/76 (92%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	L	70/76 (92%)	69 (99%)	1 (1%)	67	80
13	M	70/76 (92%)	70 (100%)	0	100	100
15	P	86/90 (96%)	86 (100%)	0	100	100
16	X	50/618 (8%)	50 (100%)	0	100	100
16	X1	125/618 (20%)	121 (97%)	4 (3%)	39	61
18	Y	59/462 (13%)	59 (100%)	0	100	100
18	Y1	128/462 (28%)	127 (99%)	1 (1%)	81	89
20	Z	150/162 (93%)	146 (97%)	4 (3%)	44	65
All	All	8122/17246 (47%)	8080 (100%)	42 (0%)	89	93

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A2	73	THR
1	A3	390	ARG
2	A4	51	THR
2	A4	62	VAL
2	A4	346	TRP
2	A4	347	CYS
2	A4	349	THR
1	B7	72	THR
4	B	124	GLN
4	B	596	ARG
4	B	598	LYS
4	B	627	LEU
4	B	628	TRP
4	B	629	GLU
4	B	731	LYS
4	B	799	LYS
5	C	120	LYS
5	C	154	LYS
5	C	200	LEU
5	C	204	GLU
5	C	295	LYS
5	C	956	ARG
6	D	268	ASN
6	D	270	ASN
6	D	309	ARG
6	D	312	VAL

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Mol	Chain	Res	Type
6	D	672	LYS
7	E	273	GLN
7	E	279	GLU
7	E	296	LYS
7	E	507	LYS
11	I	70	LYS
13	L	45	LYS
16	X1	204	LEU
16	X1	208	ARG
16	X1	213	HIS
16	X1	214	LEU
18	Y1	166	GLU
20	Z	9	ARG
20	Z	10	TYR
20	Z	122	LEU
20	Z	123	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	A2	11	GLN
2	A2	101	ASN
2	A2	329	ASN
1	A3	6	HIS
1	A3	131	GLN
1	A3	134	GLN
1	A3	195	ASN
1	A3	256	ASN
2	A4	91	GLN
2	A4	102	ASN
2	A4	228	ASN
1	A7	190	HIS
1	A7	204	ASN
1	B1	6	HIS
1	B1	131	GLN
1	B1	334	GLN
2	B2	256	GLN
2	B2	329	ASN
1	B3	15	GLN
1	B3	190	HIS
2	B4	88	HIS
2	B4	102	ASN

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Mol	Chain	Res	Type
2	B4	258	ASN
2	B4	329	ASN
1	B5	15	GLN
1	B5	99	ASN
1	B5	100	ASN
1	B5	347	ASN
1	B5	348	ASN
1	B5	384	GLN
2	B6	102	ASN
2	B6	329	ASN
1	B7	100	ASN
1	B7	334	GLN
1	B7	375	GLN
5	C	500	GLN
5	C	504	ASN
5	C	515	HIS
6	D	576	GLN
7	E	158	ASN
7	E	205	ASN
7	E	273	GLN
7	E	374	ASN
9	G	65	GLN
16	X1	240	HIS
20	Z	17	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	GDP	A3	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
21	GTP	A7	501	22	26,34,34	1.20	2 (7%)	32,54,54	1.67	7 (21%)
21	GTP	A1	501	22	26,34,34	1.13	2 (7%)	32,54,54	1.64	7 (21%)
23	GDP	A7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	5 (16%)
23	GDP	A1	503	-	24,30,30	0.95	1 (4%)	30,47,47	1.28	4 (13%)
21	GTP	A3	501	22	26,34,34	1.18	2 (7%)	32,54,54	1.72	7 (21%)
23	GDP	A5	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	5 (16%)
21	GTP	A5	501	22	26,34,34	1.22	2 (7%)	32,54,54	1.66	7 (21%)
21	GTP	B7	501	22	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)
23	GDP	B7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	5 (16%)
21	GTP	B2	501	22	26,34,34	1.19	2 (7%)	32,54,54	1.73	7 (21%)
21	GTP	B5	501	22	26,34,34	1.21	2 (7%)	32,54,54	1.62	7 (21%)
23	GDP	B5	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
23	GDP	B3	502	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
23	GDP	B1	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.34	4 (13%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	A3	502	-	-	1/12/32/32	0/3/3/3
21	GTP	A7	501	22	-	7/18/38/38	0/3/3/3
21	GTP	A1	501	22	-	5/18/38/38	0/3/3/3
23	GDP	A7	502	-	-	4/12/32/32	0/3/3/3
23	GDP	A1	503	-	-	3/12/32/32	0/3/3/3
21	GTP	A3	501	22	-	7/18/38/38	0/3/3/3
23	GDP	A5	502	-	-	1/12/32/32	0/3/3/3
21	GTP	A5	501	22	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	GTP	B7	501	22	-	6/18/38/38	0/3/3/3
23	GDP	B7	502	-	-	6/12/32/32	0/3/3/3
21	GTP	B2	501	22	-	4/18/38/38	0/3/3/3
21	GTP	B5	501	22	-	7/18/38/38	0/3/3/3
23	GDP	B5	502	-	-	4/12/32/32	0/3/3/3
23	GDP	B3	502	-	-	3/12/32/32	0/3/3/3
23	GDP	B1	501	-	-	2/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A7	501	GTP	C5-C6	-4.28	1.38	1.47
21	B7	501	GTP	C5-C6	-4.26	1.38	1.47
21	A5	501	GTP	C5-C6	-4.26	1.38	1.47
21	B5	501	GTP	C5-C6	-4.24	1.38	1.47
21	B2	501	GTP	C5-C6	-4.16	1.39	1.47
21	A3	501	GTP	C5-C6	-4.07	1.39	1.47
21	A1	501	GTP	C5-C6	-3.93	1.39	1.47
23	A3	502	GDP	C6-N1	-2.64	1.33	1.37
23	B5	502	GDP	C6-N1	-2.62	1.34	1.37
23	B1	501	GDP	C6-N1	-2.59	1.34	1.37
23	B3	502	GDP	C6-N1	-2.54	1.34	1.37
23	A7	502	GDP	C6-N1	-2.53	1.34	1.37
23	B7	502	GDP	C6-N1	-2.49	1.34	1.37
23	A5	502	GDP	C6-N1	-2.38	1.34	1.37
23	A1	503	GDP	C6-N1	-2.38	1.34	1.37
21	A1	501	GTP	C2-N3	2.21	1.38	1.33
21	A3	501	GTP	C2-N3	2.17	1.38	1.33
21	B7	501	GTP	C2-N3	2.17	1.38	1.33
21	B5	501	GTP	C2-N3	2.12	1.38	1.33
21	A5	501	GTP	C2-N3	2.12	1.38	1.33
21	B2	501	GTP	C2-N3	2.07	1.38	1.33
21	A7	501	GTP	C2-N3	2.02	1.38	1.33

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B2	501	GTP	PB-O3B-PG	-5.00	115.69	132.83
21	A5	501	GTP	PA-O3A-PB	-4.67	116.82	132.83
21	A3	501	GTP	PB-O3B-PG	-4.46	117.52	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A3	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
21	A7	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
21	B5	501	GTP	PA-O3A-PB	-4.33	117.98	132.83
21	A1	501	GTP	PA-O3A-PB	-4.06	118.90	132.83
21	A1	501	GTP	PB-O3B-PG	-3.97	119.19	132.83
23	B3	502	GDP	PA-O3A-PB	-3.93	119.34	132.83
21	B2	501	GTP	PA-O3A-PB	-3.85	119.61	132.83
21	A7	501	GTP	PB-O3B-PG	-3.82	119.72	132.83
23	B7	502	GDP	PA-O3A-PB	-3.65	120.32	132.83
21	B7	501	GTP	PB-O3B-PG	-3.63	120.38	132.83
23	B5	502	GDP	PA-O3A-PB	-3.52	120.75	132.83
21	B5	501	GTP	C5-C6-N1	3.45	120.04	113.95
21	A3	501	GTP	C5-C6-N1	3.44	120.03	113.95
23	B1	501	GDP	PA-O3A-PB	-3.43	121.06	132.83
21	B7	501	GTP	PA-O3A-PB	-3.40	121.16	132.83
21	A5	501	GTP	PB-O3B-PG	-3.37	121.25	132.83
21	A5	501	GTP	C5-C6-N1	3.31	119.80	113.95
21	B7	501	GTP	C5-C6-N1	3.30	119.78	113.95
21	B2	501	GTP	C5-C6-N1	3.30	119.78	113.95
21	A7	501	GTP	C5-C6-N1	3.28	119.75	113.95
23	B1	501	GDP	C3'-C2'-C1'	3.25	105.87	100.98
21	A1	501	GTP	C5-C6-N1	3.23	119.66	113.95
23	A1	503	GDP	PA-O3A-PB	-3.22	121.76	132.83
23	B7	502	GDP	C3'-C2'-C1'	3.20	105.80	100.98
21	B5	501	GTP	PB-O3B-PG	-3.17	121.96	132.83
23	A3	502	GDP	PA-O3A-PB	-3.15	122.01	132.83
21	B2	501	GTP	C8-N7-C5	3.11	108.91	102.99
23	A5	502	GDP	PA-O3A-PB	-3.11	122.16	132.83
21	A1	501	GTP	C8-N7-C5	3.06	108.82	102.99
23	A3	502	GDP	C3'-C2'-C1'	3.05	105.56	100.98
21	A7	501	GTP	C8-N7-C5	3.04	108.78	102.99
21	A3	501	GTP	C2-N1-C6	-3.04	119.50	125.10
21	B5	501	GTP	C2-N1-C6	-3.04	119.50	125.10
23	A1	503	GDP	C3'-C2'-C1'	3.04	105.55	100.98
21	A3	501	GTP	C8-N7-C5	3.03	108.75	102.99
21	B7	501	GTP	C2-N1-C6	-3.02	119.54	125.10
23	A5	502	GDP	C3'-C2'-C1'	3.01	105.50	100.98
21	B5	501	GTP	C8-N7-C5	2.99	108.69	102.99
21	B7	501	GTP	C8-N7-C5	2.99	108.69	102.99
21	A5	501	GTP	C8-N7-C5	2.98	108.67	102.99
23	A7	502	GDP	PA-O3A-PB	-2.96	122.66	132.83
21	B2	501	GTP	C2-N1-C6	-2.94	119.69	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A7	501	GTP	C2-N1-C6	-2.92	119.71	125.10
21	A5	501	GTP	C2-N1-C6	-2.92	119.71	125.10
21	B2	501	GTP	O4'-C1'-C2'	-2.90	102.69	106.93
23	B3	502	GDP	C3'-C2'-C1'	2.87	105.29	100.98
21	A1	501	GTP	C2-N1-C6	-2.86	119.83	125.10
23	A7	502	GDP	C3'-C2'-C1'	2.84	105.25	100.98
23	B5	502	GDP	C3'-C2'-C1'	2.77	105.14	100.98
21	B5	501	GTP	C3'-C2'-C1'	2.70	105.04	100.98
21	A5	501	GTP	C3'-C2'-C1'	2.58	104.86	100.98
21	A5	501	GTP	O6-C6-C5	-2.53	119.43	124.37
21	A1	501	GTP	C3'-C2'-C1'	2.52	104.78	100.98
21	A7	501	GTP	C3'-C2'-C1'	2.49	104.73	100.98
23	A3	502	GDP	C5-C6-N1	2.47	118.31	113.95
21	A3	501	GTP	C3'-C2'-C1'	2.43	104.64	100.98
21	A7	501	GTP	O6-C6-C5	-2.40	119.67	124.37
23	A5	502	GDP	C5-C6-N1	2.39	118.18	113.95
23	B1	501	GDP	C8-N7-C5	2.39	107.55	102.99
23	B1	501	GDP	C5-C6-N1	2.39	118.17	113.95
23	A5	502	GDP	C8-N7-C5	2.38	107.53	102.99
23	A1	503	GDP	C5-C6-N1	2.38	118.15	113.95
23	B5	502	GDP	C5-C6-N1	2.37	118.13	113.95
21	B7	501	GTP	C3'-C2'-C1'	2.36	104.53	100.98
23	B3	502	GDP	C5-C6-N1	2.35	118.10	113.95
23	A1	503	GDP	C8-N7-C5	2.32	107.42	102.99
23	B3	502	GDP	C8-N7-C5	2.31	107.40	102.99
23	A7	502	GDP	C8-N7-C5	2.31	107.39	102.99
23	B5	502	GDP	C8-N7-C5	2.29	107.35	102.99
23	A7	502	GDP	C5-C6-N1	2.29	118.00	113.95
23	B7	502	GDP	C8-N7-C5	2.29	107.34	102.99
23	B7	502	GDP	O4'-C4'-C5'	-2.28	101.86	109.37
23	B7	502	GDP	C5-C6-N1	2.28	117.98	113.95
23	A3	502	GDP	C8-N7-C5	2.27	107.32	102.99
21	B2	501	GTP	O6-C6-C5	-2.26	119.96	124.37
21	B7	501	GTP	O6-C6-C5	-2.24	120.00	124.37
21	B5	501	GTP	O6-C6-C5	-2.19	120.09	124.37
23	A3	502	GDP	O3B-PB-O3A	2.17	111.91	104.64
21	A1	501	GTP	O6-C6-C5	-2.09	120.28	124.37
21	A3	501	GTP	O6-C6-C5	-2.08	120.31	124.37
23	A7	502	GDP	O3B-PB-O3A	2.08	111.60	104.64
23	A5	502	GDP	O3B-PB-O3A	2.02	111.41	104.64

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A1	501	GTP	C5'-O5'-PA-O1A
21	A3	501	GTP	C5'-O5'-PA-O1A
21	A3	501	GTP	C5'-O5'-PA-O2A
21	A5	501	GTP	C5'-O5'-PA-O1A
21	A7	501	GTP	C5'-O5'-PA-O1A
21	A7	501	GTP	C5'-O5'-PA-O2A
21	B2	501	GTP	C5'-O5'-PA-O3A
21	B5	501	GTP	C5'-O5'-PA-O1A
21	B5	501	GTP	C5'-O5'-PA-O2A
21	B7	501	GTP	C5'-O5'-PA-O3A
21	B7	501	GTP	C5'-O5'-PA-O2A
23	A1	503	GDP	PA-O3A-PB-O3B
23	A1	503	GDP	C5'-O5'-PA-O1A
23	A7	502	GDP	PA-O3A-PB-O3B
23	B1	501	GDP	C5'-O5'-PA-O3A
23	B1	501	GDP	C5'-O5'-PA-O1A
23	B3	502	GDP	PA-O3A-PB-O3B
23	B3	502	GDP	C5'-O5'-PA-O1A
23	B5	502	GDP	C5'-O5'-PA-O1A
23	B7	502	GDP	PA-O3A-PB-O3B
23	B7	502	GDP	C5'-O5'-PA-O3A
23	B7	502	GDP	C5'-O5'-PA-O1A
23	B7	502	GDP	C3'-C4'-C5'-O5'
21	A7	501	GTP	C3'-C4'-C5'-O5'
21	A5	501	GTP	C3'-C4'-C5'-O5'
23	B7	502	GDP	O4'-C4'-C5'-O5'
21	A5	501	GTP	O4'-C4'-C5'-O5'
21	B5	501	GTP	C3'-C4'-C5'-O5'
23	B7	502	GDP	PA-O3A-PB-O1B
21	A7	501	GTP	O4'-C4'-C5'-O5'
21	A3	501	GTP	C4'-C5'-O5'-PA
21	A7	501	GTP	C4'-C5'-O5'-PA
21	B2	501	GTP	C4'-C5'-O5'-PA
21	B7	501	GTP	PB-O3A-PA-O5'
23	A1	503	GDP	PA-O3A-PB-O2B
21	A7	501	GTP	C5'-O5'-PA-O3A
21	A1	501	GTP	C4'-C5'-O5'-PA
21	B5	501	GTP	C4'-C5'-O5'-PA
21	B7	501	GTP	C4'-C5'-O5'-PA
21	A1	501	GTP	C5'-O5'-PA-O2A
21	A5	501	GTP	C5'-O5'-PA-O2A
21	B2	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
21	A5	501	GTP	C4'-C5'-O5'-PA
21	B5	501	GTP	O4'-C4'-C5'-O5'
21	A7	501	GTP	PA-O3A-PB-O2B
23	A7	502	GDP	C3'-C4'-C5'-O5'
23	B3	502	GDP	PA-O3A-PB-O1B
21	A3	501	GTP	C3'-C4'-C5'-O5'
21	B7	501	GTP	PA-O3A-PB-O1B
23	A7	502	GDP	PA-O3A-PB-O1B
23	B5	502	GDP	PA-O3A-PB-O1B
21	B2	501	GTP	PB-O3B-PG-O3G
21	A1	501	GTP	C5'-O5'-PA-O3A
21	A3	501	GTP	C5'-O5'-PA-O3A
21	A5	501	GTP	C5'-O5'-PA-O3A
21	B5	501	GTP	C5'-O5'-PA-O3A
23	B5	502	GDP	C5'-O5'-PA-O3A
21	A1	501	GTP	C3'-C4'-C5'-O5'
23	B5	502	GDP	C3'-C4'-C5'-O5'
21	A3	501	GTP	PA-O3A-PB-O1B
21	A3	501	GTP	PA-O3A-PB-O2B
21	B5	501	GTP	PA-O3A-PB-O2B
21	B7	501	GTP	PA-O3A-PB-O2B
23	A3	502	GDP	C5'-O5'-PA-O1A
23	A5	502	GDP	C5'-O5'-PA-O1A
23	A7	502	GDP	C5'-O5'-PA-O1A

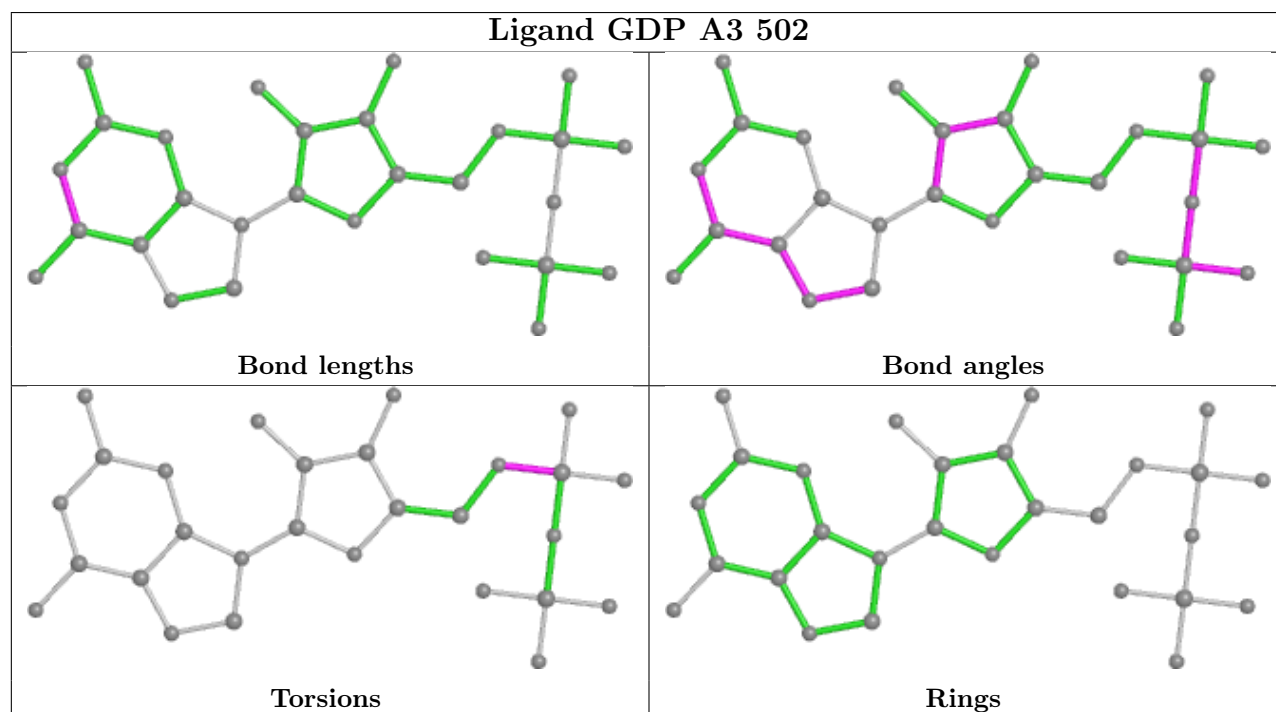
There are no ring outliers.

11 monomers are involved in 19 short contacts:

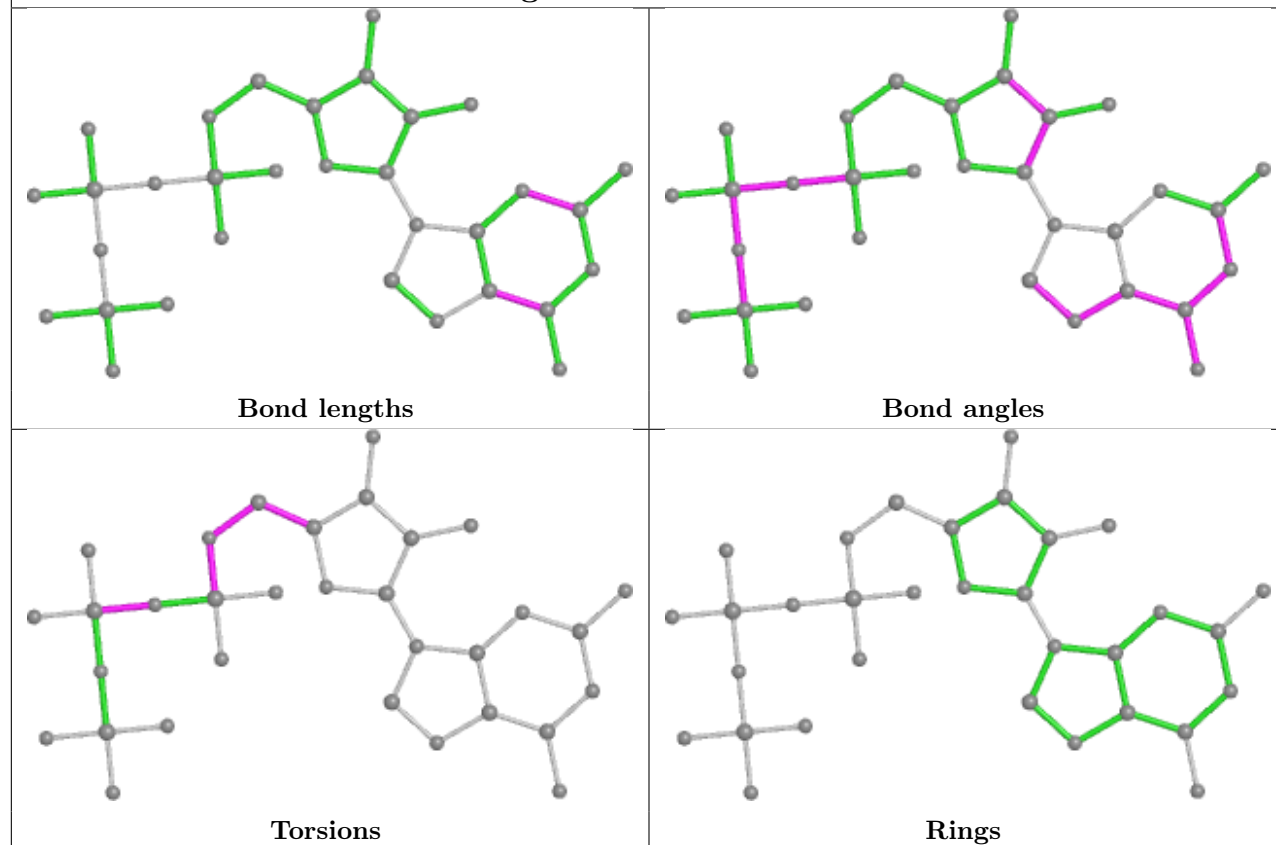
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A3	502	GDP	2	0
21	A7	501	GTP	4	0
23	A7	502	GDP	2	0
21	A3	501	GTP	1	0
21	A5	501	GTP	1	0
23	B7	502	GDP	1	0
21	B2	501	GTP	1	0
21	B5	501	GTP	1	0
23	B5	502	GDP	1	0
23	B3	502	GDP	2	0
23	B1	501	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

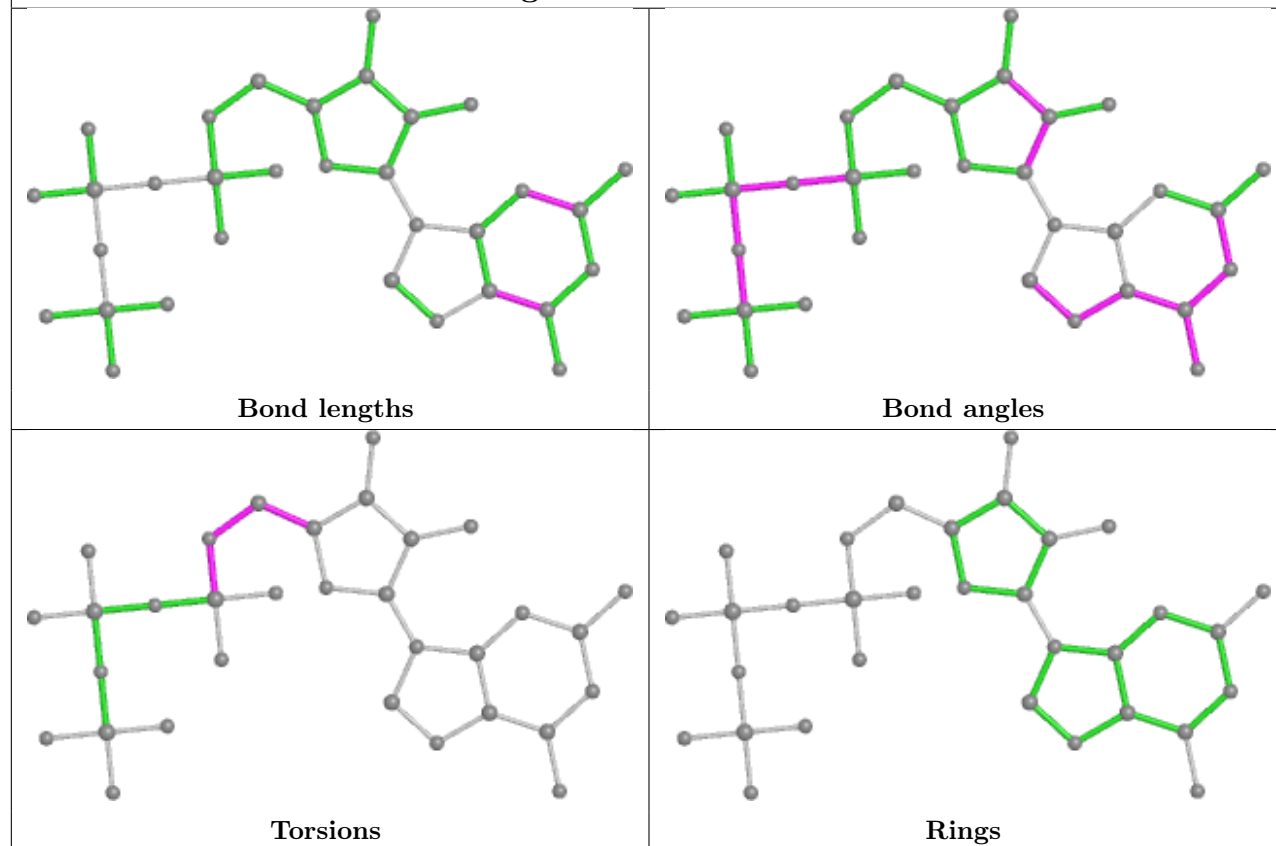
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

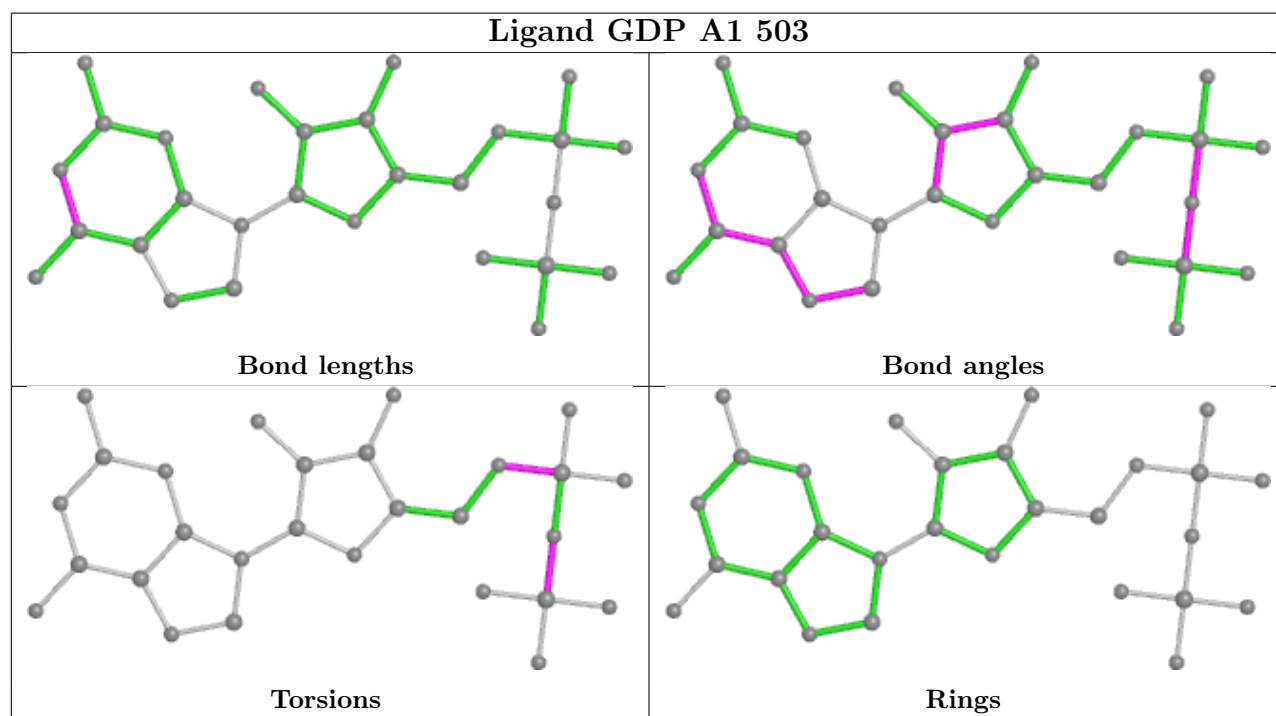
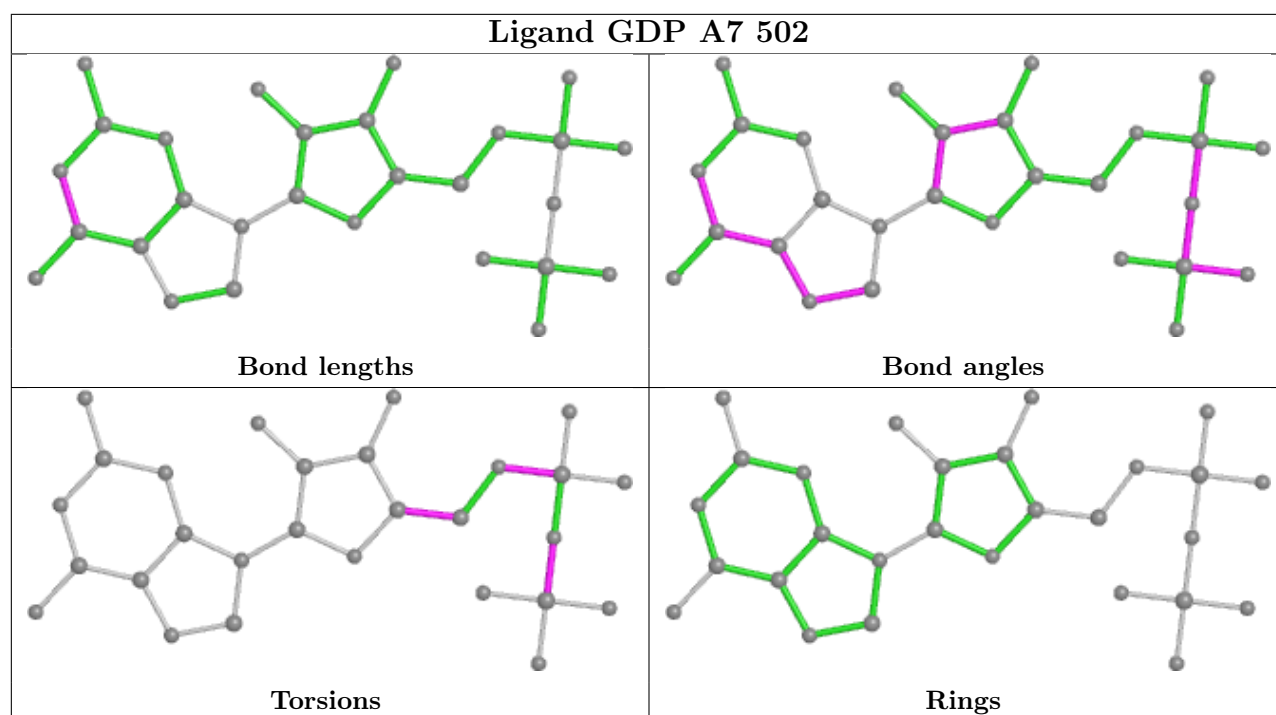


Ligand GTP A7 501

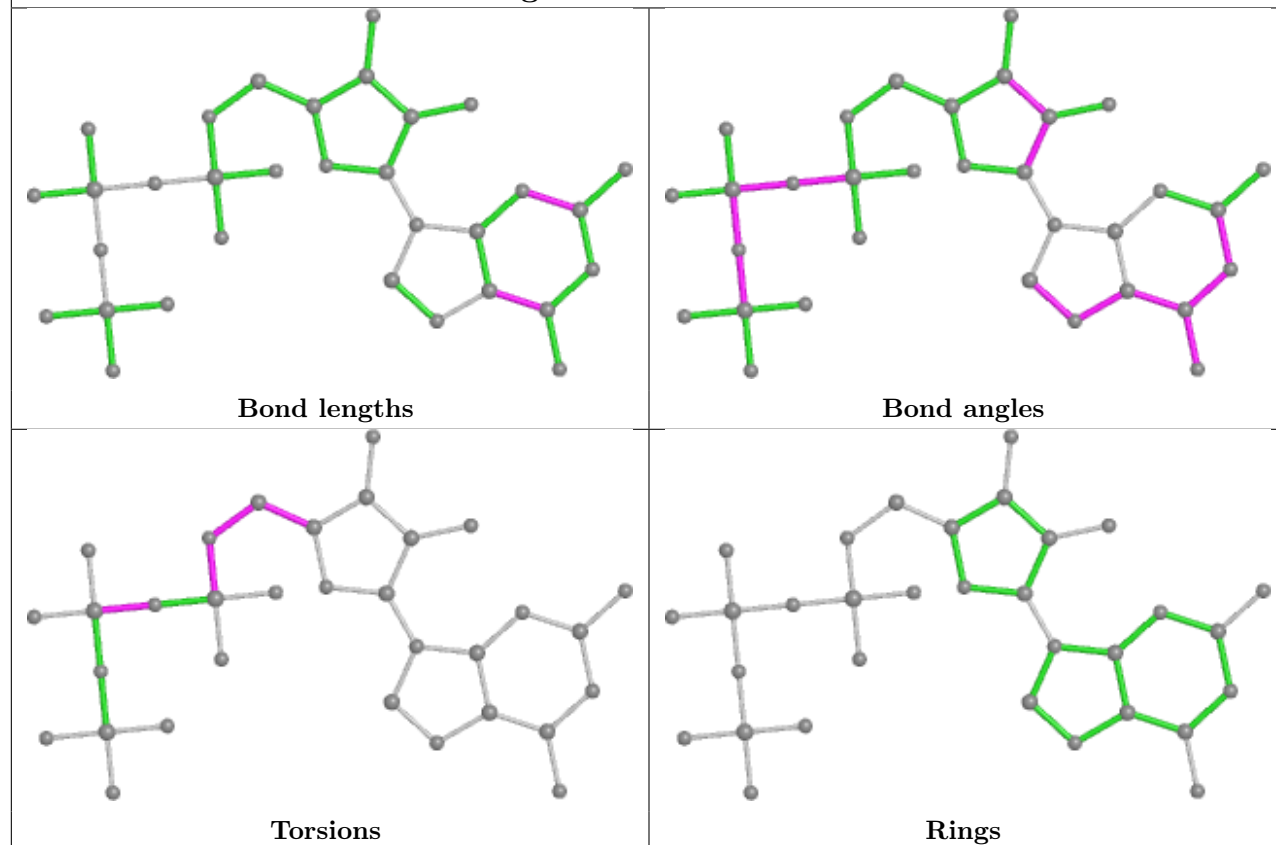


Ligand GTP A1 501

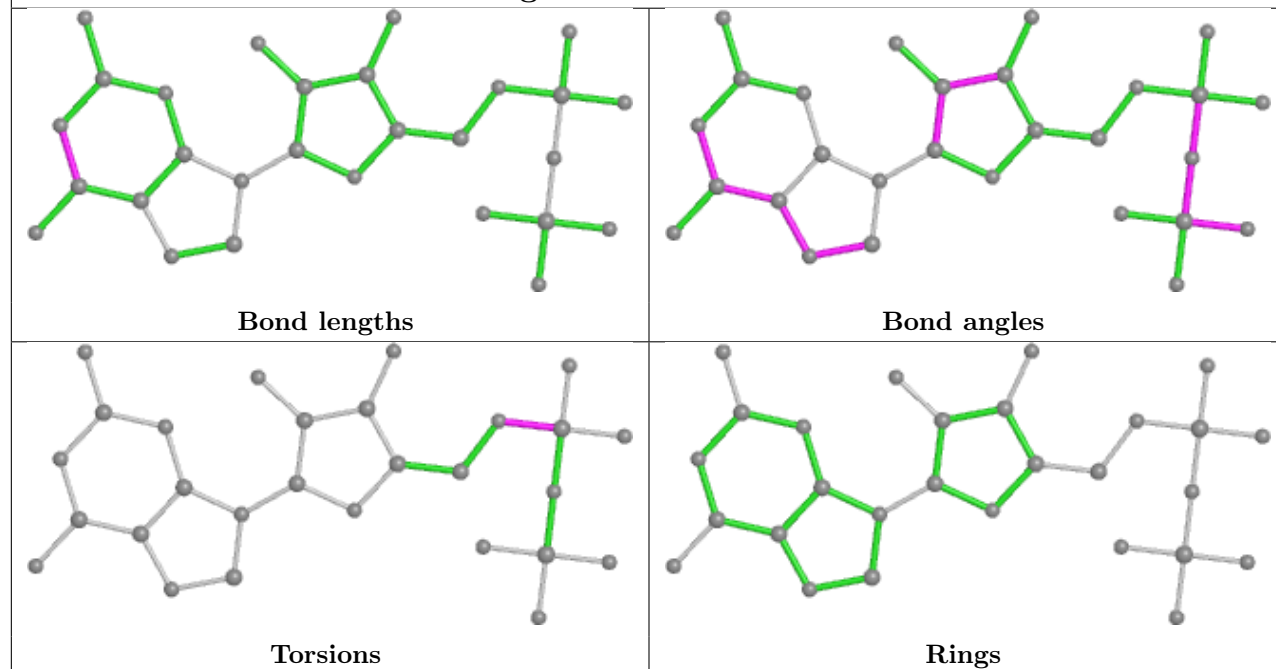




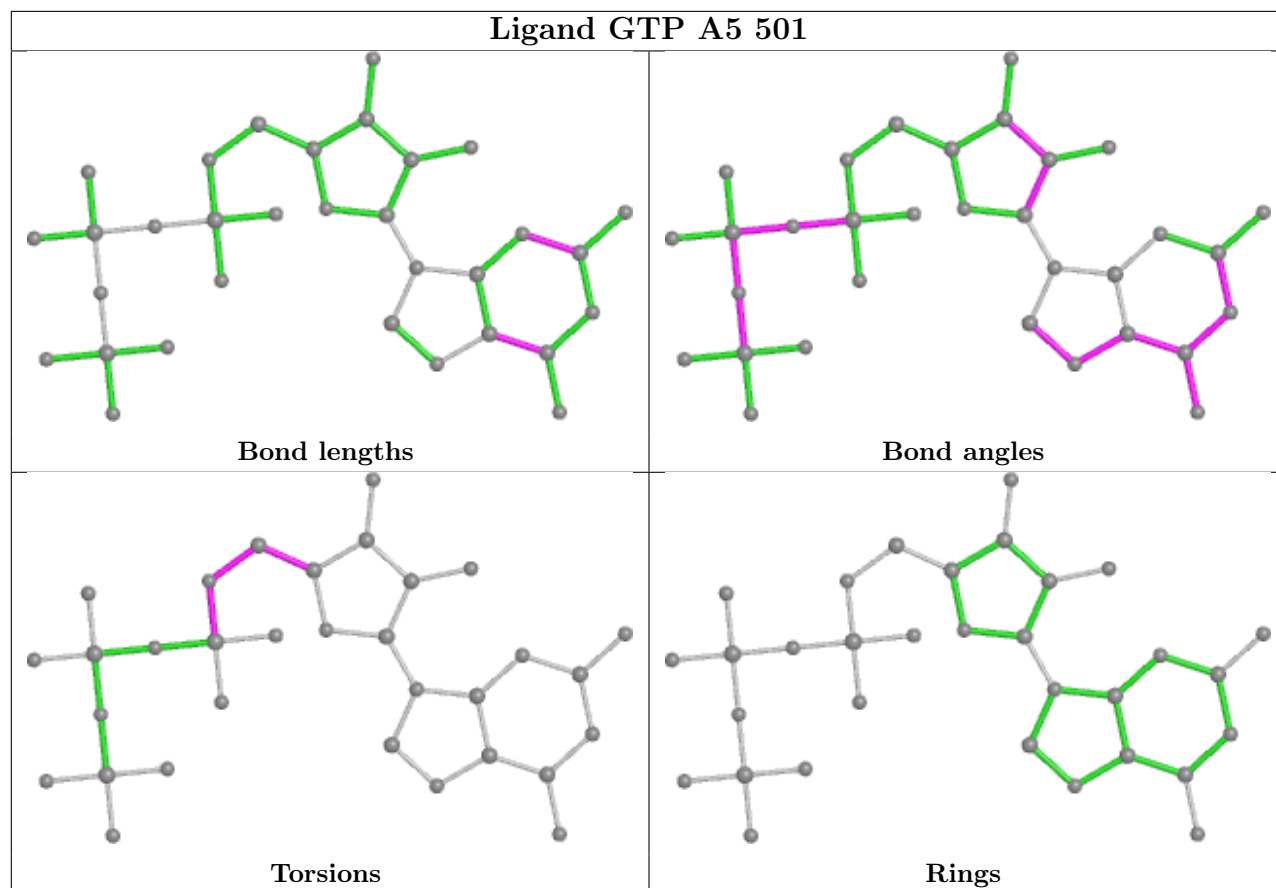
Ligand GTP A3 501



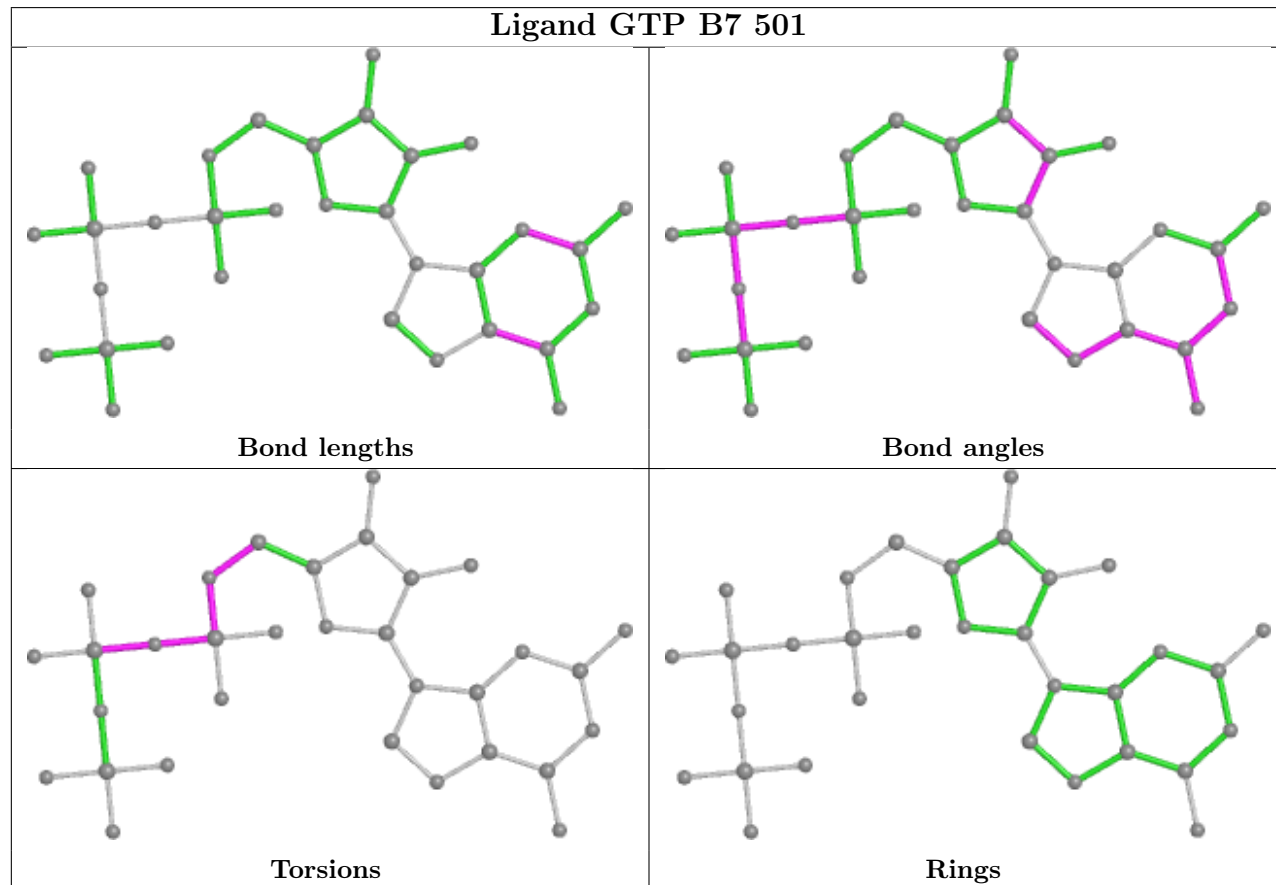
Ligand GDP A5 502



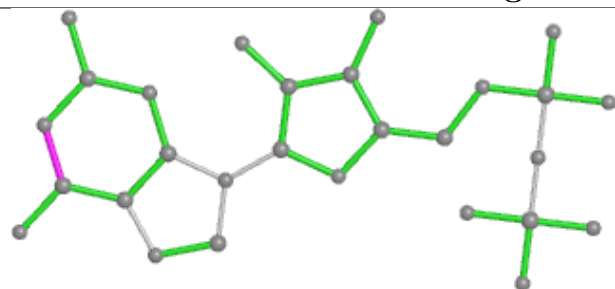
Ligand GTP A5 501



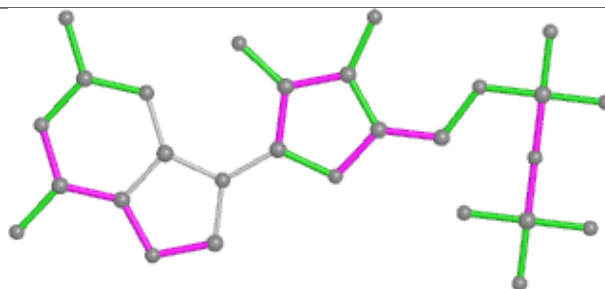
Ligand GTP B7 501



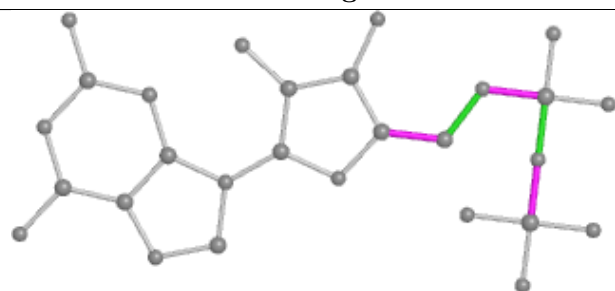
Ligand GDP B7 502



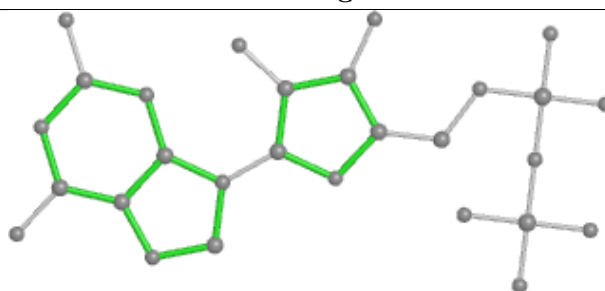
Bond lengths



Bond angles

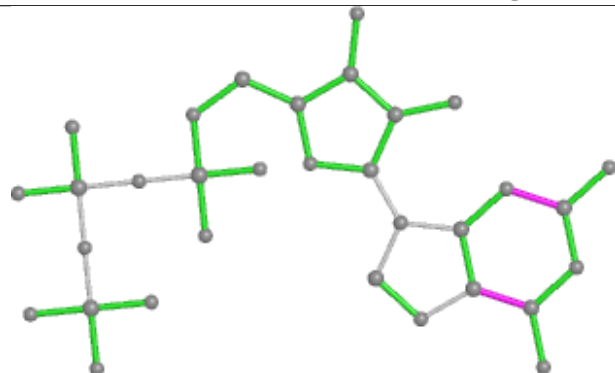


Torsions

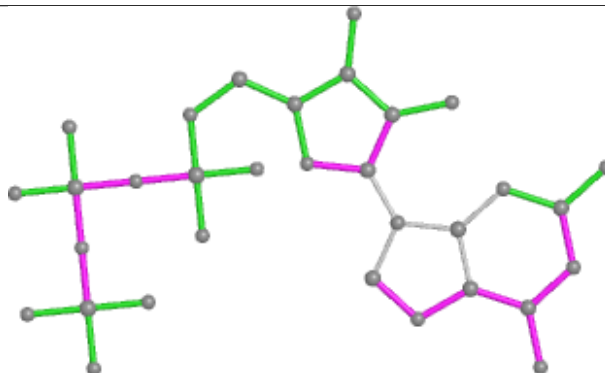


Rings

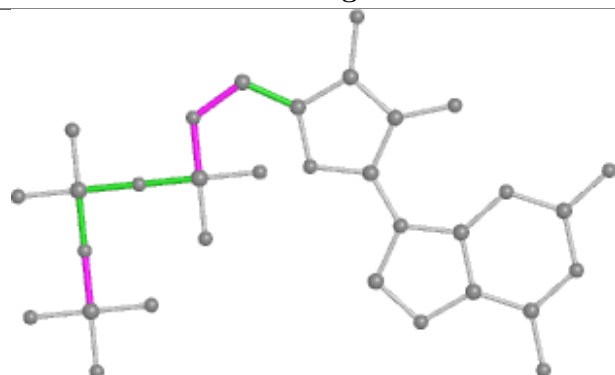
Ligand GTP B2 501



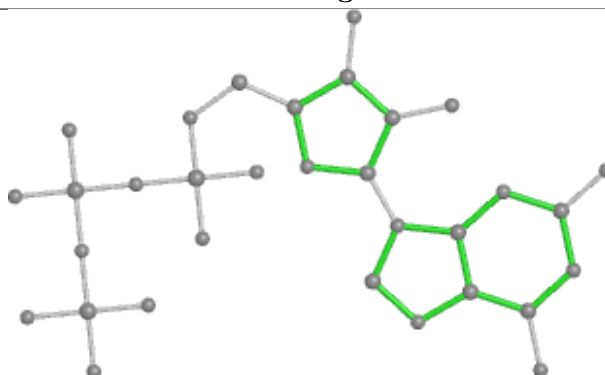
Bond lengths



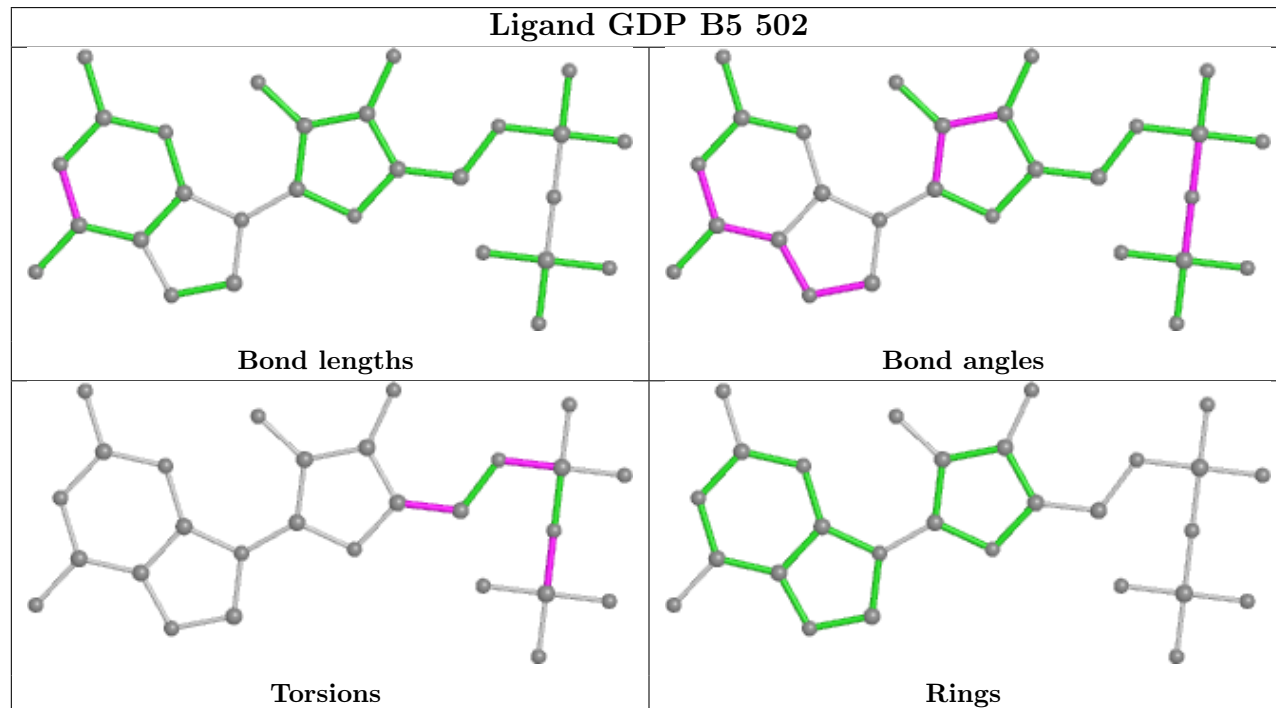
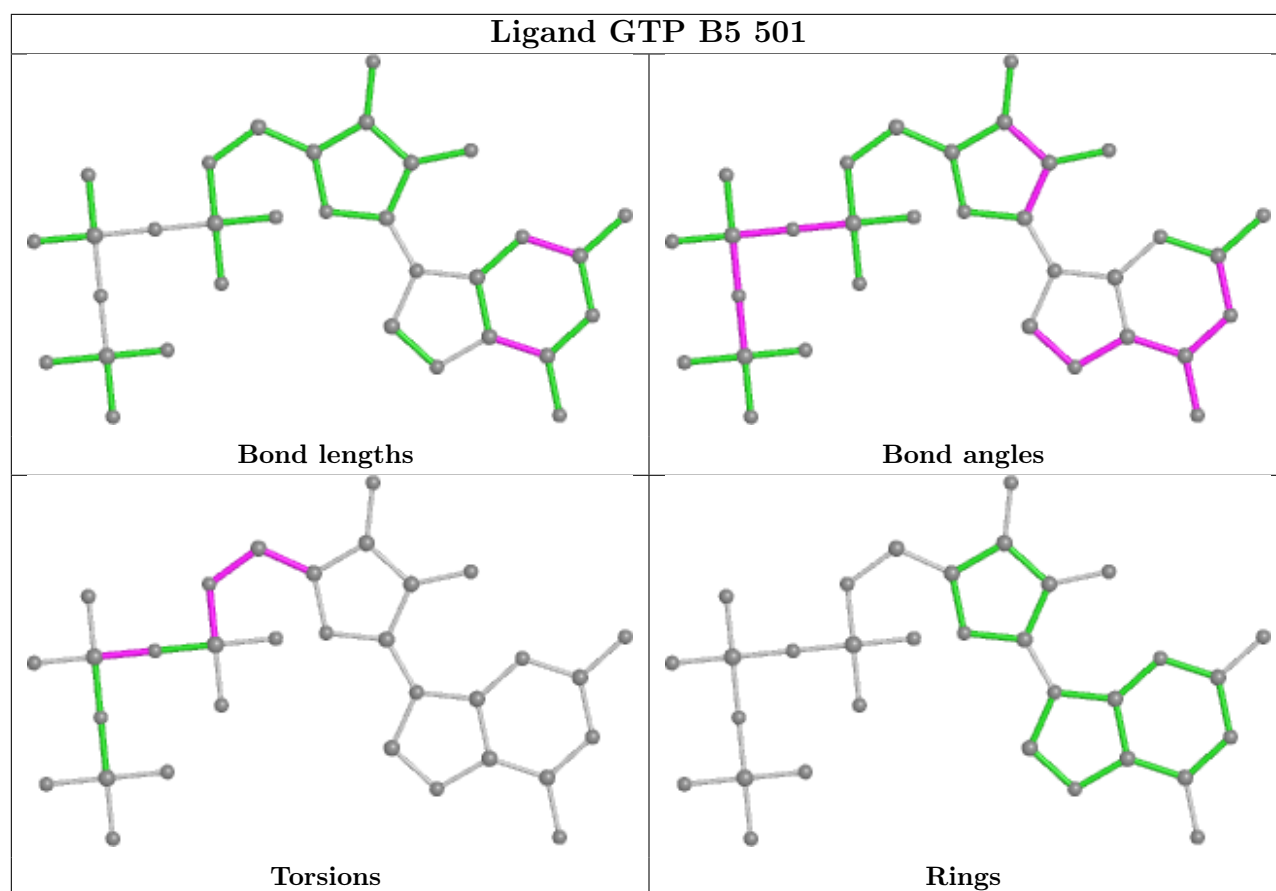
Bond angles

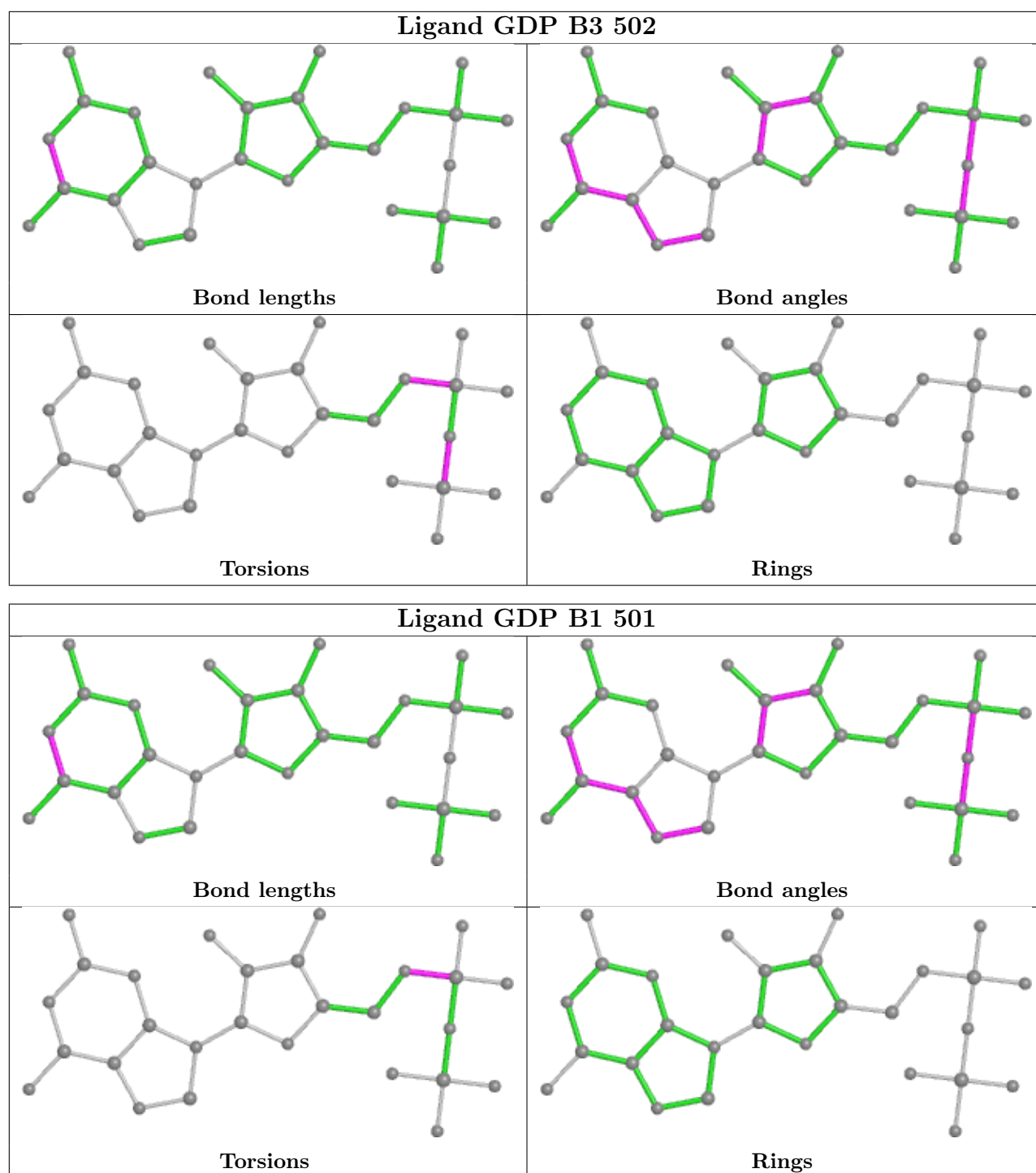


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	Y0	3
17	X0	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X0	396:UNK	C	403:UNK	N	28.65
1	Y0	387:UNK	C	394:UNK	N	22.26
1	Y0	420:UNK	C	424:UNK	N	12.82
1	X0	346:UNK	C	348:UNK	N	9.65
1	Y0	281:UNK	C	284:UNK	N	6.72

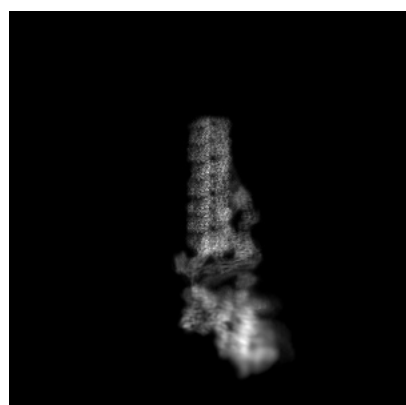
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23082. These allow visual inspection of the internal detail of the map and identification of artifacts.

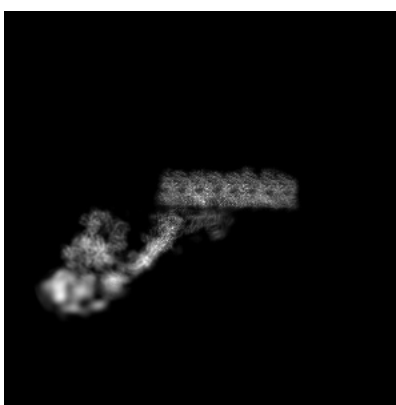
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

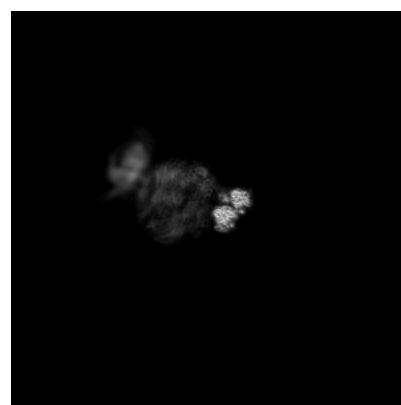
6.1.1 Primary map



X



Y

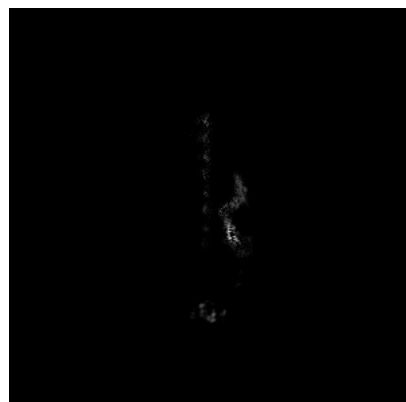


Z

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

6.2 Central slices [i](#)

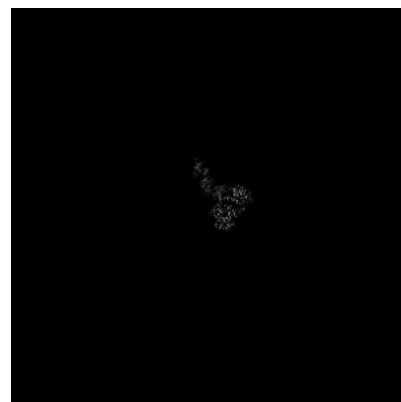
6.2.1 Primary map



X Index: 350



Y Index: 350

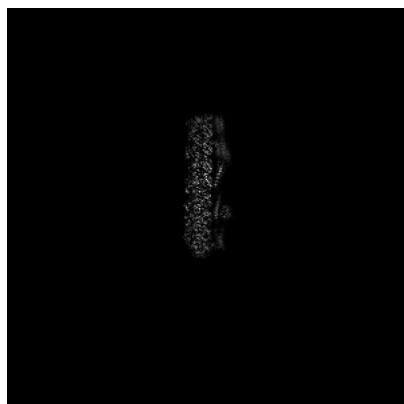


Z Index: 350

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: 372



Y Index: 347



Z Index: 294

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

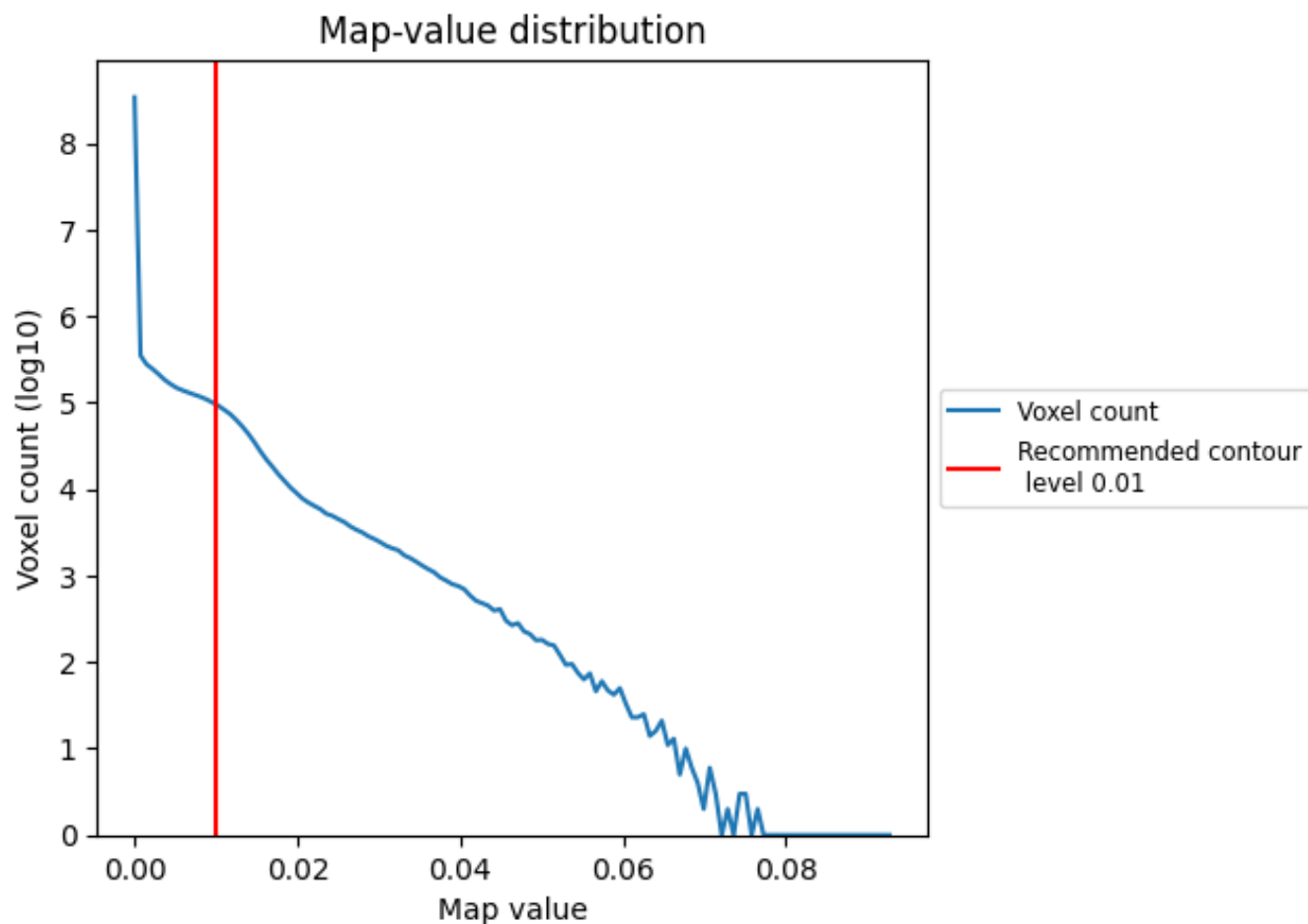
6.5 Mask visualisation

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

7 Map analysis [i](#)

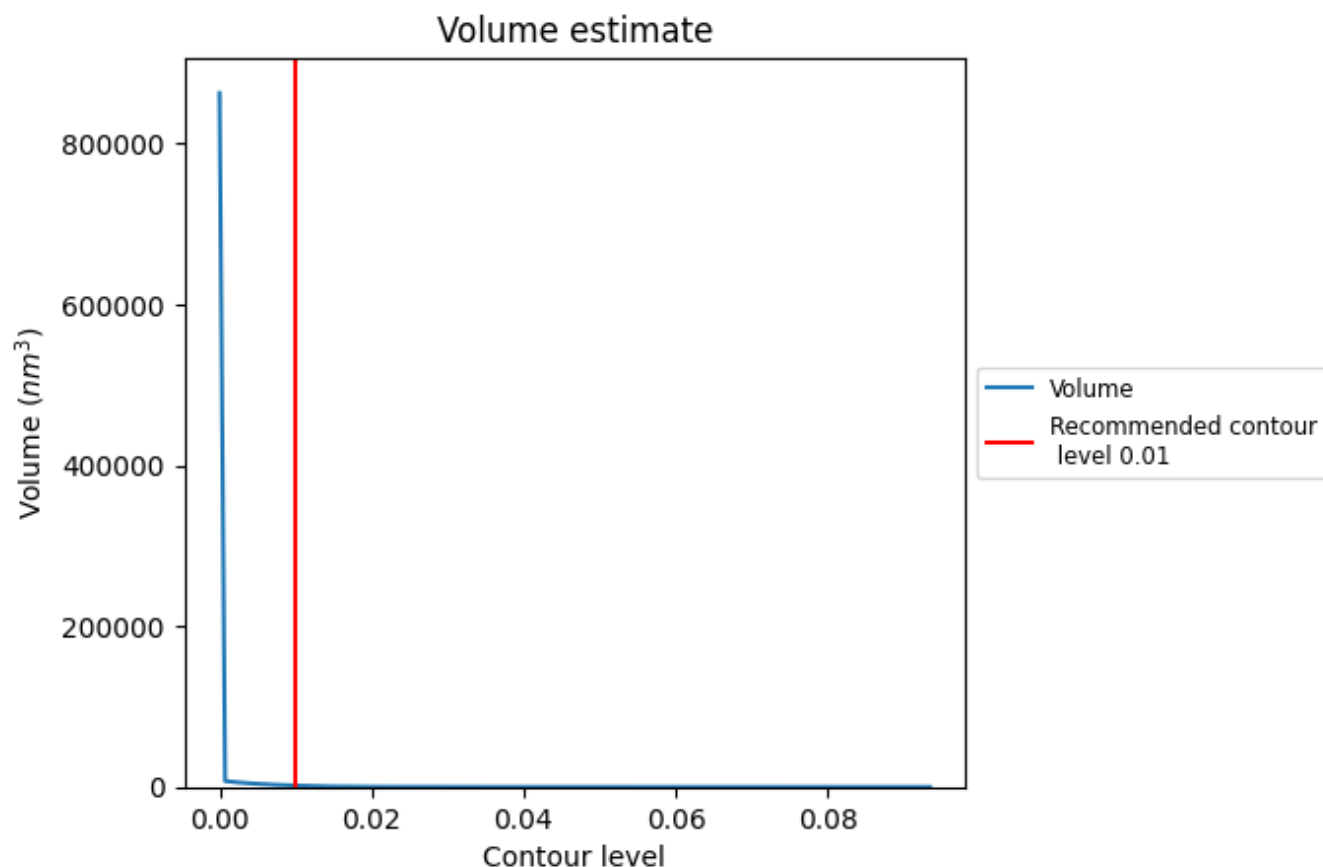
This section contains the results of statistical analysis of the map.

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.

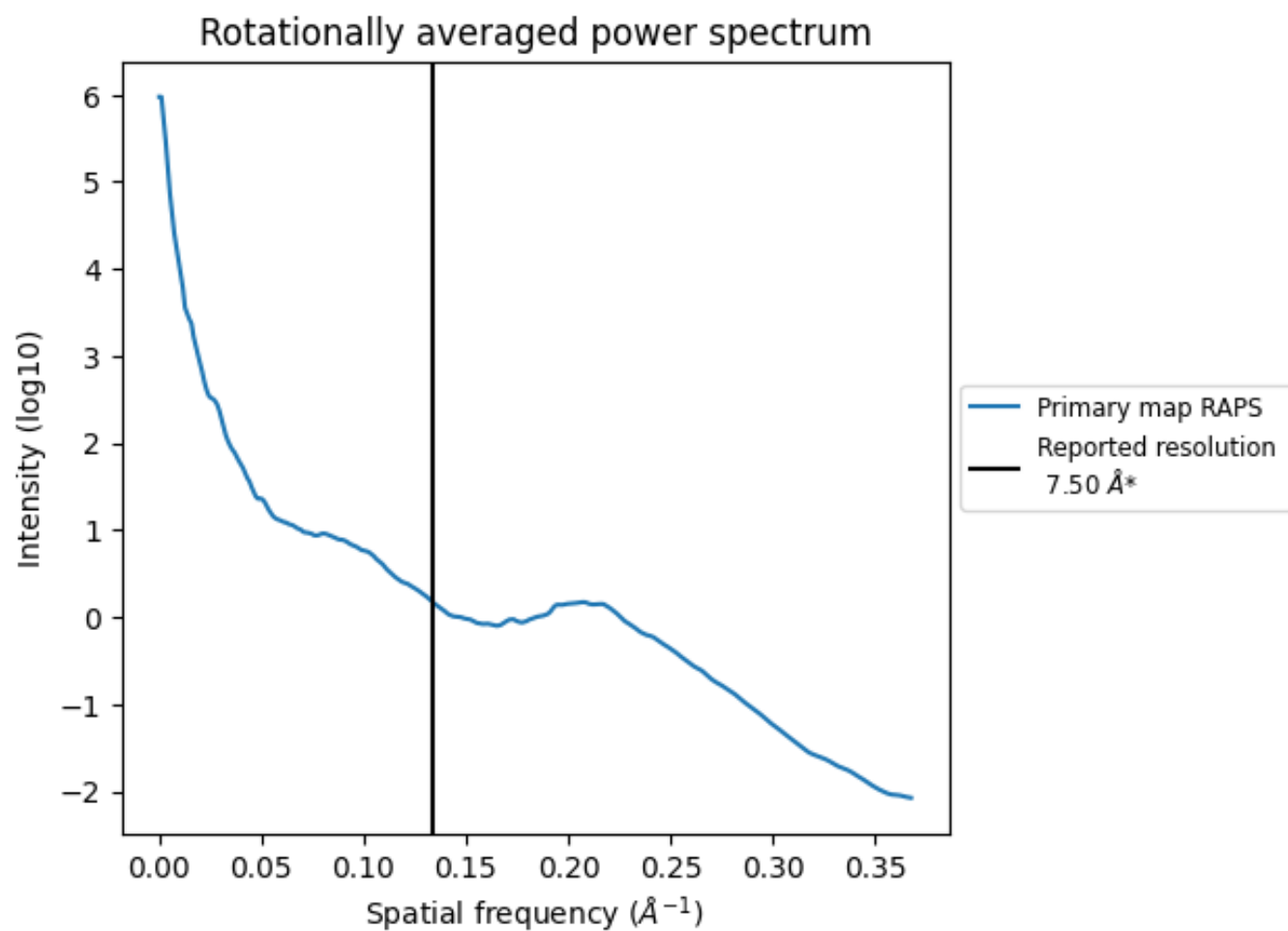
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1728 nm^3 ; this corresponds to an approximate mass of 1561 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 0.133 Å⁻¹

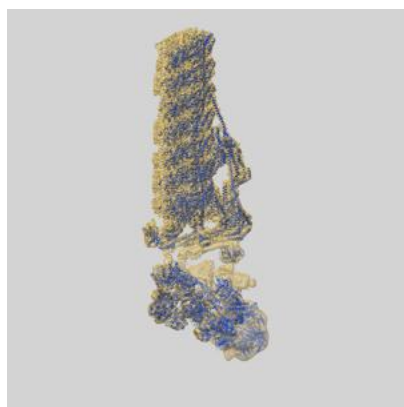
8 Fourier-Shell correlation

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

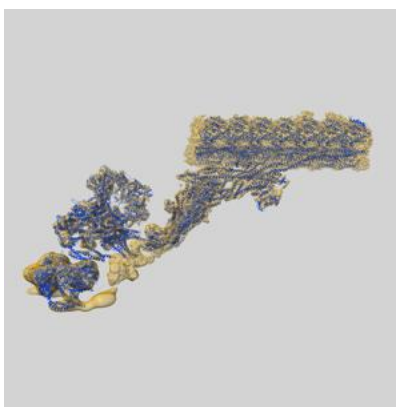
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23082 and PDB model 7KZM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

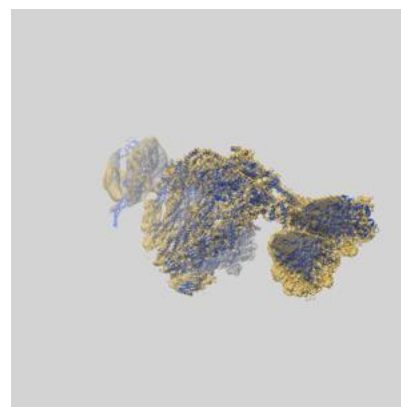
9.1 Map-model overlay [i](#)



X



Y



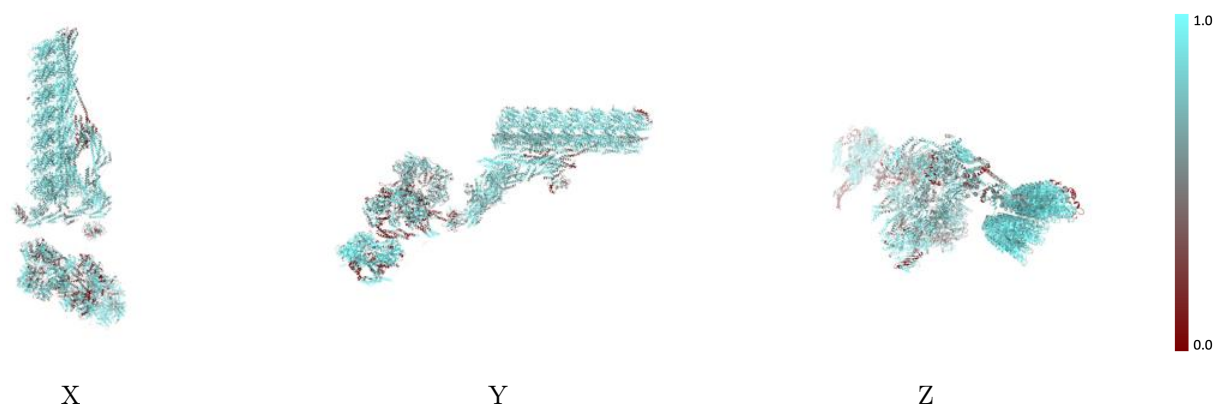
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

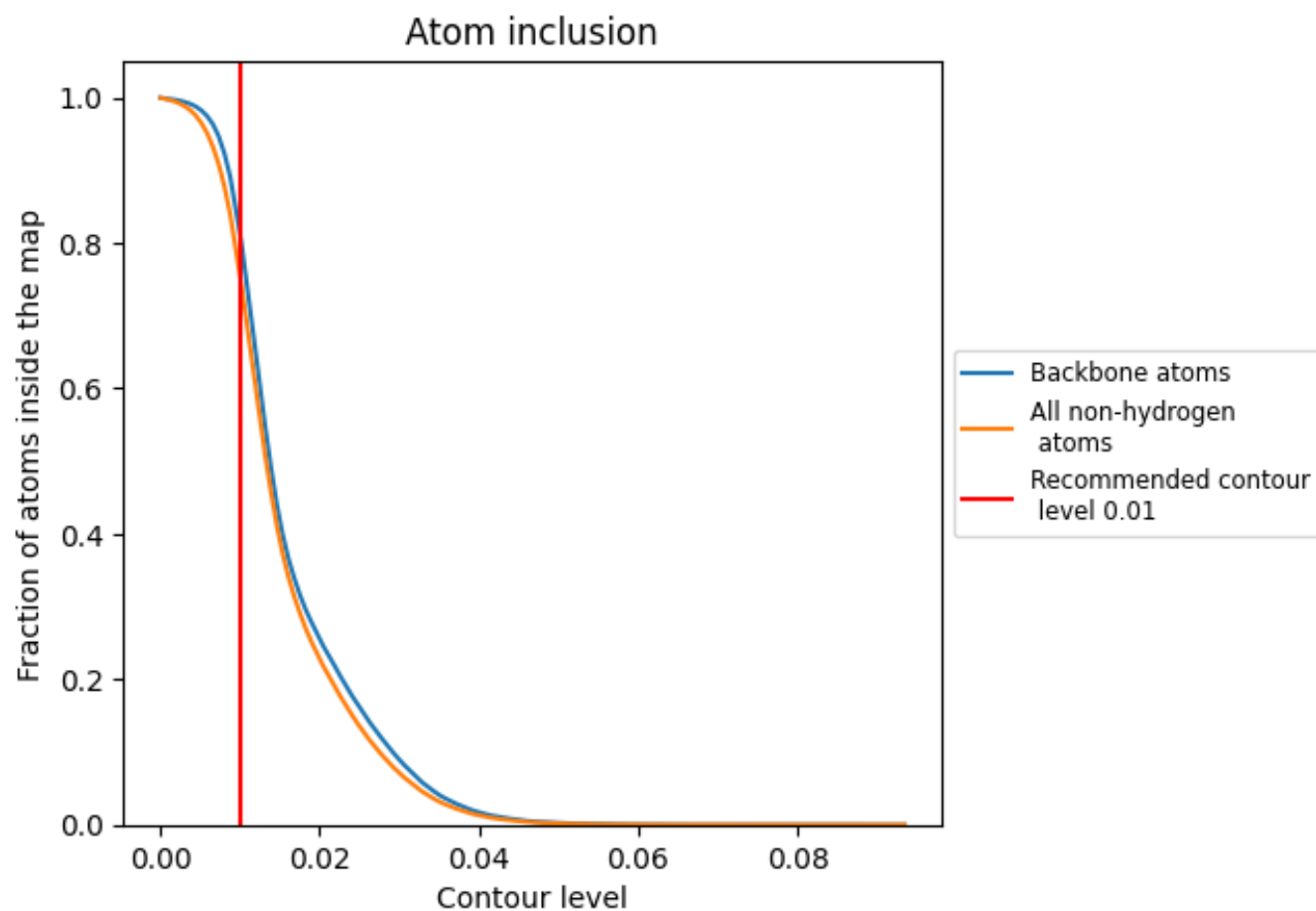
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).




































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary




The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.7538
A	 0.7811
A1	 0.8454
A2	 0.8872
A3	 0.8974
A4	 0.9156
A5	 0.8980
A6	 0.8773
A7	 0.8657
B	 0.6073
B1	 0.8395
B2	 0.8844
B3	 0.8993
B4	 0.8975
B5	 0.9162
B6	 0.8637
B7	 0.7598
C	 0.6326
D	 0.7966
E	 0.7605
F	 0.5859
G	 0.6019
H	 0.8027
I	 0.7092
J	 0.7692
K	 0.7761
L	 0.6551
M	 0.7186
N	 0.7936
O	 0.5343
P	 0.7181
X	 0.5987
X0	 0.6877
X1	 0.7474
Y	 0.6534



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Chain	Atom inclusion
Y0	 0.8321
Y1	 0.7727
Z	 0.6064