Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 05:23 PM EST

PDB ID	:	7L6N
EMDB ID	:	EMD-23206
Title	:	The Mycobacterium tuberculosis ClpB disaggregase hexamer structure with three locally refined ClpB middle domains and three DnaK nucleotide binding domains
Authors	:	Yin, Y.Y.; Feng, X.; Li, H.
Deposited on	:	2020-12-23
Resolution	:	7.00 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:

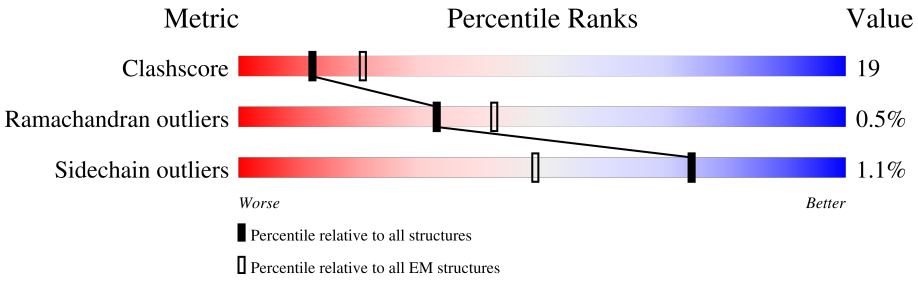
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	848	56% 22% 21%
1	B	848	7% 59% 20% 21%
1	C	848	8% 60% 19% 20%
1	D	848	51% 15% 34%
1	E	848	11% 43% 21% 35%
1	F	848	23% 44% 20% 36%
2	N	33	6% 73% 6% 21%
3	I	625	31% 26% 43%

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Mol	Chain	Length	Quality of chain
3	J	625	30% 26% 43%
3	K	625	29% 27% 43%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AGS	E	901	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 36999 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	674	Total	C	N	O	S	0	0
			5222	3253	954	1004	11		
1	B	672	Total	C	N	O	S	0	0
			5207	3241	952	1004	10		
1	C	675	Total	C	N	O	S	0	0
			5224	3251	955	1008	10		
1	D	562	Total	C	N	O	S	0	0
			4321	2701	790	821	9		
1	E	548	Total	C	N	O	S	0	0
			4230	2647	772	802	9		
1	F	546	Total	C	N	O	S	0	0
			4219	2641	770	799	9		

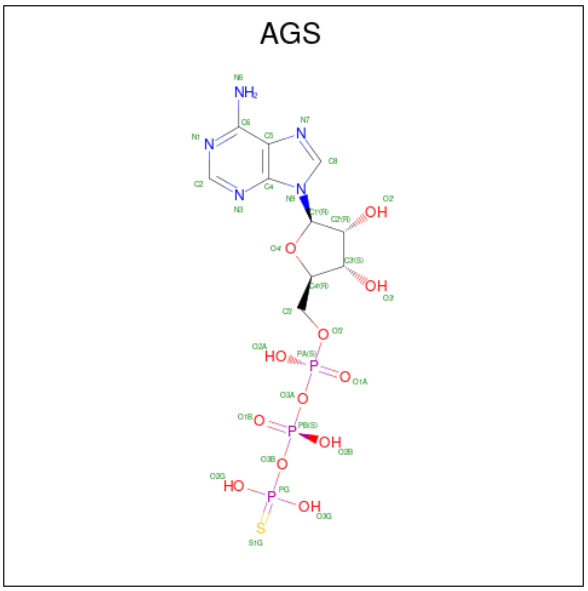
- Molecule 2 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 3 is a protein called Chaperone protein DnaK.

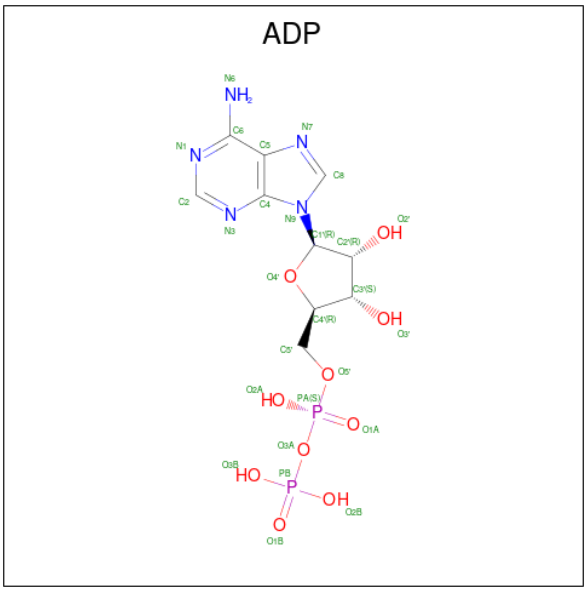
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	357	Total	C	N	O	S	0	0
			2694	1675	474	539	6		
3	J	357	Total	C	N	O	S	0	0
			2694	1675	474	539	6		
3	K	357	Total	C	N	O	S	0	0
			2694	1675	474	539	6		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

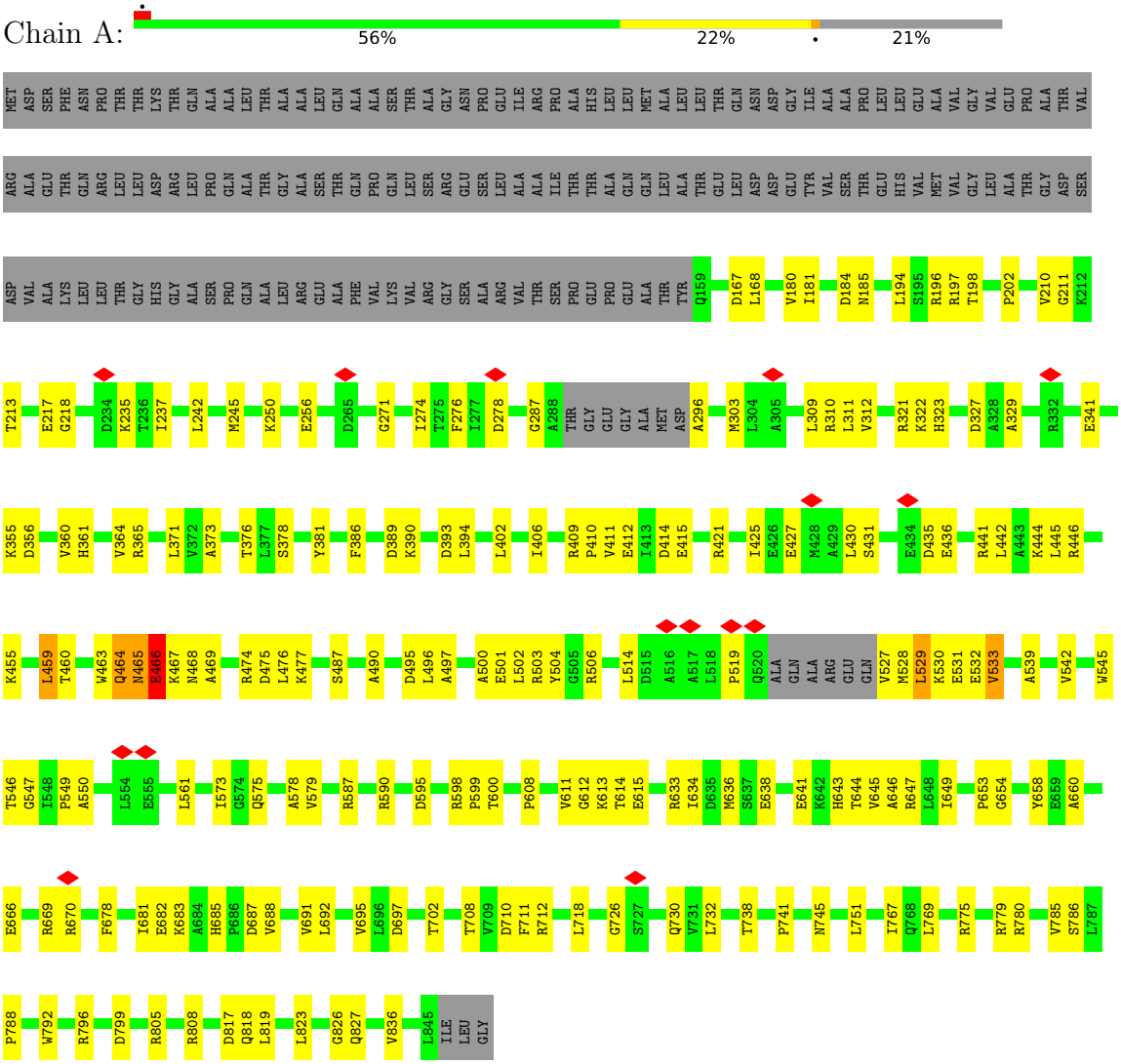


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

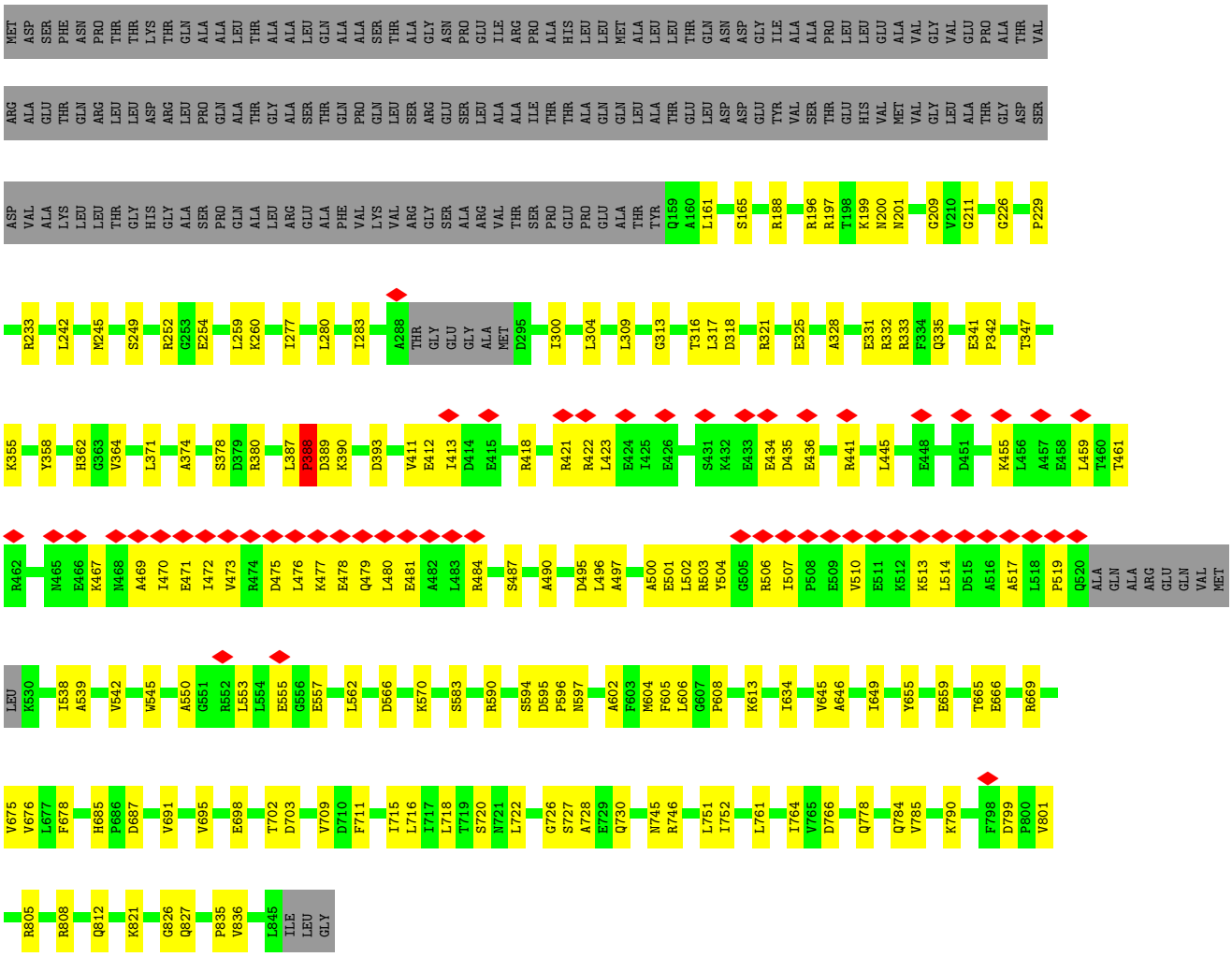
3 Residue-property plots (i)

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

• Molecule 1: Chaperone protein ClpB

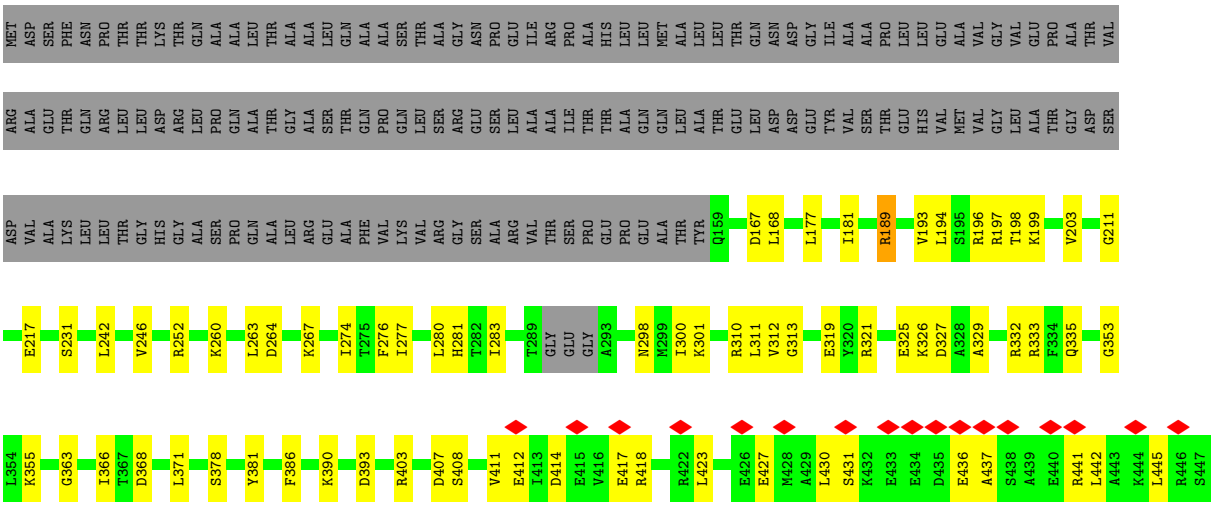


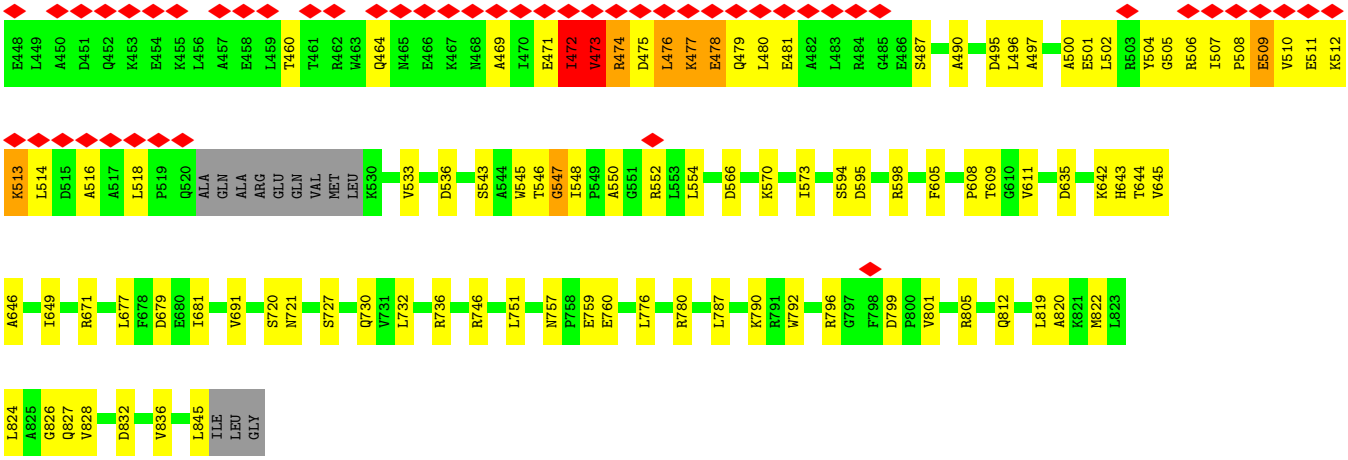
• Molecule 1: Chaperone protein ClpB



• Molecule 1: Chaperone protein ClpB

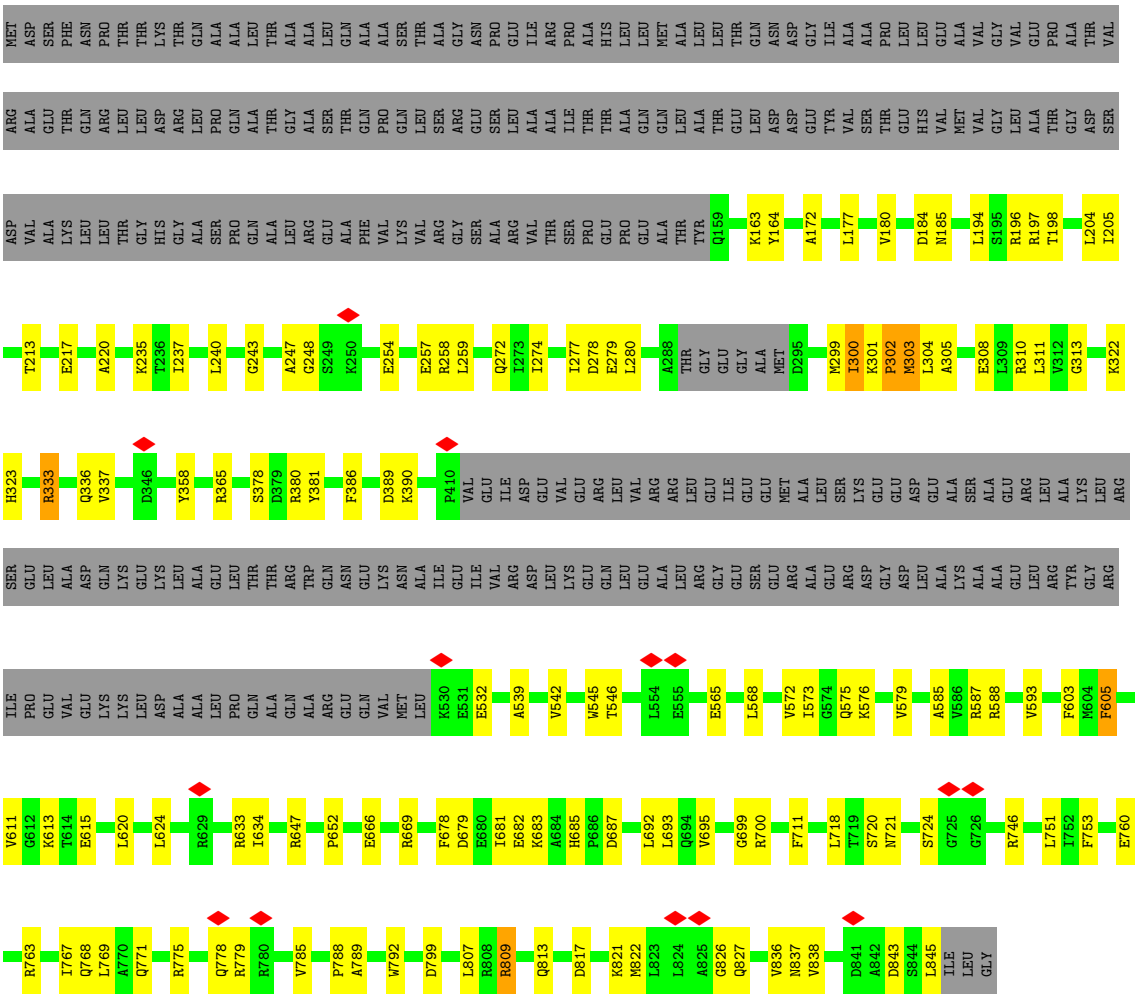
Chain C:





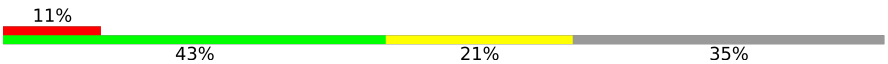
• Molecule 1: Chaperone protein ClpB

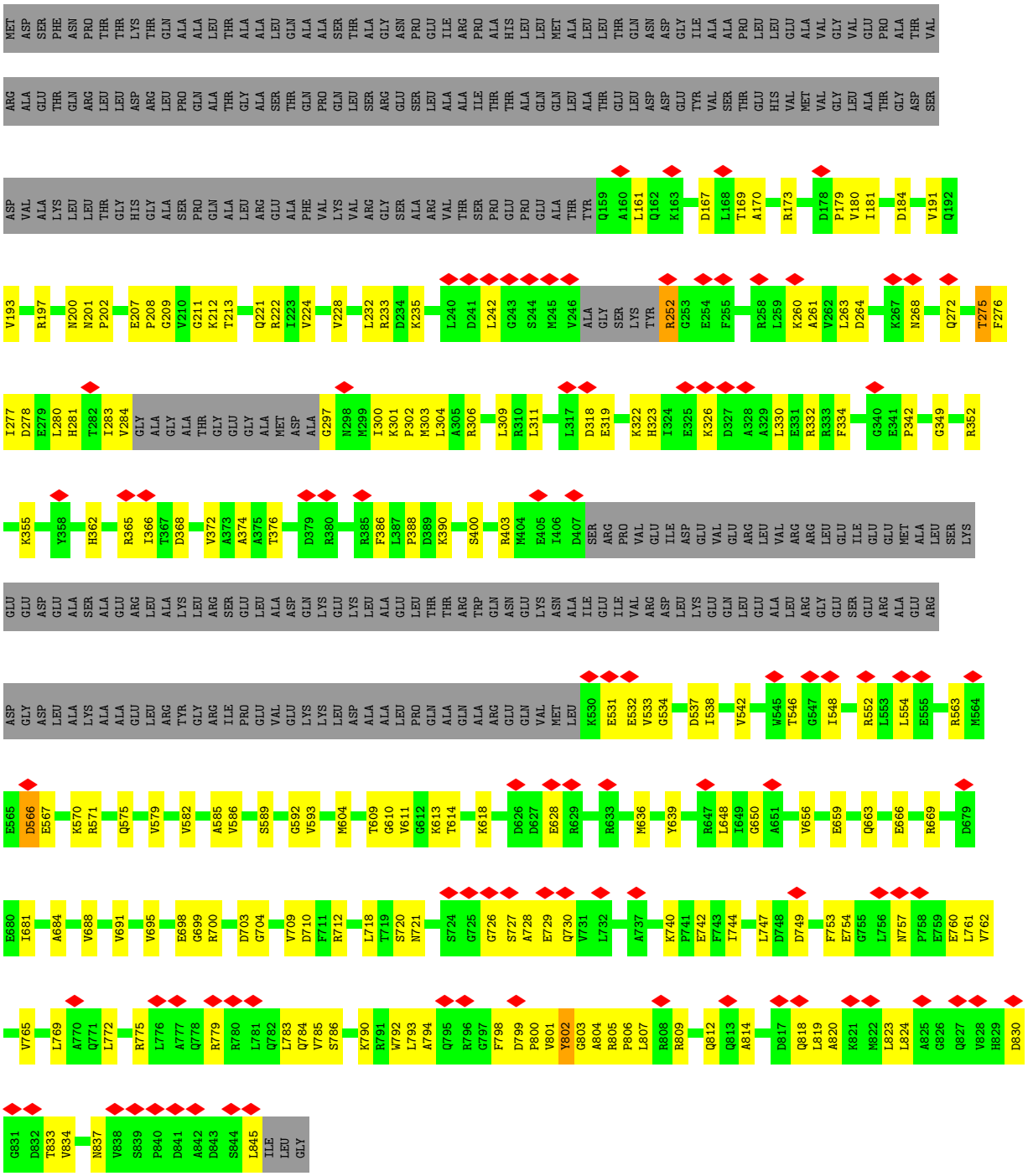
Chain D:



• Molecule 1: Chaperone protein ClpB

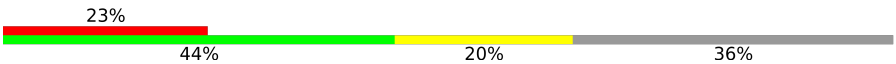
Chain E:

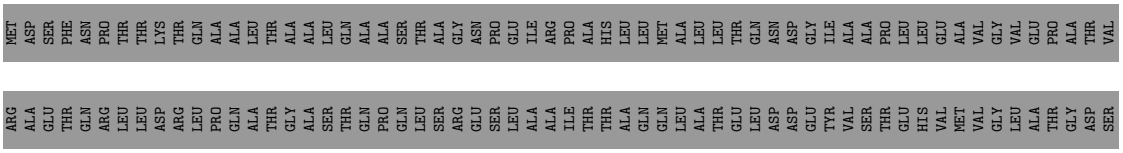


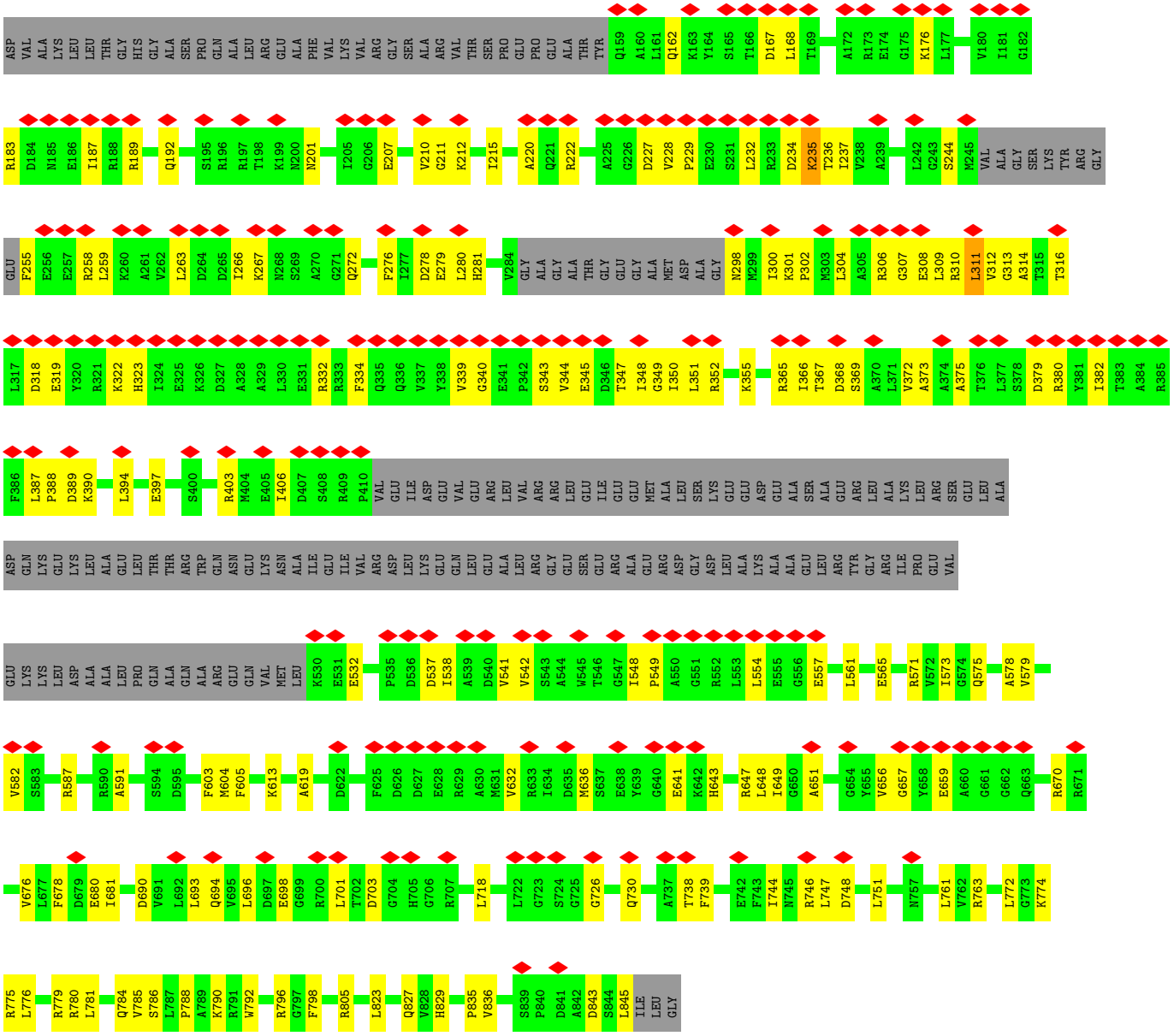


• Molecule 1: Chaperone protein ClpB

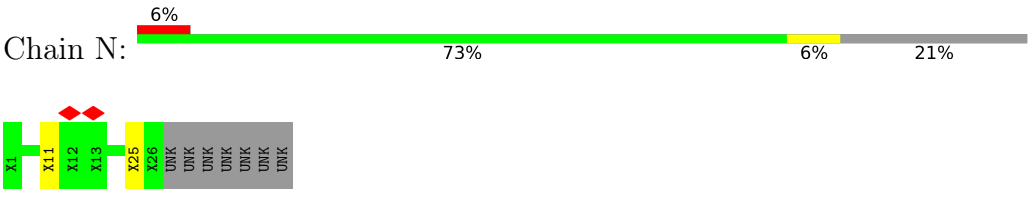
Chain F:



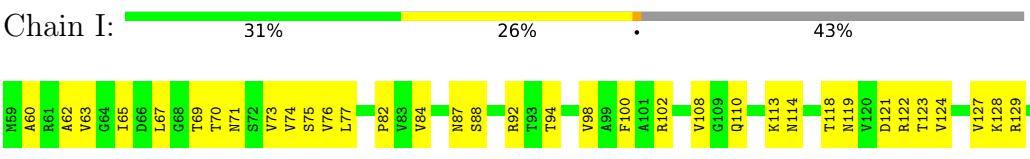


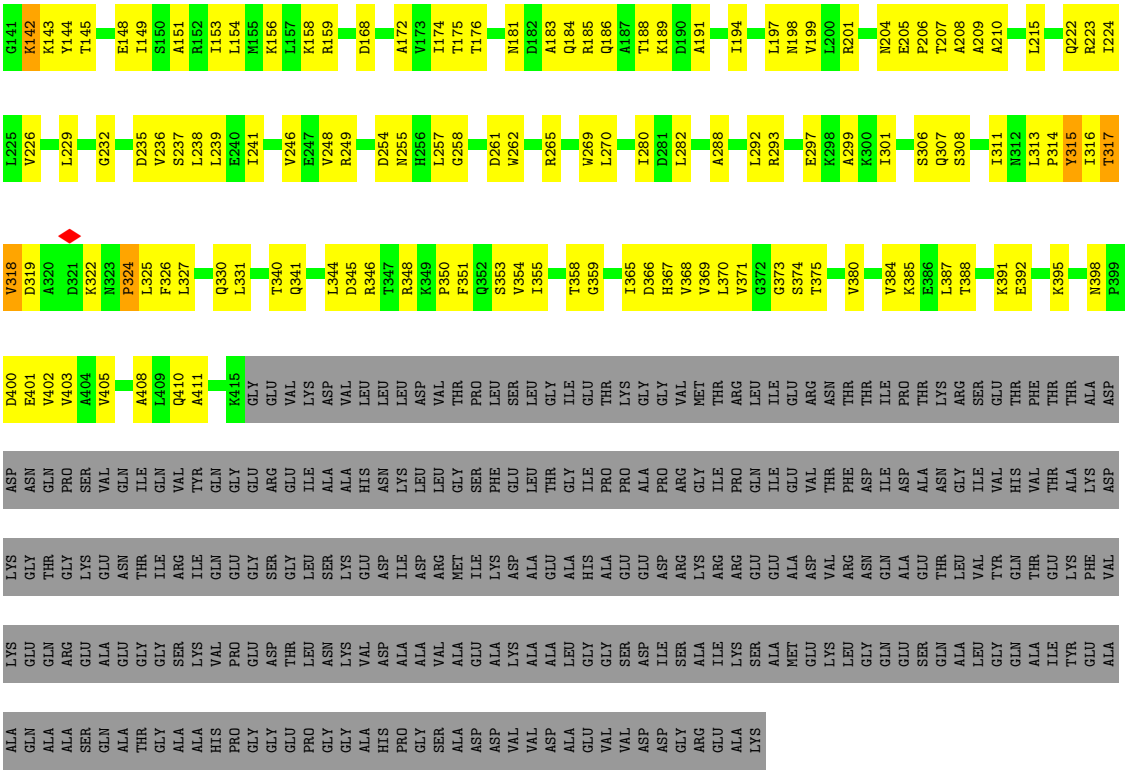


• Molecule 2: Substrate



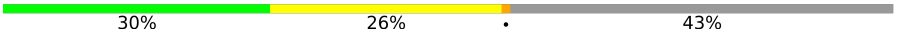
• Molecule 3: Chaperone protein DnaK

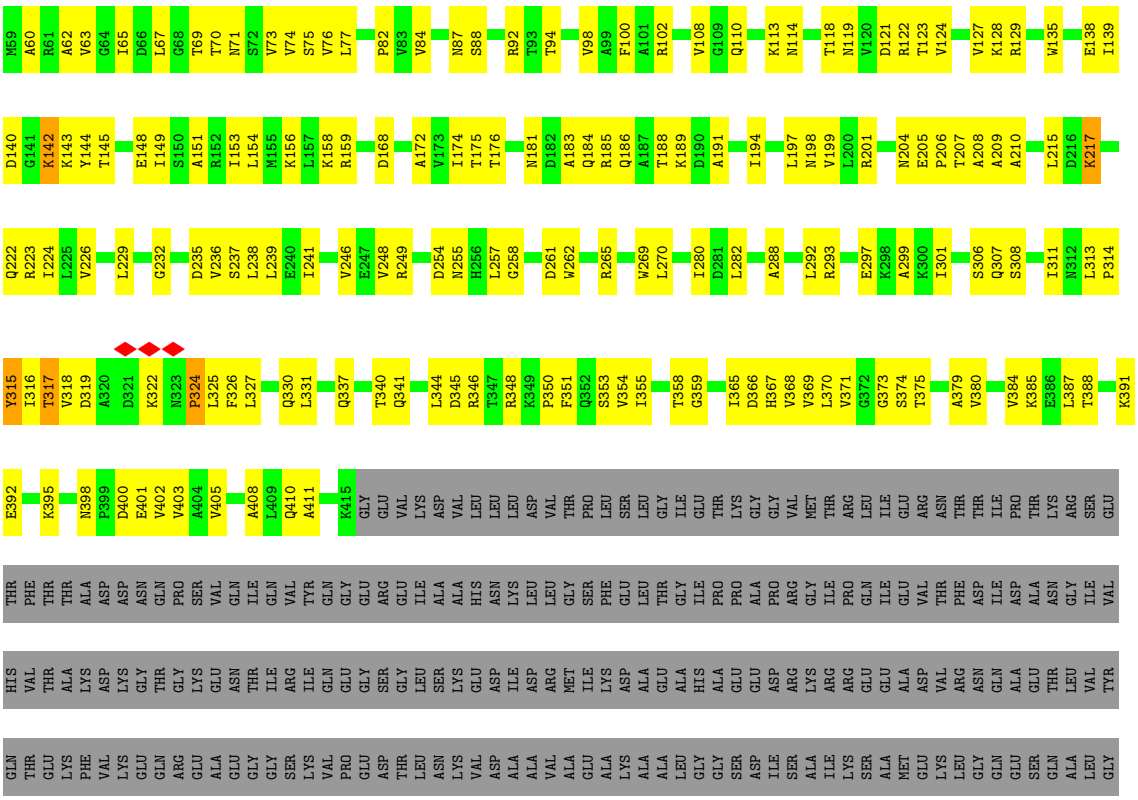


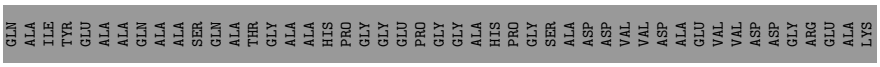


• Molecule 3: Chaperone protein DnaK

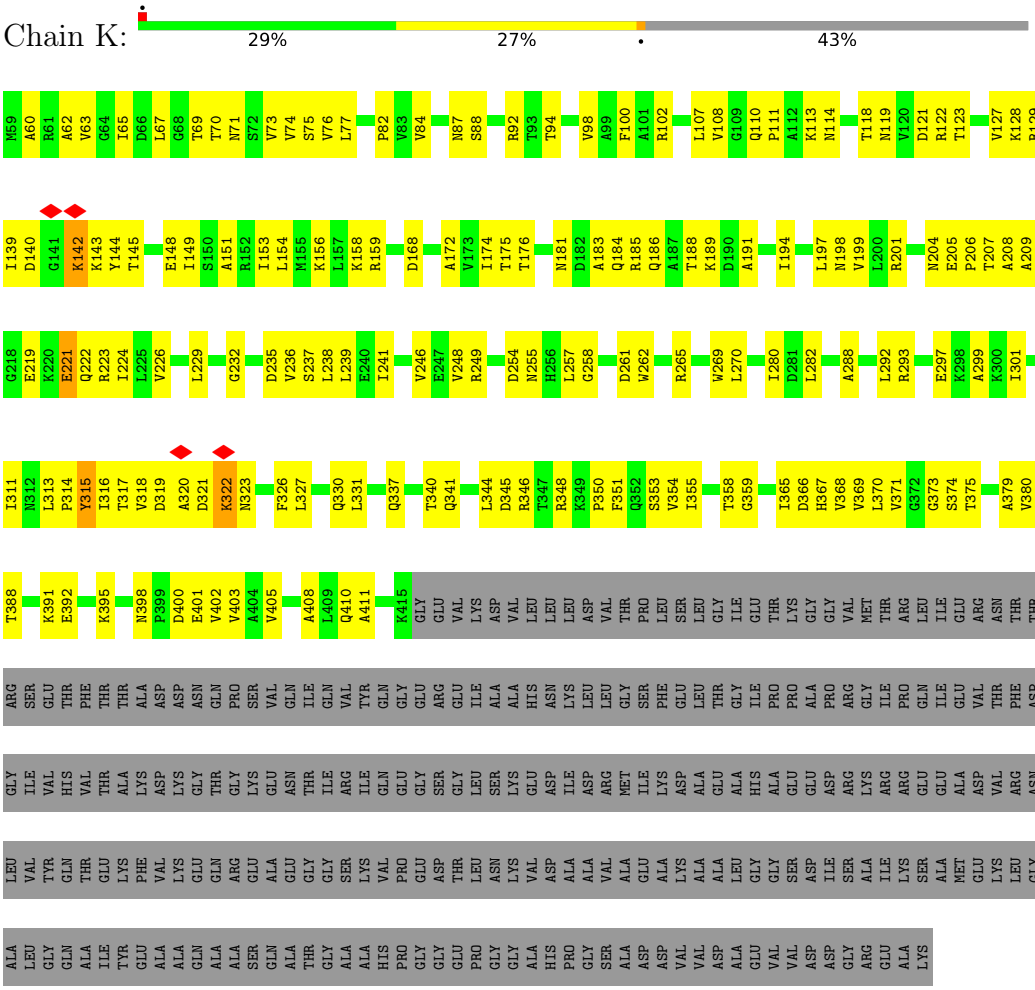
Chain J:







• Molecule 3: Chaperone protein DnaK



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	50.570	Depositor
Minimum map value	-13.833	Depositor
Average map value	0.042	Depositor
Map value standard deviation	1.510	Depositor
Recommended contour level	7.1	Depositor
Map size (Å)	386.64, 386.64, 386.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/5286	0.50	0/7126
1	B	0.32	0/5271	0.52	2/7106 (0.0%)
1	C	0.32	0/5288	0.49	0/7130
1	D	0.32	0/4380	0.50	0/5914
1	E	0.27	0/4286	0.47	0/5786
1	F	0.26	0/4276	0.46	0/5774
3	I	0.39	0/2727	0.65	0/3695
3	J	0.39	0/2727	0.65	0/3695
3	K	0.39	0/2727	0.66	0/3695
All	All	0.33	0/36968	0.53	2/49921 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	388	PRO	CA-N-CD	-9.28	98.51	111.50
1	B	388	PRO	CB-CA-C	6.38	127.95	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5222	0	5289	192	0
1	B	5207	0	5264	175	0
1	C	5224	0	5278	190	0
1	D	4321	0	4378	129	0
1	E	4230	0	4290	163	0
1	F	4219	0	4283	140	0
2	N	130	0	31	2	0
3	I	2694	0	2716	175	0
3	J	2694	0	2718	170	0
3	K	2694	0	2718	166	0
4	A	62	0	24	7	0
4	B	62	0	24	7	0
4	C	62	0	24	10	0
4	D	62	0	24	11	0
4	E	31	0	12	14	0
4	F	31	0	12	3	0
5	E	27	0	12	3	0
5	F	27	0	12	2	0
All	All	36999	0	37109	1421	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 19.

All (1421) 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)
1:E:801:VAL:HG23	1:E:802:TYR:CE1	1.38	1.55
3:I:222:GLN:NE2	3:I:241:ILE:CG2	1.69	1.54
3:I:222:GLN:NE2	3:I:241:ILE:CB	1.68	1.49
1:D:301:LYS:HG2	1:D:333:ARG:NH2	1.27	1.43
1:E:801:VAL:HG23	1:E:802:TYR:CD1	1.52	1.42
1:B:342:PRO:O	1:B:387:LEU:CD1	1.67	1.41
1:D:303:MET:CE	1:D:308:GLU:CB	1.99	1.40
1:D:301:LYS:CG	1:D:333:ARG:NH2	1.86	1.38
1:D:303:MET:CE	1:D:308:GLU:HG3	1.51	1.38
1:E:801:VAL:CG2	1:E:802:TYR:CE1	2.07	1.37
1:D:303:MET:CE	1:D:308:GLU:CG	2.02	1.36
3:I:222:GLN:NE2	3:I:241:ILE:HB	1.20	1.36
1:D:303:MET:HE1	1:D:308:GLU:CB	1.54	1.34
1:C:476:LEU:HD23	1:C:510:VAL:CG1	1.57	1.31
3:J:217:LYS:CD	3:J:366:ASP:HB3	1.67	1.24
1:C:476:LEU:CD2	1:C:510:VAL:HG13	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:MET:HE2	1:D:308:GLU:CG	1.63	1.20
3:I:319:ASP:OD2	3:I:325:LEU:HG	1.43	1.17
1:A:501:GLU:HA	3:I:315:TYR:HD2	1.11	1.16
1:B:473:VAL:HG21	1:B:517:ALA:HB1	1.20	1.16
1:C:501:GLU:HA	3:K:315:TYR:HD2	1.11	1.15
1:B:501:GLU:HA	3:J:315:TYR:HD2	1.11	1.15
1:B:342:PRO:O	1:B:387:LEU:HD13	1.39	1.13
1:B:473:VAL:HG21	1:B:517:ALA:CB	1.79	1.12
1:A:406:ILE:HD12	1:A:529:LEU:HD21	1.29	1.12
1:A:500:ALA:HB2	3:I:316:ILE:O	1.48	1.11
1:B:500:ALA:HB2	3:J:316:ILE:O	1.48	1.11
1:D:303:MET:HE2	1:D:308:GLU:CB	1.73	1.09
1:C:480:LEU:HD13	1:C:510:VAL:CG1	1.83	1.08
1:C:476:LEU:O	1:C:479:GLN:HB3	1.52	1.07
3:J:319:ASP:HB3	3:J:325:LEU:HG	1.15	1.07
3:I:222:GLN:NE2	3:I:241:ILE:HG21	1.69	1.07
1:B:342:PRO:O	1:B:387:LEU:HD11	1.56	1.06
1:D:573:ILE:O	4:D:902:AGS:N6	1.87	1.06
1:F:311:LEU:HD11	1:F:334:PHE:HZ	1.18	1.06
3:I:319:ASP:OD2	3:I:325:LEU:CG	2.04	1.06
1:C:477:LYS:HA	1:C:480:LEU:HB3	1.36	1.06
3:J:217:LYS:HD3	3:J:366:ASP:HB3	1.34	1.05
3:K:217:LYS:HE2	3:K:217:LYS:HA	1.36	1.04
1:D:303:MET:HE2	1:D:308:GLU:HG3	1.15	1.03
1:B:476:LEU:HD11	1:B:513:LYS:HD3	1.38	1.02
1:A:465:ASN:O	1:A:466:GLU:C	1.96	1.00
3:I:222:GLN:NE2	3:I:241:ILE:HG22	1.72	1.00
1:E:801:VAL:CG2	1:E:802:TYR:HE1	1.71	1.00
1:C:476:LEU:O	1:C:480:LEU:N	1.95	1.00
1:C:480:LEU:HD13	1:C:510:VAL:HG12	1.43	0.99
1:D:303:MET:HE3	1:D:308:GLU:HG3	1.41	0.99
1:E:211:GLY:N	4:E:901:AGS:O1B	1.92	0.98
3:I:222:GLN:CD	3:I:241:ILE:HB	1.84	0.98
1:B:389:ASP:OD2	1:C:332:ARG:HD2	1.64	0.98
1:D:301:LYS:CG	1:D:333:ARG:HH22	1.59	0.98
1:A:431:SER:HA	1:A:442:LEU:CD1	1.94	0.97
1:D:301:LYS:CG	1:D:333:ARG:HH21	1.70	0.97
1:D:301:LYS:HG3	1:D:333:ARG:HH21	1.28	0.96
1:E:180:VAL:HA	4:E:901:AGS:C2	1.94	0.95
3:I:319:ASP:CG	3:I:325:LEU:HG	1.87	0.95
1:B:378:SER:O	1:B:390:LYS:HE3	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LYS:HA	1:C:480:LEU:CB	1.96	0.94
1:D:303:MET:HE1	1:D:308:GLU:HB3	0.94	0.93
1:A:431:SER:HA	1:A:442:LEU:HD11	1.51	0.92
3:J:319:ASP:CB	3:J:325:LEU:HG	1.97	0.92
1:C:476:LEU:HD21	1:C:510:VAL:HG22	1.49	0.92
1:D:303:MET:HE2	1:D:308:GLU:HB2	1.49	0.92
1:D:303:MET:CE	1:D:308:GLU:HB2	1.98	0.92
3:I:222:GLN:HG2	3:I:241:ILE:O	1.70	0.92
1:C:501:GLU:HA	3:K:315:TYR:CD2	2.04	0.91
1:A:501:GLU:HA	3:I:315:TYR:CD2	2.04	0.91
3:I:313:LEU:O	3:I:326:PHE:HB2	1.71	0.91
1:A:406:ILE:HD12	1:A:529:LEU:CD2	2.00	0.91
1:D:303:MET:CE	1:D:308:GLU:HB3	1.79	0.91
3:K:313:LEU:O	3:K:326:PHE:HB2	1.71	0.91
1:B:387:LEU:HB3	1:B:388:PRO:HD2	1.53	0.90
1:B:501:GLU:HA	3:J:315:TYR:CD2	2.04	0.90
1:D:301:LYS:HG3	1:D:333:ARG:NH2	1.79	0.90
3:J:313:LEU:O	3:J:326:PHE:HB2	1.71	0.90
1:F:304:LEU:HD22	1:F:311:LEU:CD2	2.02	0.90
1:A:427:GLU:OE2	1:A:446:ARG:NH2	2.05	0.89
3:K:280:ILE:HG21	3:K:317:THR:HG21	1.54	0.89
1:E:804:ALA:CB	1:E:807:LEU:HD12	2.03	0.89
1:C:471:GLU:O	1:C:475:ASP:CB	2.21	0.88
1:A:466:GLU:OE1	1:A:466:GLU:N	2.07	0.88
1:C:476:LEU:O	1:C:479:GLN:CB	2.20	0.88
1:F:311:LEU:HD11	1:F:334:PHE:CZ	2.07	0.87
1:E:209:GLY:HA2	4:E:901:AGS:O2G	1.72	0.87
1:D:301:LYS:HG2	1:D:333:ARG:HH22	0.77	0.87
1:C:472:ILE:HD12	1:C:473:VAL:H	1.41	0.85
1:E:801:VAL:HG21	1:E:802:TYR:HE1	1.42	0.85
1:C:476:LEU:CD2	1:C:510:VAL:HG22	2.07	0.84
3:J:318:VAL:CG2	3:J:322:LYS:HA	2.05	0.84
1:E:801:VAL:CG2	1:E:802:TYR:CD1	2.49	0.84
1:A:465:ASN:O	1:A:467:LYS:N	2.09	0.84
1:E:801:VAL:HG21	1:E:802:TYR:CE1	2.12	0.83
1:C:473:VAL:O	1:C:514:LEU:HD21	1.79	0.83
1:B:473:VAL:HG13	1:B:514:LEU:HD13	1.58	0.83
1:B:280:LEU:HD23	1:B:313:GLY:HA3	1.59	0.82
1:B:476:LEU:HD21	1:B:510:VAL:CG1	2.10	0.82
1:B:476:LEU:CD1	1:B:513:LYS:HD3	2.09	0.82
3:J:217:LYS:HD2	3:J:366:ASP:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ALA:HB2	3:J:316:ILE:C	2.00	0.82
1:C:471:GLU:O	1:C:475:ASP:N	2.12	0.81
1:A:532:GLU:N	1:A:532:GLU:OE1	2.13	0.81
1:F:605:PHE:HB3	1:F:751:LEU:HB2	1.62	0.81
3:K:217:LYS:O	3:K:217:LYS:NZ	2.13	0.81
1:A:500:ALA:HB2	3:I:316:ILE:C	2.00	0.80
1:A:442:LEU:HD23	1:A:442:LEU:O	1.81	0.80
1:C:476:LEU:O	1:C:479:GLN:CA	2.29	0.80
3:I:319:ASP:OD2	3:I:325:LEU:CD1	2.29	0.80
1:D:573:ILE:HD11	1:D:763:ARG:NH1	1.98	0.79
1:A:406:ILE:CD1	1:A:529:LEU:HD21	2.10	0.79
1:C:500:ALA:HB2	3:K:316:ILE:O	1.82	0.79
1:E:757:ASN:HB3	1:E:760:GLU:HB2	1.65	0.79
1:E:180:VAL:HA	4:E:901:AGS:N1	1.98	0.78
3:I:222:GLN:CG	3:I:241:ILE:HB	2.14	0.78
1:A:466:GLU:O	1:A:469:ALA:N	2.16	0.78
1:C:280:LEU:HD23	1:C:313:GLY:HA3	1.65	0.78
1:C:501:GLU:CA	3:K:315:TYR:HD2	1.97	0.76
4:D:901:AGS:S1G	1:E:332:ARG:NH1	2.59	0.76
3:J:217:LYS:HD3	3:J:366:ASP:CB	2.13	0.76
1:E:805:ARG:CB	1:E:806:PRO:CD	2.64	0.76
3:J:318:VAL:HG22	3:J:322:LYS:HA	1.68	0.76
1:D:572:VAL:HG22	1:D:615:GLU:OE1	1.86	0.76
3:I:308:SER:OG	3:I:331:LEU:O	2.03	0.76
1:B:473:VAL:CG1	1:B:514:LEU:CD1	2.64	0.76
1:C:513:LYS:HA	1:C:513:LYS:HE3	1.68	0.76
3:J:280:ILE:HG21	3:J:317:THR:HG21	1.68	0.75
1:F:304:LEU:HD22	1:F:311:LEU:HD21	1.68	0.75
1:B:476:LEU:HD21	1:B:510:VAL:HG13	1.69	0.75
4:B:902:AGS:S1G	1:C:746:ARG:NH2	2.60	0.75
3:I:280:ILE:HG21	3:I:317:THR:HG21	1.68	0.75
3:J:308:SER:OG	3:J:331:LEU:O	2.03	0.74
1:B:501:GLU:CA	3:J:315:TYR:HD2	1.97	0.74
1:E:804:ALA:HB2	1:E:807:LEU:HD12	1.70	0.74
3:I:159:ARG:NH1	3:I:168:ASP:OD2	2.21	0.74
1:A:501:GLU:CA	3:I:315:TYR:HD2	1.97	0.74
3:I:100:PHE:CD2	3:I:139:ILE:HG21	2.23	0.73
3:K:100:PHE:CD2	3:K:139:ILE:HG21	2.23	0.73
1:B:476:LEU:HD12	1:B:513:LYS:NZ	2.02	0.73
3:J:159:ARG:NH1	3:J:168:ASP:OD2	2.21	0.73
3:J:100:PHE:CD2	3:J:139:ILE:HG21	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:901:AGS:S1G	1:D:746:ARG:NH2	2.61	0.73
1:C:547:GLY:H	1:C:671:ARG:HH21	1.35	0.73
1:A:504:TYR:CE1	3:I:318:VAL:HB	2.24	0.73
1:C:504:TYR:CE1	3:K:318:VAL:HB	2.24	0.73
1:E:283:ILE:HG22	1:E:284:VAL:HG13	1.70	0.73
3:K:159:ARG:NH1	3:K:168:ASP:OD2	2.21	0.73
3:K:217:LYS:HA	3:K:217:LYS:CE	2.18	0.73
1:A:427:GLU:HG2	1:A:445:LEU:HD22	1.70	0.72
3:I:235:ASP:OD1	3:I:237:SER:OG	2.07	0.72
1:B:342:PRO:C	1:B:387:LEU:HD13	2.08	0.72
1:B:378:SER:O	1:B:390:LYS:CE	2.36	0.72
1:C:477:LYS:O	1:C:480:LEU:N	2.23	0.72
1:F:236:THR:OG1	1:F:272:GLN:O	2.07	0.72
1:F:681:ILE:HG12	1:F:718:LEU:HD23	1.71	0.72
3:I:176:THR:OG1	3:I:204:ASN:OD1	2.07	0.72
3:J:235:ASP:OD1	3:J:237:SER:OG	2.07	0.72
1:C:469:ALA:O	1:C:473:VAL:HG22	1.90	0.72
3:I:129:ARG:NH2	3:I:232:GLY:O	2.24	0.71
1:D:545:TRP:HD1	1:D:546:THR:HG23	1.53	0.71
1:F:212:LYS:HD3	1:F:314:ALA:HB1	1.72	0.71
3:J:217:LYS:CE	3:J:366:ASP:HB3	2.20	0.71
3:K:176:THR:OG1	3:K:204:ASN:OD1	2.07	0.71
3:J:209:ALA:HB1	3:J:369:VAL:HG11	1.73	0.71
3:K:129:ARG:NH2	3:K:232:GLY:O	2.24	0.71
3:K:209:ALA:HB1	3:K:369:VAL:HG11	1.73	0.71
1:C:822:MET:HB3	1:C:828:VAL:HG21	1.72	0.71
4:C:902:AGS:S1G	1:D:333:ARG:NH1	2.64	0.71
1:D:301:LYS:HG2	1:D:301:LYS:O	1.89	0.71
3:J:129:ARG:NH2	3:J:232:GLY:O	2.23	0.71
3:K:235:ASP:OD1	3:K:237:SER:OG	2.07	0.71
3:K:308:SER:OG	3:K:331:LEU:O	2.03	0.71
1:A:427:GLU:HB2	1:A:445:LEU:HD21	1.72	0.70
1:E:805:ARG:CB	1:E:806:PRO:HD3	2.21	0.70
1:F:573:ILE:H	4:F:901:AGS:HN62	1.39	0.70
1:D:573:ILE:HG22	4:D:902:AGS:N1	2.05	0.70
1:E:802:TYR:HB2	1:E:805:ARG:HD2	1.72	0.70
3:J:176:THR:OG1	3:J:204:ASN:OD1	2.07	0.70
1:E:180:VAL:HA	4:E:901:AGS:H2	1.72	0.70
1:D:775:ARG:NH1	1:E:593:VAL:O	2.25	0.69
1:E:804:ALA:HB1	1:E:807:LEU:HD12	1.72	0.69
4:B:901:AGS:S1G	1:C:333:ARG:NH1	2.62	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:209:ALA:HB1	3:I:369:VAL:HG11	1.73	0.69
3:K:128:LYS:NZ	3:K:205:GLU:OE2	2.23	0.69
1:A:469:ALA:HB1	1:A:519:PRO:HG3	1.73	0.69
1:B:341:GLU:HG3	1:B:387:LEU:HD12	1.74	0.69
1:C:472:ILE:O	1:C:473:VAL:C	2.30	0.69
1:E:613:LYS:HA	1:E:753:PHE:HE2	1.57	0.69
1:C:471:GLU:O	1:C:475:ASP:HB2	1.93	0.69
1:A:561:LEU:O	1:A:587:ARG:NH2	2.25	0.69
3:J:217:LYS:CD	3:J:366:ASP:CB	2.60	0.69
1:A:445:LEU:O	1:A:445:LEU:HD23	1.91	0.69
1:B:501:GLU:OE2	1:B:506:ARG:NH2	2.25	0.69
1:A:501:GLU:OE2	1:A:506:ARG:NH2	2.25	0.69
1:C:501:GLU:OE2	1:C:506:ARG:NH2	2.25	0.69
1:E:207:GLU:HB3	1:E:208:PRO:HD2	1.75	0.69
3:K:63:VAL:HG12	3:K:76:VAL:HG12	1.75	0.69
1:E:784:GLN:HE22	1:E:786:SER:HB3	1.58	0.69
3:I:122:ARG:NH1	3:I:140:ASP:OD1	2.26	0.69
1:E:228:VAL:O	1:E:233:ARG:NH2	2.26	0.68
1:A:465:ASN:O	1:A:468:ASN:N	2.26	0.68
3:J:63:VAL:HG12	3:J:76:VAL:HG12	1.75	0.68
3:I:142:LYS:CG	3:I:143:LYS:N	2.57	0.68
3:J:122:ARG:NH1	3:J:140:ASP:OD1	2.26	0.68
1:A:410:PRO:HG3	1:A:463:TRP:CD1	2.29	0.68
1:C:478:GLU:OE2	1:C:478:GLU:HA	1.93	0.68
3:K:122:ARG:NH1	3:K:140:ASP:OD1	2.27	0.68
3:K:142:LYS:CG	3:K:143:LYS:N	2.57	0.68
1:C:473:VAL:HA	1:C:514:LEU:CD2	2.24	0.68
1:F:693:LEU:O	1:F:746:ARG:NH1	2.27	0.68
3:I:63:VAL:HG12	3:I:76:VAL:HG12	1.75	0.68
1:D:301:LYS:H	1:D:302:PRO:HD3	1.59	0.68
1:E:211:GLY:H	4:E:901:AGS:PB	2.17	0.68
1:A:194:LEU:O	1:A:310:ARG:NH1	2.27	0.68
1:C:566:ASP:O	1:C:570:LYS:NZ	2.27	0.68
3:I:223:ARG:HD2	3:I:238:LEU:HD22	1.76	0.68
1:C:199:LYS:HD2	1:C:333:ARG:HA	1.76	0.67
3:J:223:ARG:HD2	3:J:238:LEU:HD22	1.76	0.67
3:K:223:ARG:HD2	3:K:238:LEU:HD22	1.76	0.67
1:A:287:GLY:O	1:B:252:ARG:NH2	2.27	0.67
3:I:371:VAL:HG12	3:I:402:VAL:HG11	1.76	0.67
1:A:442:LEU:HD23	1:A:442:LEU:C	2.15	0.67
1:E:669:ARG:HB3	1:E:709:VAL:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ASN:HB2	1:F:310:ARG:O	1.93	0.67
1:F:304:LEU:CD2	1:F:311:LEU:HD21	2.25	0.67
1:F:575:GLN:HB3	1:F:578:ALA:HB3	1.76	0.67
1:B:476:LEU:C	1:B:476:LEU:HD23	2.14	0.67
3:I:119:ASN:O	3:I:123:THR:N	2.28	0.67
3:I:181:ASN:ND2	3:I:184:GLN:OE1	2.28	0.67
1:C:518:LEU:N	1:C:518:LEU:HD12	2.10	0.67
1:F:302:PRO:O	1:F:306:ARG:NH1	2.28	0.67
3:K:371:VAL:HG12	3:K:402:VAL:HG11	1.76	0.67
3:J:142:LYS:CG	3:J:143:LYS:N	2.57	0.67
3:K:119:ASN:O	3:K:123:THR:N	2.28	0.67
1:B:473:VAL:HG13	1:B:514:LEU:CD1	2.25	0.67
3:J:181:ASN:ND2	3:J:184:GLN:OE1	2.27	0.67
3:K:181:ASN:ND2	3:K:184:GLN:OE1	2.27	0.67
3:I:254:ASP:OD2	3:I:346:ARG:NE	2.28	0.67
1:B:341:GLU:HG3	1:B:387:LEU:CD1	2.25	0.66
1:D:301:LYS:N	1:D:302:PRO:HD3	2.10	0.66
3:I:340:THR:O	3:I:344:LEU:N	2.28	0.66
1:C:476:LEU:CD2	1:C:510:VAL:CG1	2.49	0.66
1:C:476:LEU:HD21	1:C:510:VAL:CG2	2.24	0.66
3:K:113:LYS:NZ	3:K:297:GLU:OE1	2.19	0.66
3:K:340:THR:O	3:K:344:LEU:N	2.28	0.66
1:A:476:LEU:HB2	1:A:514:LEU:HD13	1.77	0.66
1:A:775:ARG:NH2	1:B:595:ASP:OD1	2.29	0.66
3:K:219:GLU:CD	3:K:219:GLU:H	1.96	0.66
3:I:128:LYS:NZ	3:I:205:GLU:OE2	2.23	0.66
3:J:119:ASN:O	3:J:123:THR:N	2.28	0.66
3:K:77:LEU:HD11	3:K:408:ALA:O	1.95	0.66
1:B:604:MET:HB2	1:B:718:LEU:HB2	1.77	0.66
1:B:209:GLY:HA2	1:B:389:ASP:OD2	1.95	0.66
1:C:476:LEU:HD23	1:C:510:VAL:CB	2.26	0.66
1:F:394:LEU:HD21	1:F:538:ILE:HG23	1.78	0.66
3:I:77:LEU:HD11	3:I:408:ALA:O	1.96	0.66
3:J:371:VAL:HG12	3:J:402:VAL:HG11	1.76	0.66
1:C:477:LYS:C	1:C:479:GLN:N	2.47	0.66
3:J:77:LEU:HD11	3:J:408:ALA:O	1.95	0.66
3:J:110:GLN:O	3:J:114:ASN:ND2	2.29	0.65
3:J:340:THR:O	3:J:344:LEU:N	2.28	0.65
3:K:110:GLN:O	3:K:114:ASN:ND2	2.29	0.65
1:A:167:ASP:OD1	1:A:168:LEU:N	2.30	0.65
1:A:427:GLU:CG	1:A:445:LEU:HD22	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:254:ASP:OD2	3:K:346:ARG:NE	2.28	0.65
1:D:575:GLN:NE2	1:D:611:VAL:HG12	2.12	0.65
1:F:220:ALA:HB2	1:F:237:ILE:HD11	1.79	0.65
1:C:836:VAL:HG12	1:C:845:LEU:HG	1.78	0.65
1:F:229:PRO:HG2	1:F:232:LEU:HD13	1.77	0.65
1:D:301:LYS:N	1:D:302:PRO:CD	2.60	0.65
1:E:362:HIS:O	1:E:403:ARG:NH1	2.29	0.65
3:K:280:ILE:HG21	3:K:317:THR:CG2	2.27	0.65
1:D:301:LYS:O	1:D:333:ARG:NH2	2.29	0.64
1:A:406:ILE:CD1	1:A:529:LEU:CD2	2.72	0.64
1:C:473:VAL:O	1:C:514:LEU:CD2	2.45	0.64
1:C:476:LEU:O	1:C:479:GLN:C	2.36	0.64
1:E:639:TYR:OH	1:E:663:GLN:OE1	2.14	0.64
3:J:254:ASP:OD2	3:J:346:ARG:NE	2.28	0.64
1:A:702:THR:HG22	1:A:708:THR:HG22	1.79	0.64
1:B:566:ASP:O	1:B:570:LYS:NZ	2.28	0.64
1:E:284:VAL:HG12	1:E:297:GLY:HA2	1.78	0.64
1:E:805:ARG:HB3	1:E:806:PRO:HD3	1.78	0.64
3:I:110:GLN:O	3:I:114:ASN:ND2	2.29	0.64
1:F:565:GLU:OE2	1:F:587:ARG:NH2	2.30	0.64
3:K:129:ARG:NE	3:K:255:ASN:O	2.31	0.64
1:C:727:SER:HB3	1:C:730:GLN:HE21	1.62	0.64
1:F:280:LEU:HD22	1:F:313:GLY:HA3	1.80	0.64
3:I:129:ARG:NE	3:I:255:ASN:O	2.31	0.64
1:F:304:LEU:CD2	1:F:311:LEU:CD2	2.75	0.64
1:A:430:LEU:HD23	1:A:445:LEU:HD13	1.80	0.64
1:E:386:PHE:O	1:E:390:LYS:CB	2.45	0.64
1:F:304:LEU:HD13	1:F:311:LEU:HD23	1.78	0.64
3:J:129:ARG:NE	3:J:255:ASN:O	2.31	0.64
1:B:605:PHE:HB3	1:B:751:LEU:HB2	1.78	0.64
3:K:60:ALA:HB2	3:K:77:LEU:HD12	1.80	0.64
3:K:142:LYS:HG3	3:K:143:LYS:H	1.63	0.64
1:E:610:GLY:HA3	1:E:803:GLY:HA3	1.80	0.64
1:F:696:LEU:O	1:F:746:ARG:NH1	2.31	0.64
3:I:60:ALA:HB2	3:I:77:LEU:HD12	1.80	0.64
3:J:92:ARG:NE	3:J:401:GLU:OE2	2.29	0.64
3:J:128:LYS:NZ	3:J:205:GLU:OE2	2.23	0.64
1:A:647:ARG:NH2	1:B:702:THR:O	2.31	0.63
3:K:145:THR:OG1	3:K:148:GLU:OE1	2.16	0.63
1:A:638:GLU:OE1	1:A:647:ARG:NH2	2.31	0.63
1:B:805:ARG:NH1	4:B:902:AGS:S1G	2.70	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:ASP:OD2	1:C:552:ARG:NH2	2.32	0.63
3:I:142:LYS:HG3	3:I:143:LYS:H	1.63	0.63
3:J:113:LYS:NZ	3:J:297:GLU:OE1	2.19	0.63
3:J:142:LYS:HG3	3:J:143:LYS:H	1.63	0.63
3:I:92:ARG:NE	3:I:401:GLU:OE2	2.29	0.63
3:J:60:ALA:HB2	3:J:77:LEU:HD12	1.80	0.63
1:A:256:GLU:OE1	1:A:256:GLU:N	2.26	0.63
1:C:476:LEU:HD23	1:C:510:VAL:HG13	0.72	0.63
1:E:252:ARG:HH12	2:N:11:UNK:HA	1.62	0.63
1:E:609:THR:OG1	5:E:902:ADP:O2B	2.17	0.63
1:E:666:GLU:OE2	1:E:669:ARG:NH2	2.32	0.63
1:F:304:LEU:HD22	1:F:311:LEU:HD22	1.80	0.63
1:B:473:VAL:CG2	1:B:517:ALA:HB1	2.13	0.63
1:D:568:LEU:HD23	1:D:579:VAL:HG13	1.79	0.63
1:E:209:GLY:CA	4:E:901:AGS:O2G	2.41	0.63
3:K:219:GLU:OE2	3:K:219:GLU:N	2.26	0.63
4:C:902:AGS:O2G	4:C:902:AGS:O1B	2.17	0.63
3:J:145:THR:OG1	3:J:148:GLU:OE1	2.16	0.63
4:B:901:AGS:O2G	4:B:901:AGS:O1B	2.17	0.63
1:C:476:LEU:CD2	1:C:510:VAL:CG2	2.76	0.63
1:D:573:ILE:HG22	4:D:902:AGS:C6	2.28	0.63
3:J:172:ALA:N	3:J:198:ASN:O	2.32	0.63
1:A:466:GLU:O	1:A:468:ASN:N	2.32	0.62
1:A:503:ARG:NH2	3:I:316:ILE:O	2.32	0.62
1:C:472:ILE:HD12	1:C:473:VAL:N	2.14	0.62
1:E:769:LEU:HA	1:E:772:LEU:HG	1.80	0.62
3:J:355:ILE:O	3:J:359:GLY:N	2.31	0.62
1:B:665:THR:HG23	1:B:709:VAL:HG21	1.81	0.62
3:I:145:THR:OG1	3:I:148:GLU:OE1	2.16	0.62
3:I:172:ALA:N	3:I:198:ASN:O	2.32	0.62
3:I:319:ASP:OD2	3:I:325:LEU:HD11	1.98	0.62
1:B:503:ARG:NH2	3:J:316:ILE:O	2.32	0.62
4:D:901:AGS:O2A	4:D:901:AGS:O2B	2.18	0.62
3:K:355:ILE:O	3:K:359:GLY:N	2.31	0.62
3:J:368:VAL:HG23	3:J:391:LYS:HE3	1.81	0.62
1:A:460:THR:O	1:A:464:GLN:HB2	2.00	0.62
1:C:472:ILE:O	1:C:475:ASP:N	2.33	0.62
1:C:605:PHE:HB3	1:C:751:LEU:HB2	1.81	0.62
1:B:476:LEU:HA	1:B:479:GLN:HE21	1.63	0.62
1:F:316:THR:OG1	1:F:318:ASP:OD1	2.14	0.62
3:I:142:LYS:HG3	3:I:143:LYS:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:280:ILE:CG2	3:K:317:THR:HG21	2.27	0.62
1:A:210:VAL:HG13	1:A:341:GLU:HA	1.82	0.62
1:C:197:ARG:HG2	1:C:198:THR:HG23	1.80	0.62
1:A:466:GLU:O	1:A:467:LYS:C	2.38	0.62
3:K:368:VAL:HG23	3:K:391:LYS:HE3	1.81	0.62
3:I:113:LYS:NZ	3:I:297:GLU:OE1	2.19	0.62
3:I:236:VAL:HG11	3:I:351:PHE:HA	1.82	0.61
3:K:172:ALA:N	3:K:198:ASN:O	2.32	0.61
1:E:184:ASP:OD1	1:E:222:ARG:NH1	2.33	0.61
3:K:217:LYS:HE2	3:K:217:LYS:CA	2.21	0.61
3:K:385:LYS:NZ	3:K:392:GLU:OE1	2.33	0.61
1:A:608:PRO:O	1:A:613:LYS:NZ	2.33	0.61
3:I:355:ILE:O	3:I:359:GLY:N	2.31	0.61
3:J:385:LYS:NZ	3:J:392:GLU:OE1	2.33	0.61
3:K:142:LYS:HG3	3:K:143:LYS:N	2.15	0.61
1:A:378:SER:OG	1:A:390:LYS:HG3	2.01	0.61
3:K:221:GLU:HA	3:K:241:ILE:O	2.01	0.61
1:A:409:ARG:NH2	1:A:414:ASP:OD1	2.32	0.61
1:B:477:LYS:O	1:B:480:LEU:HB3	2.01	0.61
3:J:139:ILE:HG22	3:J:139:ILE:O	2.00	0.61
3:J:142:LYS:HG3	3:J:143:LYS:N	2.15	0.61
3:K:139:ILE:HG22	3:K:139:ILE:O	2.00	0.61
1:A:365:ARG:O	1:A:532:GLU:HB2	2.01	0.61
1:B:473:VAL:HG11	1:B:514:LEU:CD1	2.31	0.61
1:F:603:PHE:HB3	1:F:748:ASP:HB2	1.82	0.61
3:I:139:ILE:HG22	3:I:139:ILE:O	2.00	0.61
1:C:393:ASP:OD1	1:D:196:ARG:NH2	2.28	0.61
1:D:788:PRO:HB2	1:D:838:VAL:HG21	1.82	0.61
1:E:374:ALA:HB2	1:E:538:ILE:HD13	1.83	0.61
1:C:476:LEU:CD2	1:C:510:VAL:CB	2.79	0.61
1:C:496:LEU:HD21	3:K:316:ILE:HG23	1.82	0.61
3:K:236:VAL:HG11	3:K:351:PHE:HA	1.83	0.61
1:E:563:ARG:HH21	1:E:567:GLU:HB2	1.66	0.61
3:I:63:VAL:CG1	3:I:76:VAL:HG12	2.31	0.61
3:I:368:VAL:HG23	3:I:391:LYS:HE3	1.81	0.61
3:J:236:VAL:HG11	3:J:351:PHE:HA	1.83	0.61
3:K:63:VAL:CG1	3:K:76:VAL:HG12	2.31	0.61
1:B:341:GLU:CG	1:B:387:LEU:HD12	2.30	0.60
1:C:167:ASP:OD1	1:C:168:LEU:N	2.34	0.60
1:E:281:HIS:O	1:E:323:HIS:ND1	2.26	0.60
4:B:902:AGS:O1B	4:B:902:AGS:O2G	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:VAL:CG2	1:D:615:GLU:OE1	2.49	0.60
3:I:385:LYS:NZ	3:I:392:GLU:OE1	2.33	0.60
3:K:92:ARG:NE	3:K:401:GLU:OE2	2.28	0.60
3:K:307:GLN:OE1	3:K:307:GLN:N	2.34	0.60
1:A:435:ASP:OD1	1:A:436:GLU:N	2.34	0.60
1:C:477:LYS:O	1:C:478:GLU:C	2.38	0.60
1:C:480:LEU:HB2	1:C:510:VAL:HG11	1.84	0.60
1:E:659:GLU:OE1	1:E:659:GLU:N	2.33	0.60
3:J:307:GLN:N	3:J:307:GLN:OE1	2.34	0.60
3:K:314:PRO:O	3:K:315:TYR:O	2.20	0.60
1:E:818:GLN:HE21	1:E:845:LEU:HD12	1.66	0.60
3:I:307:GLN:OE1	3:I:307:GLN:N	2.34	0.60
1:E:386:PHE:O	1:E:390:LYS:HB2	2.01	0.60
4:A:901:AGS:O2G	4:A:901:AGS:O1B	2.18	0.60
1:B:473:VAL:CG1	1:B:514:LEU:HD13	2.27	0.60
1:C:608:PRO:HG2	1:C:611:VAL:HG21	1.84	0.60
1:D:380:ARG:NH1	1:D:381:TYR:OH	2.35	0.60
1:E:546:THR:HG23	1:E:548:ILE:H	1.67	0.60
1:A:365:ARG:HH21	1:A:531:GLU:HB2	1.67	0.59
1:D:300:ILE:HD13	1:D:300:ILE:O	2.01	0.59
1:F:538:ILE:O	1:F:542:VAL:HG23	2.02	0.59
1:F:548:ILE:HD12	1:F:549:PRO:HD2	1.84	0.59
3:J:63:VAL:CG1	3:J:76:VAL:HG12	2.31	0.59
3:J:314:PRO:O	3:J:315:TYR:O	2.20	0.59
1:A:427:GLU:OE2	1:A:446:ARG:CZ	2.50	0.59
1:F:311:LEU:HD12	1:F:311:LEU:O	2.02	0.59
1:C:476:LEU:O	1:C:479:GLN:N	2.36	0.59
4:C:901:AGS:O1B	4:C:901:AGS:O2G	2.20	0.59
3:I:314:PRO:O	3:I:315:TYR:O	2.20	0.59
3:J:108:VAL:O	3:J:156:LYS:NZ	2.36	0.59
1:B:411:VAL:O	1:B:412:GLU:HG2	2.01	0.59
4:D:902:AGS:O1B	4:D:902:AGS:O2G	2.19	0.59
1:F:779:ARG:HH21	1:F:823:LEU:HG	1.66	0.59
1:C:414:ASP:OD1	1:C:418:ARG:NH1	2.36	0.59
1:C:477:LYS:O	1:C:479:GLN:N	2.36	0.59
1:B:242:LEU:HD11	1:B:283:ILE:HG13	1.85	0.59
4:B:902:AGS:O2A	4:B:902:AGS:O2B	2.20	0.59
3:K:184:GLN:O	3:K:188:THR:HG23	2.03	0.59
1:B:726:GLY:HA3	1:B:730:GLN:HB2	1.85	0.59
1:C:480:LEU:HD13	1:C:510:VAL:HG11	1.78	0.59
1:E:698:GLU:OE2	1:E:700:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:VAL:HG13	1:F:375:ALA:HB1	1.85	0.59
1:F:345:GLU:HA	1:F:348:ILE:HD12	1.85	0.59
1:A:654:GLY:HA2	1:F:656:VAL:HB	1.84	0.58
1:F:267:LYS:NZ	1:F:308:GLU:OE2	2.26	0.58
3:K:258:GLY:N	3:K:261:ASP:OD1	2.36	0.58
1:A:545:TRP:CD1	1:A:546:THR:HG23	2.38	0.58
1:A:702:THR:O	1:F:647:ARG:NH2	2.36	0.58
1:E:765:VAL:O	1:E:769:LEU:HG	2.03	0.58
3:I:184:GLN:O	3:I:188:THR:HG23	2.03	0.58
3:J:258:GLY:N	3:J:261:ASP:OD1	2.36	0.58
1:A:196:ARG:NH2	1:F:397:GLU:OE2	2.36	0.58
1:A:427:GLU:CG	1:A:445:LEU:CD2	2.80	0.58
1:B:645:VAL:HG11	1:B:691:VAL:HG21	1.84	0.58
1:C:471:GLU:O	1:C:475:ASP:CA	2.51	0.58
1:E:221:GLN:HA	1:E:224:VAL:HG12	1.85	0.58
3:K:100:PHE:HB2	3:K:139:ILE:HD12	1.84	0.58
1:A:785:VAL:HA	1:A:836:VAL:HG22	1.84	0.58
1:B:808:ARG:HH22	1:C:598:ARG:HD2	1.68	0.58
3:I:108:VAL:O	3:I:156:LYS:NZ	2.36	0.58
1:E:263:LEU:HD23	1:E:303:MET:HG3	1.85	0.58
1:F:189:ARG:NH1	1:F:192:GLN:OE1	2.36	0.58
1:A:670:ARG:HD3	1:B:317:LEU:HD21	1.84	0.58
1:C:518:LEU:HD12	1:C:518:LEU:H	1.69	0.58
4:C:901:AGS:O2A	4:C:901:AGS:O2B	2.19	0.58
3:I:258:GLY:N	3:I:261:ASP:OD1	2.36	0.58
3:K:108:VAL:O	3:K:156:LYS:NZ	2.36	0.58
1:A:779:ARG:HH22	1:A:823:LEU:HD21	1.69	0.58
3:J:184:GLN:O	3:J:188:THR:HG23	2.03	0.58
3:J:341:GLN:O	3:J:341:GLN:NE2	2.37	0.58
1:A:666:GLU:O	1:A:670:ARG:NH1	2.36	0.58
1:E:805:ARG:HB3	1:E:806:PRO:CD	2.32	0.58
3:I:100:PHE:HB2	3:I:139:ILE:HD12	1.85	0.58
1:A:415:GLU:OE2	1:B:188:ARG:NH2	2.36	0.57
3:K:341:GLN:O	3:K:341:GLN:NE2	2.37	0.57
1:A:250:LYS:NZ	1:B:254:GLU:OE1	2.32	0.57
1:A:500:ALA:CB	3:I:316:ILE:C	2.71	0.57
1:A:321:ARG:HB3	1:F:670:ARG:HH22	1.70	0.57
3:I:206:PRO:HA	3:I:226:VAL:HG11	1.87	0.57
3:J:350:PRO:O	3:J:353:SER:OG	2.19	0.57
1:A:427:GLU:OE2	1:A:446:ARG:NE	2.38	0.57
1:A:465:ASN:O	1:A:466:GLU:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:341:GLN:O	3:I:341:GLN:NE2	2.37	0.57
1:A:653:PRO:HA	1:A:658:TYR:CZ	2.40	0.57
1:C:274:ILE:HG12	1:C:310:ARG:HD3	1.85	0.57
3:K:350:PRO:O	3:K:353:SER:OG	2.19	0.57
1:B:469:ALA:O	1:B:472:ILE:HG22	2.04	0.57
1:D:769:LEU:HD13	1:D:785:VAL:HG21	1.87	0.57
1:E:571:ARG:NH2	1:E:628:GLU:OE1	2.32	0.57
1:F:279:GLU:HB3	1:F:281:HIS:NE2	2.20	0.57
3:J:100:PHE:HB2	3:J:139:ILE:HD12	1.85	0.57
3:K:209:ALA:HB2	3:K:371:VAL:HG11	1.87	0.57
1:A:411:VAL:O	1:A:412:GLU:HG2	2.05	0.57
1:C:472:ILE:CD1	1:C:473:VAL:H	2.13	0.57
1:C:518:LEU:H	1:C:518:LEU:CD1	2.18	0.57
3:I:209:ALA:HB2	3:I:371:VAL:HG11	1.87	0.57
1:B:161:LEU:O	1:B:165:SER:OG	2.19	0.57
1:B:500:ALA:CB	3:J:316:ILE:C	2.71	0.57
1:D:299:MET:O	1:D:302:PRO:CD	2.53	0.57
3:I:67:LEU:O	3:I:128:LYS:NZ	2.26	0.57
3:K:313:LEU:HB2	3:K:316:ILE:HD11	1.86	0.57
1:A:378:SER:HB2	1:A:394:LEU:HD11	1.87	0.57
1:C:757:ASN:HB2	1:C:760:GLU:HG3	1.87	0.57
3:K:185:ARG:NH2	3:K:204:ASN:OD1	2.38	0.57
3:K:341:GLN:NE2	3:K:345:ASP:OD1	2.38	0.57
1:C:505:GLY:O	1:C:509:GLU:HB2	2.05	0.56
3:I:341:GLN:NE2	3:I:345:ASP:OD1	2.38	0.56
3:K:207:THR:HG23	3:K:246:VAL:HG11	1.87	0.56
1:C:476:LEU:HG	1:C:479:GLN:OE1	2.04	0.56
3:J:102:ARG:NH2	3:J:121:ASP:OD1	2.39	0.56
1:A:496:LEU:HD22	3:I:288:ALA:HA	1.86	0.56
1:A:549:PRO:HB2	1:A:590:ARG:HH12	1.70	0.56
1:A:669:ARG:NH2	1:B:325:GLU:OE1	2.30	0.56
1:E:691:VAL:O	1:E:695:VAL:HG23	2.04	0.56
1:E:802:TYR:CD1	1:E:802:TYR:N	2.73	0.56
1:F:604:MET:HB2	1:F:718:LEU:HB2	1.87	0.56
3:I:392:GLU:OE2	3:I:395:LYS:NZ	2.37	0.56
3:J:113:LYS:O	3:J:293:ARG:NH2	2.38	0.56
3:J:206:PRO:HA	3:J:226:VAL:HG11	1.87	0.56
1:A:202:PRO:HG2	1:A:312:VAL:HG23	1.88	0.56
3:I:113:LYS:O	3:I:293:ARG:NH2	2.38	0.56
3:I:185:ARG:NH2	3:I:204:ASN:OD1	2.38	0.56
3:K:102:ARG:NH2	3:K:121:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:206:PRO:HA	3:K:226:VAL:HG11	1.87	0.56
1:B:473:VAL:HG11	1:B:514:LEU:HD12	1.87	0.56
1:C:496:LEU:HD22	3:K:288:ALA:HA	1.86	0.56
1:E:772:LEU:HA	1:E:775:ARG:HG2	1.88	0.56
3:K:257:LEU:HD12	3:K:258:GLY:H	1.71	0.56
3:I:257:LEU:HD12	3:I:258:GLY:H	1.70	0.56
3:J:185:ARG:NH2	3:J:204:ASN:OD1	2.38	0.56
3:J:341:GLN:NE2	3:J:345:ASP:OD1	2.38	0.56
1:A:769:LEU:HD13	1:A:785:VAL:HG21	1.88	0.56
1:E:180:VAL:CA	4:E:901:AGS:N1	2.68	0.56
1:F:603:PHE:HA	1:F:747:LEU:HD22	1.87	0.56
3:I:191:ALA:HA	3:I:194:ILE:HD12	1.87	0.56
3:I:207:THR:HG23	3:I:246:VAL:HG11	1.87	0.56
3:J:207:THR:HG23	3:J:246:VAL:HG11	1.87	0.56
3:J:380:VAL:O	3:J:384:VAL:HG23	2.06	0.56
3:K:191:ALA:HA	3:K:194:ILE:HD12	1.88	0.56
1:B:341:GLU:CD	1:B:387:LEU:HG	2.27	0.56
1:B:341:GLU:OE1	1:B:387:LEU:HG	2.06	0.56
1:B:476:LEU:HD21	1:B:510:VAL:HG12	1.88	0.56
3:K:113:LYS:O	3:K:293:ARG:NH2	2.38	0.56
1:C:326:LYS:NZ	1:C:327:ASP:OD1	2.35	0.56
1:C:476:LEU:HD21	1:C:510:VAL:HA	1.87	0.56
1:E:801:VAL:C	1:E:802:TYR:CD1	2.79	0.56
3:I:102:ARG:NH2	3:I:121:ASP:OD1	2.39	0.56
3:I:380:VAL:O	3:I:384:VAL:HG23	2.06	0.56
1:B:347:THR:HG23	1:B:388:PRO:HD3	1.88	0.56
1:B:608:PRO:O	1:B:613:LYS:NZ	2.39	0.56
1:A:595:ASP:OD2	1:F:775:ARG:NH2	2.39	0.55
1:B:471:GLU:OE1	1:B:471:GLU:HA	2.04	0.55
1:C:471:GLU:O	1:C:475:ASP:HB3	2.05	0.55
1:E:167:ASP:OD1	1:E:170:ALA:N	2.31	0.55
1:E:726:GLY:HA3	1:E:730:GLN:HG3	1.87	0.55
1:F:786:SER:HB2	1:F:788:PRO:HD2	1.88	0.55
3:J:326:PHE:CD1	3:J:327:LEU:N	2.74	0.55
3:K:261:ASP:O	3:K:265:ARG:NH1	2.39	0.55
1:A:235:LYS:NZ	1:A:271:GLY:O	2.30	0.55
1:A:465:ASN:C	1:A:467:LYS:N	2.58	0.55
1:E:720:SER:OG	1:E:721:ASN:N	2.39	0.55
3:I:319:ASP:HB3	3:I:325:LEU:HD12	1.86	0.55
1:A:431:SER:CA	1:A:442:LEU:HD11	2.30	0.55
1:B:480:LEU:HG	1:B:484:ARG:CZ	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ASP:OD2	1:D:700:ARG:NH1	2.35	0.55
3:J:261:ASP:O	3:J:265:ARG:NH1	2.39	0.55
1:B:496:LEU:HD22	3:J:288:ALA:HA	1.86	0.55
1:D:767:ILE:O	1:D:771:GLN:HG3	2.07	0.55
3:J:209:ALA:HB2	3:J:371:VAL:HG11	1.87	0.55
3:J:392:GLU:OE2	3:J:395:LYS:NZ	2.37	0.55
1:E:275:THR:OG1	1:E:276:PHE:N	2.37	0.55
1:F:310:ARG:HA	1:F:310:ARG:HE	1.71	0.55
3:I:208:ALA:HB3	3:I:403:VAL:HG13	1.89	0.55
3:I:261:ASP:O	3:I:265:ARG:NH1	2.39	0.55
3:J:208:ALA:HB3	3:J:403:VAL:HG13	1.89	0.55
1:A:410:PRO:CD	1:A:463:TRP:NE1	2.69	0.55
1:A:561:LEU:HD21	1:A:590:ARG:HG3	1.89	0.55
1:D:575:GLN:HE21	1:D:611:VAL:HG12	1.71	0.55
3:I:326:PHE:CD1	3:I:327:LEU:N	2.74	0.55
1:B:703:ASP:OD1	1:B:703:ASP:N	2.39	0.55
1:E:656:VAL:HG22	2:N:25:UNK:HA	1.89	0.55
3:J:257:LEU:HD12	3:J:258:GLY:H	1.70	0.55
3:K:208:ALA:HB3	3:K:403:VAL:HG13	1.89	0.55
1:A:442:LEU:HD21	1:A:446:ARG:CZ	2.37	0.55
1:E:814:ALA:O	1:E:818:GLN:HB3	2.06	0.55
3:J:191:ALA:HA	3:J:194:ILE:HD12	1.87	0.55
3:K:282:LEU:HD12	3:K:292:LEU:HD11	1.89	0.55
3:K:326:PHE:CD1	3:K:327:LEU:N	2.74	0.55
1:A:276:PHE:HD1	1:A:312:VAL:HG13	1.71	0.55
1:B:347:THR:CG2	1:B:388:PRO:HD3	2.37	0.55
1:B:476:LEU:HA	1:B:479:GLN:HB3	1.88	0.55
1:E:566:ASP:O	1:E:570:LYS:N	2.39	0.55
1:E:726:GLY:H	1:E:730:GLN:HE21	1.55	0.55
1:A:287:GLY:HA2	1:A:296:ALA:HB3	1.88	0.54
1:D:299:MET:O	1:D:302:PRO:HD3	2.08	0.54
3:K:392:GLU:OE2	3:K:395:LYS:NZ	2.37	0.54
1:A:181:ILE:HD12	1:A:181:ILE:H	1.72	0.54
3:I:350:PRO:O	3:I:353:SER:OG	2.19	0.54
3:J:67:LEU:O	3:J:128:LYS:NZ	2.26	0.54
1:A:504:TYR:CD1	3:I:318:VAL:HB	2.41	0.54
3:K:380:VAL:O	3:K:384:VAL:HG23	2.06	0.54
1:B:545:TRP:HB2	1:C:189:ARG:NH2	2.22	0.54
1:C:509:GLU:OE1	1:C:509:GLU:HA	2.06	0.54
1:E:191:VAL:HG23	1:E:232:LEU:HD13	1.89	0.54
1:F:310:ARG:HA	1:F:310:ARG:NE	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ARG:NH1	4:A:902:AGS:O3'	2.40	0.54
1:B:557:GLU:OE1	1:B:590:ARG:NH2	2.41	0.54
1:C:476:LEU:C	1:C:479:GLN:HB3	2.25	0.54
1:D:163:LYS:NZ	1:D:164:TYR:OH	2.41	0.54
1:B:504:TYR:CE2	3:J:317:THR:HA	2.42	0.54
1:C:263:LEU:HD11	1:C:300:ILE:HG22	1.88	0.54
1:E:805:ARG:HB2	1:E:806:PRO:CD	2.38	0.54
4:D:901:AGS:O2G	4:D:901:AGS:O1B	2.26	0.54
1:E:809:ARG:HA	1:E:812:GLN:HG2	1.89	0.54
1:A:614:THR:OG1	4:A:902:AGS:O1B	2.24	0.54
1:B:476:LEU:CD1	1:B:513:LYS:CD	2.83	0.54
1:D:565:GLU:OE2	1:D:587:ARG:NH2	2.31	0.54
1:D:685:HIS:O	1:D:687:ASP:N	2.34	0.54
1:F:613:LYS:NZ	4:F:901:AGS:O3G	2.37	0.54
4:A:902:AGS:O1B	4:A:902:AGS:O2G	2.24	0.54
1:B:476:LEU:CD2	1:B:510:VAL:HG13	2.38	0.54
1:B:799:ASP:O	1:B:801:VAL:N	2.33	0.54
1:C:298:ASN:HB2	1:C:301:LYS:HE3	1.90	0.54
1:D:799:ASP:N	1:D:799:ASP:OD1	2.42	0.54
1:E:342:PRO:HG2	1:E:388:PRO:HG3	1.89	0.53
1:E:611:VAL:C	5:E:902:ADP:N7	2.61	0.53
3:I:282:LEU:HD12	3:I:292:LEU:HD11	1.89	0.53
1:A:634:ILE:HD11	1:A:678:PHE:HE1	1.73	0.53
1:D:575:GLN:NE2	1:D:611:VAL:CG1	2.71	0.53
1:B:476:LEU:O	1:B:480:LEU:N	2.40	0.53
3:K:186:GLN:OE1	3:K:189:LYS:NZ	2.39	0.53
1:B:501:GLU:HG3	3:J:315:TYR:CD2	2.44	0.53
1:C:194:LEU:HD21	1:C:274:ILE:HG21	1.91	0.53
1:C:477:LYS:HG3	1:C:480:LEU:CD2	2.39	0.53
1:F:318:ASP:O	1:F:322:LYS:HG2	2.08	0.53
1:A:501:GLU:HG3	3:I:315:TYR:CD2	2.44	0.53
1:A:741:PRO:O	1:A:745:ASN:HB2	2.09	0.53
1:C:501:GLU:HG3	3:K:315:TYR:CD2	2.44	0.53
1:F:222:ARG:HH22	1:F:228:VAL:HG12	1.72	0.53
1:F:843:ASP:N	1:F:843:ASP:OD1	2.41	0.53
1:A:786:SER:OG	1:A:788:PRO:HD2	2.09	0.53
1:D:386:PHE:O	1:D:390:LYS:HB3	2.09	0.53
3:K:84:VAL:HG12	3:K:92:ARG:HB3	1.91	0.53
3:K:148:GLU:HG3	3:K:194:ILE:HD13	1.91	0.53
3:K:321:ASP:O	3:K:322:LYS:HB2	2.08	0.53
1:B:300:ILE:HD11	1:B:309:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:TYR:CE2	3:I:317:THR:HA	2.43	0.53
1:C:826:GLY:O	1:C:827:GLN:HG2	2.08	0.53
1:D:573:ILE:O	1:D:573:ILE:HG23	2.08	0.53
1:E:819:LEU:O	1:E:823:LEU:HG	2.08	0.53
3:I:297:GLU:O	3:I:301:ILE:HD12	2.09	0.53
1:A:726:GLY:HA3	1:A:730:GLN:HB2	1.91	0.53
1:C:507:ILE:O	1:C:511:GLU:HG3	2.09	0.53
1:D:539:ALA:HA	1:D:542:VAL:HG12	1.91	0.53
1:E:740:LYS:HG3	1:E:742:GLU:HG3	1.90	0.53
1:F:234:ASP:O	1:F:236:THR:N	2.42	0.53
3:K:100:PHE:CG	3:K:139:ILE:HG13	2.44	0.53
1:A:196:ARG:HG2	1:A:197:ARG:H	1.74	0.53
1:C:381:TYR:HE2	1:C:550:ALA:HB2	1.72	0.53
3:J:186:GLN:OE1	3:J:189:LYS:NZ	2.38	0.53
3:K:373:GLY:N	3:K:400:ASP:OD1	2.42	0.53
1:A:445:LEU:HD23	1:A:445:LEU:C	2.29	0.52
1:C:430:LEU:HD22	1:C:442:LEU:HD13	1.91	0.52
1:C:477:LYS:CA	1:C:480:LEU:H	2.21	0.52
1:C:513:LYS:HE3	1:C:513:LYS:CA	2.37	0.52
1:D:681:ILE:HG21	1:D:718:LEU:HD12	1.90	0.52
1:E:242:LEU:HD11	1:E:283:ILE:HD11	1.92	0.52
1:E:181:ILE:H	1:E:181:ILE:HD12	1.74	0.52
1:E:301:LYS:HE2	1:E:330:LEU:HD13	1.91	0.52
1:E:805:ARG:HB2	1:E:806:PRO:HD3	1.90	0.52
1:F:210:VAL:HG11	1:F:339:VAL:HG21	1.91	0.52
3:J:282:LEU:HD12	3:J:292:LEU:HD11	1.89	0.52
3:I:84:VAL:HG12	3:I:92:ARG:HB3	1.91	0.52
3:K:67:LEU:O	3:K:128:LYS:NZ	2.26	0.52
1:B:476:LEU:HD12	1:B:513:LYS:HZ3	1.73	0.52
1:B:646:ALA:HA	1:B:649:ILE:HG22	1.91	0.52
1:E:801:VAL:C	1:E:802:TYR:HD1	2.13	0.52
3:J:84:VAL:HG12	3:J:92:ARG:HB3	1.91	0.52
1:C:477:LYS:HG3	1:C:480:LEU:HD23	1.91	0.52
1:D:826:GLY:O	1:D:827:GLN:HG2	2.10	0.52
3:I:100:PHE:CG	3:I:139:ILE:HG13	2.44	0.52
3:J:217:LYS:HD2	3:J:366:ASP:CB	2.37	0.52
3:K:241:ILE:HG12	3:K:246:VAL:HG13	1.91	0.52
1:B:476:LEU:O	1:B:479:GLN:HB3	2.10	0.52
3:J:297:GLU:O	3:J:301:ILE:HD12	2.09	0.52
1:E:213:THR:OG1	4:E:901:AGS:O2A	2.23	0.52
3:I:241:ILE:HG12	3:I:246:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:100:PHE:CG	3:J:139:ILE:HG13	2.44	0.52
3:J:241:ILE:HG12	3:J:246:VAL:HG13	1.91	0.52
1:B:341:GLU:CG	1:B:387:LEU:CD1	2.87	0.52
1:C:720:SER:OG	1:C:721:ASN:N	2.40	0.52
1:D:303:MET:HE3	1:D:308:GLU:CG	2.11	0.52
1:F:319:GLU:O	1:F:323:HIS:HB2	2.10	0.52
1:D:692:LEU:HA	1:D:695:VAL:HB	1.92	0.52
1:F:352:ARG:O	1:F:355:LYS:NZ	2.33	0.52
3:K:297:GLU:O	3:K:301:ILE:HD12	2.09	0.52
1:A:710:ASP:OD1	1:A:710:ASP:N	2.40	0.52
4:A:902:AGS:S1G	1:B:746:ARG:NH2	2.75	0.52
1:F:308:GLU:N	1:F:308:GLU:OE1	2.43	0.52
1:F:350:ILE:HG12	5:F:902:ADP:N1	2.24	0.52
1:F:403:ARG:HA	1:F:406:ILE:HD12	1.91	0.52
1:B:480:LEU:HG	1:B:484:ARG:NH1	2.25	0.51
1:C:477:LYS:HA	1:C:480:LEU:HB2	1.90	0.51
3:I:280:ILE:HG21	3:I:317:THR:CG2	2.39	0.51
3:J:148:GLU:HG3	3:J:194:ILE:HD13	1.91	0.51
1:C:472:ILE:HA	1:C:475:ASP:HB3	1.92	0.51
1:E:167:ASP:OD1	1:E:169:THR:N	2.43	0.51
1:F:785:VAL:HA	1:F:836:VAL:HG12	1.92	0.51
3:K:326:PHE:HD1	3:K:327:LEU:N	2.08	0.51
1:A:213:THR:O	1:A:217:GLU:HG2	2.10	0.51
1:B:455:LYS:HG3	1:B:459:LEU:HD13	1.91	0.51
1:E:710:ASP:OD1	1:E:710:ASP:N	2.42	0.51
1:A:476:LEU:CB	1:A:514:LEU:HD13	2.39	0.51
1:B:480:LEU:HD11	1:B:507:ILE:HG23	1.92	0.51
1:B:504:TYR:CB	3:J:324:PRO:HG3	2.41	0.51
1:E:179:PRO:O	4:E:901:AGS:H2	2.11	0.51
1:A:361:HIS:CD2	1:B:197:ARG:HB2	2.46	0.51
1:C:546:THR:O	1:C:548:ILE:N	2.43	0.51
1:C:732:LEU:O	1:C:736:ARG:NH2	2.43	0.51
1:D:763:ARG:O	1:D:767:ILE:HG12	2.10	0.51
1:E:614:THR:O	1:E:618:LYS:HG3	2.11	0.51
1:F:579:VAL:HA	1:F:582:VAL:HG12	1.93	0.51
3:J:308:SER:OG	3:J:330:GLN:NE2	2.44	0.51
1:A:504:TYR:CB	3:I:324:PRO:HG3	2.41	0.51
1:A:745:ASN:ND2	1:F:805:ARG:HD2	2.25	0.51
1:E:318:ASP:OD1	1:E:319:GLU:N	2.42	0.51
1:E:805:ARG:N	1:E:806:PRO:HD2	2.25	0.51
3:I:326:PHE:HD1	3:I:327:LEU:N	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:326:PHE:HD1	3:J:327:LEU:N	2.09	0.51
1:D:205:ILE:HD12	1:D:336:GLN:HB3	1.93	0.51
1:D:633:ARG:NH2	1:D:679:ASP:OD2	2.44	0.51
3:I:223:ARG:N	3:I:366:ASP:OD2	2.43	0.51
1:B:434:GLU:OE1	1:B:434:GLU:N	2.43	0.51
1:D:277:ILE:HD12	1:D:311:LEU:HD11	1.92	0.51
3:I:148:GLU:HG3	3:I:194:ILE:HD13	1.91	0.51
1:A:194:LEU:HD11	1:A:310:ARG:HB3	1.93	0.51
1:A:666:GLU:HB3	1:A:670:ARG:HH12	1.75	0.51
1:E:386:PHE:O	1:E:390:LYS:HB3	2.11	0.51
3:I:71:ASN:ND2	3:I:400:ASP:OD1	2.44	0.51
3:K:71:ASN:ND2	3:K:400:ASP:OD1	2.44	0.51
1:B:441:ARG:NH2	1:C:368:ASP:OD1	2.44	0.50
1:B:487:SER:HA	1:B:502:LEU:HD13	1.94	0.50
1:B:504:TYR:HB2	3:J:324:PRO:HG3	1.93	0.50
1:F:232:LEU:O	1:F:234:ASP:N	2.42	0.50
3:I:158:LYS:NZ	3:I:168:ASP:OD2	2.45	0.50
3:J:71:ASN:ND2	3:J:400:ASP:OD1	2.44	0.50
3:J:280:ILE:HG21	3:J:317:THR:CG2	2.39	0.50
3:J:299:ALA:HB2	3:J:311:ILE:HD11	1.93	0.50
1:A:386:PHE:C	1:A:390:LYS:HD2	2.32	0.50
1:C:643:HIS:HD2	1:D:652:PRO:HG3	1.76	0.50
1:C:799:ASP:O	1:C:801:VAL:N	2.38	0.50
1:E:355:LYS:HG3	1:E:366:ILE:HG13	1.92	0.50
3:J:158:LYS:NZ	3:J:168:ASP:OD2	2.45	0.50
3:K:299:ALA:HB2	3:K:311:ILE:HD11	1.93	0.50
1:A:421:ARG:O	1:A:425:ILE:HG13	2.11	0.50
3:I:299:ALA:HB2	3:I:311:ILE:HD11	1.93	0.50
3:J:62:ALA:HB3	3:J:411:ALA:HB1	1.94	0.50
3:K:308:SER:OG	3:K:330:GLN:NE2	2.44	0.50
1:C:487:SER:HA	1:C:502:LEU:HD13	1.94	0.50
1:D:322:LYS:HE3	1:D:323:HIS:CD2	2.46	0.50
1:D:785:VAL:HA	1:D:836:VAL:HG22	1.94	0.50
1:E:563:ARG:NH2	1:E:567:GLU:HB2	2.25	0.50
1:F:222:ARG:HH11	1:F:227:ASP:HB2	1.76	0.50
3:J:257:LEU:HD12	3:J:258:GLY:N	2.26	0.50
1:A:643:HIS:HB2	1:B:655:TYR:CZ	2.47	0.50
1:B:470:ILE:CB	1:B:519:PRO:HG2	2.41	0.50
3:K:217:LYS:CE	3:K:217:LYS:CA	2.86	0.50
3:K:257:LEU:HD12	3:K:258:GLY:N	2.26	0.50
1:A:410:PRO:HD3	1:A:463:TRP:NE1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:O	1:A:459:LEU:HB2	2.11	0.50
1:A:692:LEU:HA	1:A:695:VAL:HB	1.94	0.50
1:B:476:LEU:CD2	1:B:510:VAL:CG1	2.85	0.50
1:D:259:LEU:HD23	1:D:299:MET:SD	2.52	0.50
1:A:321:ARG:HB3	1:F:670:ARG:NH2	2.25	0.50
3:I:257:LEU:HD12	3:I:258:GLY:N	2.26	0.50
3:K:127:VAL:HG23	3:K:135:TRP:CD1	2.47	0.50
1:A:410:PRO:HG3	1:A:463:TRP:NE1	2.27	0.50
1:C:242:LEU:HD11	1:C:283:ILE:HG13	1.93	0.50
1:C:518:LEU:N	1:C:518:LEU:CD1	2.73	0.50
1:E:650:GLY:O	1:E:704:GLY:HA3	2.12	0.50
3:K:158:LYS:NZ	3:K:168:ASP:OD2	2.45	0.50
1:A:487:SER:HA	1:A:502:LEU:HD13	1.94	0.50
1:C:822:MET:HG2	1:C:827:GLN:HE21	1.77	0.50
1:F:779:ARG:HE	1:F:823:LEU:HD21	1.77	0.50
1:B:812:GLN:HE22	1:C:594:SER:HA	1.77	0.49
1:C:460:THR:O	1:C:464:GLN:HG2	2.12	0.49
1:C:554:LEU:HD23	1:C:554:LEU:H	1.77	0.49
1:C:812:GLN:HB3	1:D:588:ARG:NH1	2.27	0.49
1:E:534:GLY:H	1:E:537:ASP:HB3	1.77	0.49
3:K:100:PHE:CB	3:K:139:ILE:HD12	2.42	0.49
1:D:172:ALA:HB2	1:D:177:LEU:HD12	1.93	0.49
1:D:194:LEU:HD11	1:D:310:ARG:HB3	1.94	0.49
1:D:605:PHE:HB3	1:D:751:LEU:HB2	1.94	0.49
1:E:804:ALA:HB1	1:E:807:LEU:HB2	1.93	0.49
1:E:820:ALA:HA	1:E:823:LEU:HD12	1.94	0.49
1:F:537:ASP:O	1:F:541:VAL:HG23	2.12	0.49
3:I:62:ALA:HB3	3:I:411:ALA:HB1	1.94	0.49
3:I:84:VAL:HG11	3:I:401:GLU:HG2	1.94	0.49
3:I:100:PHE:CB	3:I:139:ILE:HD12	2.42	0.49
1:B:423:LEU:HD22	1:B:445:LEU:HD11	1.94	0.49
1:F:183:ARG:NH1	1:F:340:GLY:O	2.41	0.49
1:C:436:GLU:OE2	1:C:780:ARG:NH1	2.44	0.49
1:C:573:ILE:H	4:C:901:AGS:HN62	1.60	0.49
1:D:720:SER:OG	1:D:721:ASN:N	2.46	0.49
1:E:784:GLN:NE2	1:E:785:VAL:O	2.45	0.49
3:I:308:SER:OG	3:I:330:GLN:NE2	2.44	0.49
1:A:504:TYR:HB2	3:I:324:PRO:HG3	1.93	0.49
1:E:365:ARG:HH11	1:E:532:GLU:HB3	1.77	0.49
1:E:761:LEU:HD12	1:E:794:ALA:HB1	1.94	0.49
3:K:62:ALA:HB3	3:K:411:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:87:ASN:OD1	3:I:88:SER:N	2.46	0.49
3:I:127:VAL:HG23	3:I:135:TRP:CD1	2.47	0.49
1:A:646:ALA:HA	1:A:649:ILE:HG22	1.95	0.49
1:E:681:ILE:HG12	1:E:718:LEU:HD23	1.93	0.49
1:F:387:LEU:HA	1:F:390:LYS:HE2	1.95	0.49
3:I:148:GLU:OE1	3:I:148:GLU:N	2.46	0.49
3:J:69:THR:HG21	3:J:232:GLY:O	2.12	0.49
3:K:69:THR:HG21	3:K:232:GLY:O	2.12	0.49
1:A:608:PRO:HG2	1:A:611:VAL:HG21	1.94	0.49
1:B:539:ALA:HA	1:B:542:VAL:HG12	1.94	0.49
1:C:645:VAL:HG21	1:C:691:VAL:HG21	1.95	0.49
3:I:69:THR:HG21	3:I:232:GLY:O	2.12	0.49
1:C:355:LYS:HD3	1:C:371:LEU:HD11	1.95	0.49
1:D:299:MET:HG2	1:D:300:ILE:N	2.28	0.49
1:F:571:ARG:HG2	1:F:619:ALA:HB2	1.95	0.49
3:J:84:VAL:HG11	3:J:401:GLU:HG2	1.94	0.49
3:J:127:VAL:HG23	3:J:135:TRP:CD1	2.47	0.49
3:J:373:GLY:N	3:J:400:ASP:OD1	2.42	0.49
3:K:87:ASN:OD1	3:K:88:SER:N	2.46	0.49
1:D:304:LEU:HD21	1:D:311:LEU:HD22	1.95	0.49
1:E:837:ASN:N	1:E:845:LEU:O	2.44	0.49
3:J:87:ASN:OD1	3:J:88:SER:N	2.46	0.49
3:J:174:ILE:HG13	3:J:199:VAL:HG22	1.94	0.49
3:K:84:VAL:HG11	3:K:401:GLU:HG2	1.94	0.49
3:K:257:LEU:HD11	3:K:262:TRP:NE1	2.28	0.49
1:B:475:ASP:O	1:B:479:GLN:N	2.45	0.48
1:E:365:ARG:NH1	1:E:531:GLU:O	2.46	0.48
1:B:539:ALA:HB1	1:B:550:ALA:O	2.13	0.48
1:B:685:HIS:O	1:B:687:ASP:N	2.44	0.48
1:C:477:LYS:C	1:C:480:LEU:H	2.16	0.48
1:F:201:ASN:CB	1:F:310:ARG:O	2.59	0.48
1:F:304:LEU:CD1	1:F:311:LEU:HD23	2.43	0.48
3:K:174:ILE:HG13	3:K:199:VAL:HG22	1.94	0.48
1:C:414:ASP:O	1:C:417:GLU:HG3	2.14	0.48
1:A:180:VAL:HG11	1:A:218:GLY:HA3	1.94	0.48
1:D:248:GLY:O	1:D:258:ARG:NH2	2.39	0.48
1:D:278:ASP:OD1	1:D:279:GLU:N	2.46	0.48
3:I:186:GLN:OE1	3:I:189:LYS:NZ	2.39	0.48
3:J:100:PHE:CB	3:J:139:ILE:HD12	2.42	0.48
3:J:148:GLU:OE1	3:J:148:GLU:N	2.46	0.48
1:B:355:LYS:HD3	1:B:371:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:HIS:O	1:B:364:VAL:N	2.46	0.48
1:D:778:GLN:HG2	1:D:779:ARG:HD2	1.94	0.48
3:I:239:LEU:HG	3:I:248:VAL:HG22	1.95	0.48
3:I:373:GLY:N	3:I:400:ASP:OD1	2.42	0.48
1:A:477:LYS:HE3	1:A:514:LEU:HD11	1.96	0.48
1:B:678:PHE:HB2	1:B:718:LEU:HD23	1.94	0.48
1:C:203:VAL:HG22	1:C:280:LEU:HD21	1.96	0.48
3:K:148:GLU:OE1	3:K:148:GLU:N	2.46	0.48
1:C:260:LYS:HA	1:C:260:LYS:HD3	1.71	0.48
1:D:613:LYS:HG2	1:D:753:PHE:CD2	2.48	0.48
1:D:817:ASP:O	1:D:821:LYS:HG2	2.14	0.48
1:F:350:ILE:HG23	5:F:902:ADP:C2	2.48	0.48
1:F:792:TRP:HE1	1:F:796:ARG:HH11	1.62	0.48
3:K:368:VAL:HG23	3:K:391:LYS:CE	2.44	0.48
1:C:500:ALA:HB2	3:K:316:ILE:C	2.33	0.48
1:E:575:GLN:NE2	1:E:754:GLU:O	2.46	0.48
3:I:100:PHE:O	3:I:122:ARG:NE	2.47	0.48
3:I:176:THR:HG21	3:I:185:ARG:HG2	1.96	0.48
1:C:476:LEU:HA	1:C:479:GLN:HB3	1.95	0.48
1:E:193:VAL:HG11	1:E:202:PRO:HB3	1.95	0.48
1:E:582:VAL:O	1:E:586:VAL:HG23	2.13	0.48
3:J:257:LEU:HD11	3:J:262:TRP:NE1	2.28	0.48
4:A:901:AGS:O2A	4:A:901:AGS:O2B	2.32	0.48
1:C:181:ILE:CD1	1:C:353:GLY:HA3	2.44	0.48
1:D:386:PHE:O	1:D:390:LYS:CB	2.62	0.48
1:D:768:GLN:HG3	1:D:807:LEU:HD22	1.96	0.48
1:F:222:ARG:HD2	1:F:227:ASP:HB2	1.96	0.48
3:K:215:LEU:O	3:K:222:GLN:NE2	2.45	0.48
5:E:902:ADP:H2'	5:E:902:ADP:N3	2.29	0.47
3:I:174:ILE:HG13	3:I:199:VAL:HG22	1.95	0.47
3:I:257:LEU:HD11	3:I:262:TRP:NE1	2.28	0.47
3:J:151:ALA:HA	3:J:154:LEU:HD12	1.96	0.47
1:B:500:ALA:HB3	3:J:316:ILE:N	2.29	0.47
1:D:235:LYS:HE2	1:D:272:GLN:HA	1.95	0.47
1:D:573:ILE:N	4:D:902:AGS:HN62	2.12	0.47
3:K:239:LEU:HG	3:K:248:VAL:HG22	1.96	0.47
1:B:727:SER:OG	1:B:728:ALA:N	2.47	0.47
1:C:477:LYS:CG	1:C:480:LEU:HD23	2.44	0.47
1:D:545:TRP:O	1:D:546:THR:OG1	2.31	0.47
1:F:648:LEU:HD12	1:F:649:ILE:HG12	1.96	0.47
3:J:215:LEU:HD13	3:J:367:HIS:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:PHE:HB2	1:A:718:LEU:HG	1.96	0.47
1:C:490:ALA:O	1:C:495:ASP:N	2.46	0.47
1:E:684:ALA:HB1	1:E:688:VAL:HG11	1.97	0.47
1:F:389:ASP:OD1	1:F:390:LYS:N	2.47	0.47
3:J:176:THR:HG21	3:J:185:ARG:HG2	1.96	0.47
3:J:239:LEU:HG	3:J:248:VAL:HG22	1.95	0.47
3:J:368:VAL:HG23	3:J:391:LYS:CE	2.44	0.47
3:K:282:LEU:HD13	3:K:288:ALA:HB1	1.96	0.47
1:A:381:TYR:HD2	1:A:542:VAL:HG11	1.80	0.47
1:B:695:VAL:HG13	1:B:711:PHE:HD2	1.79	0.47
1:F:207:GLU:O	1:F:210:VAL:HG23	2.14	0.47
3:I:223:ARG:HG3	3:I:365:ILE:HG23	1.97	0.47
3:I:282:LEU:HD13	3:I:288:ALA:HB1	1.96	0.47
1:A:612:GLY:O	1:A:615:GLU:N	2.48	0.47
1:C:594:SER:OG	1:C:595:ASP:N	2.48	0.47
1:D:575:GLN:OE1	1:D:575:GLN:HA	2.15	0.47
1:E:648:LEU:HA	1:E:663:GLN:H	1.79	0.47
1:E:749:ASP:OD1	1:E:749:ASP:N	2.47	0.47
3:J:100:PHE:O	3:J:122:ARG:NE	2.47	0.47
3:K:151:ALA:HA	3:K:154:LEU:HD12	1.96	0.47
1:A:184:ASP:OD1	1:A:185:ASN:N	2.47	0.47
1:A:393:ASP:OD2	1:B:335:GLN:NE2	2.47	0.47
1:A:634:ILE:HD11	1:A:678:PHE:CE1	2.49	0.47
1:B:761:LEU:HD12	1:B:764:ILE:HB	1.97	0.47
1:C:646:ALA:HA	1:C:649:ILE:HG22	1.97	0.47
1:D:177:LEU:HD22	1:D:217:GLU:HG2	1.95	0.47
1:D:634:ILE:HD11	1:D:678:PHE:CE2	2.50	0.47
1:E:538:ILE:O	1:E:542:VAL:HG23	2.15	0.47
1:E:727:SER:OG	1:E:728:ALA:N	2.48	0.47
1:E:769:LEU:HD11	1:E:790:LYS:HG2	1.97	0.47
1:F:349:GLY:HA2	1:F:352:ARG:HD2	1.95	0.47
3:I:368:VAL:HG23	3:I:391:LYS:CE	2.44	0.47
3:J:217:LYS:HE3	3:J:366:ASP:HB3	1.93	0.47
3:J:282:LEU:HD13	3:J:288:ALA:HB1	1.96	0.47
3:K:370:LEU:HD13	3:K:375:THR:O	2.15	0.47
1:A:490:ALA:O	1:A:495:ASP:N	2.46	0.47
1:D:666:GLU:OE2	1:D:669:ARG:NH2	2.48	0.47
1:E:542:VAL:O	1:E:546:THR:HG22	2.15	0.47
3:K:87:ASN:HD22	3:K:94:THR:HG1	1.63	0.47
1:B:594:SER:OG	1:B:595:ASP:N	2.47	0.47
1:B:821:LYS:HB2	1:B:821:LYS:HE3	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HG2	1:D:198:THR:HG23	1.96	0.47
1:F:368:ASP:O	1:F:372:VAL:HG22	2.15	0.47
1:F:403:ARG:HD2	1:F:406:ILE:HD12	1.97	0.47
3:K:100:PHE:O	3:K:122:ARG:NE	2.47	0.47
1:D:682:GLU:HG2	1:D:683:LYS:HD2	1.97	0.47
3:K:215:LEU:HD13	3:K:367:HIS:CB	2.44	0.47
3:K:371:VAL:HG12	3:K:402:VAL:CG1	2.44	0.47
1:C:477:LYS:O	1:C:481:GLU:N	2.37	0.46
1:D:301:LYS:CD	1:D:333:ARG:NH2	2.71	0.46
3:I:215:LEU:HD13	3:I:367:HIS:CB	2.44	0.46
3:I:370:LEU:HD13	3:I:375:THR:O	2.15	0.46
3:I:371:VAL:HG12	3:I:402:VAL:CG1	2.44	0.46
3:K:176:THR:HG21	3:K:185:ARG:HG2	1.96	0.46
3:K:223:ARG:HG3	3:K:365:ILE:HG23	1.97	0.46
1:A:276:PHE:CD1	1:A:312:VAL:HG13	2.51	0.46
1:A:356:ASP:O	1:A:360:VAL:HG23	2.15	0.46
1:B:229:PRO:O	1:B:233:ARG:HG3	2.15	0.46
1:C:437:ALA:O	1:C:441:ARG:NH1	2.48	0.46
1:C:480:LEU:HD13	1:C:510:VAL:CB	2.43	0.46
3:J:139:ILE:HB	3:J:144:TYR:CE2	2.51	0.46
1:A:459:LEU:HD22	1:A:459:LEU:HA	1.76	0.46
1:E:613:LYS:HA	1:E:753:PHE:CE2	2.45	0.46
3:I:151:ALA:HA	3:I:154:LEU:HD12	1.96	0.46
3:J:384:VAL:O	3:J:388:THR:OG1	2.31	0.46
3:K:139:ILE:HB	3:K:144:TYR:CE2	2.51	0.46
1:A:500:ALA:HB3	3:I:316:ILE:N	2.30	0.46
1:A:685:HIS:O	1:A:687:ASP:N	2.43	0.46
1:A:695:VAL:HG13	1:A:711:PHE:HD2	1.80	0.46
1:B:342:PRO:O	1:B:387:LEU:HD12	1.95	0.46
1:B:606:LEU:HB3	1:B:720:SER:HB3	1.98	0.46
3:I:158:LYS:HB2	3:I:197:LEU:HD21	1.98	0.46
3:K:257:LEU:HD11	3:K:262:TRP:CD1	2.50	0.46
1:B:676:VAL:HB	1:B:716:LEU:HD23	1.98	0.46
4:C:902:AGS:O2A	4:C:902:AGS:O2B	2.34	0.46
3:K:87:ASN:ND2	3:K:94:THR:OG1	2.47	0.46
1:A:373:ALA:HA	1:A:376:THR:HG22	1.97	0.46
1:E:263:LEU:HD21	1:E:300:ILE:HG22	1.96	0.46
1:E:798:PHE:CE2	1:E:800:PRO:HB3	2.49	0.46
3:J:370:LEU:HD13	3:J:375:THR:O	2.15	0.46
3:K:82:PRO:CB	3:K:405:VAL:HG13	2.46	0.46
1:B:785:VAL:HA	1:B:836:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:792:TRP:HE1	1:C:796:ARG:NH2	2.14	0.46
1:D:809:ARG:NH1	1:D:813:GLN:HB3	2.31	0.46
1:E:792:TRP:HE3	1:E:793:LEU:HD12	1.81	0.46
3:I:82:PRO:CB	3:I:405:VAL:HG13	2.46	0.46
3:I:257:LEU:HD11	3:I:262:TRP:CD1	2.51	0.46
3:J:223:ARG:HG3	3:J:365:ILE:HG23	1.97	0.46
1:B:476:LEU:HD12	1:B:513:LYS:HZ2	1.80	0.46
1:C:378:SER:OG	1:C:390:LYS:HG3	2.16	0.46
1:D:305:ALA:HB2	1:D:333:ARG:CG	2.46	0.46
1:F:276:PHE:HA	1:F:312:VAL:HG13	1.97	0.46
1:A:365:ARG:NH2	1:A:531:GLU:HB2	2.29	0.46
1:D:789:ALA:HB2	1:D:838:VAL:HG22	1.98	0.46
3:I:139:ILE:HB	3:I:144:TYR:CE2	2.51	0.46
1:A:805:ARG:HD2	1:B:745:ASN:ND2	2.31	0.46
1:B:490:ALA:O	1:B:495:ASP:N	2.46	0.46
1:C:277:ILE:HD12	1:C:311:LEU:HD11	1.97	0.46
1:E:585:ALA:O	1:E:589:SER:OG	2.22	0.46
3:K:221:GLU:HG2	3:K:222:GLN:N	2.31	0.46
3:K:318:VAL:HG22	3:K:320:ALA:H	1.81	0.46
3:K:341:GLN:HA	3:K:344:LEU:HD12	1.98	0.46
1:B:358:TYR:HE1	1:C:197:ARG:HH21	1.63	0.45
1:B:380:ARG:NH2	1:B:596:PRO:O	2.49	0.45
1:F:234:ASP:C	1:F:236:THR:H	2.19	0.45
1:F:786:SER:O	1:F:790:LYS:HG3	2.16	0.45
3:J:82:PRO:CB	3:J:405:VAL:HG13	2.46	0.45
3:J:215:LEU:O	3:J:222:GLN:NE2	2.45	0.45
3:K:181:ASN:N	3:K:184:GLN:OE1	2.46	0.45
1:B:659:GLU:CD	1:B:659:GLU:H	2.19	0.45
1:D:220:ALA:HB2	1:D:237:ILE:HD11	1.97	0.45
1:E:161:LEU:HD22	1:E:261:ALA:HB1	1.97	0.45
1:F:255:PHE:O	1:F:258:ARG:HG2	2.17	0.45
1:A:278:ASP:OD1	1:A:278:ASP:N	2.49	0.45
1:A:633:ARG:NH2	1:B:698:GLU:OE2	2.49	0.45
1:B:497:ALA:HA	3:J:315:TYR:O	2.16	0.45
3:J:238:LEU:CB	3:J:358:THR:HG21	2.47	0.45
3:J:325:LEU:HD23	3:J:325:LEU:HA	1.85	0.45
3:K:319:ASP:N	3:K:323:ASN:O	2.32	0.45
3:K:384:VAL:O	3:K:388:THR:OG1	2.32	0.45
1:A:474:ARG:NH1	1:A:475:ASP:OD1	2.45	0.45
1:A:681:ILE:HG12	1:A:718:LEU:HD23	1.98	0.45
1:B:666:GLU:OE2	1:B:669:ARG:NE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:GLY:HA2	1:D:711:PHE:HB2	1.97	0.45
1:D:822:MET:HG3	1:D:827:GLN:HE21	1.81	0.45
1:F:263:LEU:HD23	1:F:266:ILE:HD12	1.99	0.45
1:F:373:ALA:HB3	1:F:538:ILE:HD12	1.98	0.45
1:F:382:ILE:HD11	1:F:542:VAL:HA	1.99	0.45
3:I:102:ARG:NH2	3:I:118:THR:O	2.45	0.45
3:I:238:LEU:CB	3:I:358:THR:HG21	2.46	0.45
3:J:257:LEU:HD11	3:J:262:TRP:CD1	2.50	0.45
1:D:778:GLN:NE2	1:E:592:GLY:O	2.49	0.45
3:K:238:LEU:CB	3:K:358:THR:HG21	2.46	0.45
1:B:249:SER:HB2	1:C:252:ARG:HH21	1.82	0.45
3:K:201:ARG:NH1	3:K:410:GLN:OE1	2.50	0.45
1:A:389:ASP:OD1	1:A:390:LYS:N	2.49	0.45
1:E:726:GLY:N	1:E:730:GLN:HE21	2.15	0.45
1:E:744:ILE:HA	1:E:747:LEU:HD13	1.98	0.45
3:J:181:ASN:N	3:J:184:GLN:OE1	2.46	0.45
1:A:497:ALA:HA	3:I:315:TYR:O	2.16	0.45
1:B:473:VAL:CG2	1:B:517:ALA:CB	2.72	0.45
1:C:427:GLU:O	1:C:431:SER:OG	2.29	0.45
1:E:304:LEU:HA	1:E:309:LEU:HD21	1.97	0.45
1:E:322:LYS:O	1:E:326:LYS:HG2	2.16	0.45
1:F:379:ASP:OD1	1:F:380:ARG:N	2.45	0.45
1:F:573:ILE:HG23	1:F:763:ARG:HH21	1.80	0.45
3:J:201:ARG:NH1	3:J:410:GLN:OE1	2.50	0.45
3:J:371:VAL:HG12	3:J:402:VAL:CG1	2.44	0.45
3:K:158:LYS:HB2	3:K:197:LEU:HD21	1.97	0.45
1:A:364:VAL:HG21	1:A:402:LEU:HD23	1.99	0.45
1:D:180:VAL:HA	4:D:901:AGS:N1	2.32	0.45
1:E:200:ASN:OD1	1:E:201:ASN:ND2	2.49	0.45
1:F:298:ASN:N	1:F:301:LYS:HD3	2.32	0.45
1:F:694:GLN:NE2	1:F:701:LEU:HA	2.32	0.45
3:I:398:ASN:O	3:I:402:VAL:N	2.50	0.45
3:J:158:LYS:HB2	3:J:197:LEU:HD21	1.97	0.45
1:A:427:GLU:CB	1:A:445:LEU:HD21	2.43	0.45
1:B:196:ARG:HG3	1:B:200:ASN:HB3	1.98	0.45
1:B:387:LEU:HB3	1:B:388:PRO:CD	2.35	0.45
1:C:177:LEU:HD13	1:C:217:GLU:HG2	1.99	0.45
1:C:231:SER:O	1:C:231:SER:OG	2.35	0.45
1:D:545:TRP:CD1	1:D:546:THR:HG23	2.43	0.45
1:F:367:THR:OG1	1:F:369:SER:OG	2.27	0.45
1:F:561:LEU:O	1:F:587:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:224:ILE:HD12	3:I:367:HIS:HB2	1.99	0.45
3:J:215:LEU:HD13	3:J:367:HIS:HB3	1.99	0.45
1:A:406:ILE:HD12	1:A:529:LEU:HD11	1.97	0.44
1:A:769:LEU:HD23	1:A:769:LEU:HA	1.80	0.44
1:C:193:VAL:O	1:C:196:ARG:HG2	2.16	0.44
1:C:407:ASP:CG	1:C:408:SER:H	2.20	0.44
1:C:497:ALA:HA	3:K:315:TYR:O	2.16	0.44
1:F:726:GLY:HA3	1:F:730:GLN:HB2	1.99	0.44
3:K:398:ASN:O	3:K:402:VAL:N	2.50	0.44
1:C:267:LYS:HB3	1:C:267:LYS:HE2	1.80	0.44
1:C:609:THR:OG1	4:C:901:AGS:S1G	2.71	0.44
1:C:776:LEU:HD11	1:C:819:LEU:HD21	1.98	0.44
1:C:805:ARG:NH2	4:C:901:AGS:S1G	2.89	0.44
1:C:805:ARG:NH2	1:D:746:ARG:HH21	2.16	0.44
1:F:162:GLN:OE1	1:F:162:GLN:N	2.48	0.44
3:K:207:THR:CG2	3:K:246:VAL:HG11	2.47	0.44
1:A:463:TRP:CD2	1:A:463:TRP:O	2.70	0.44
1:A:799:ASP:OD1	1:A:799:ASP:N	2.48	0.44
1:C:473:VAL:CA	1:C:514:LEU:CD2	2.94	0.44
1:C:476:LEU:HD21	1:C:510:VAL:CA	2.48	0.44
1:E:762:VAL:HA	1:E:765:VAL:HG12	1.99	0.44
1:F:167:ASP:OD1	1:F:168:LEU:N	2.51	0.44
3:I:98:VAL:CG2	3:I:153:ILE:HD11	2.48	0.44
3:I:201:ARG:NH1	3:I:410:GLN:OE1	2.50	0.44
3:I:207:THR:CG2	3:I:246:VAL:HG11	2.47	0.44
3:I:341:GLN:HA	3:I:344:LEU:HD12	1.98	0.44
3:J:65:ILE:HG12	3:J:74:VAL:HG13	1.99	0.44
3:J:102:ARG:NH2	3:J:118:THR:O	2.45	0.44
3:J:207:THR:CG2	3:J:246:VAL:HG11	2.47	0.44
3:I:384:VAL:O	3:I:388:THR:OG1	2.32	0.44
3:J:98:VAL:CG2	3:J:153:ILE:HD11	2.48	0.44
1:B:328:ALA:HA	1:B:331:GLU:HG3	1.99	0.44
1:C:545:TRP:O	1:C:546:THR:OG1	2.36	0.44
1:C:644:THR:O	1:C:644:THR:OG1	2.35	0.44
1:E:277:ILE:HG22	1:E:280:LEU:HB3	1.99	0.44
1:E:372:VAL:O	1:E:376:THR:HG23	2.17	0.44
3:J:341:GLN:HA	3:J:344:LEU:HD12	1.98	0.44
3:J:398:ASN:O	3:J:402:VAL:N	2.50	0.44
3:K:181:ASN:OD1	3:K:183:ALA:HB3	2.18	0.44
1:A:303:MET:HB3	1:A:309:LEU:HD13	2.00	0.44
1:A:365:ARG:C	1:A:532:GLU:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:808:ARG:HH22	1:C:598:ARG:HH11	1.65	0.44
1:D:693:LEU:O	1:D:746:ARG:NH1	2.50	0.44
1:E:729:GLU:OE1	1:E:729:GLU:N	2.51	0.44
3:J:224:ILE:HD12	3:J:367:HIS:HB2	1.99	0.44
3:K:65:ILE:HG12	3:K:74:VAL:HG13	1.99	0.44
3:K:224:ILE:HD12	3:K:367:HIS:HB2	1.99	0.44
3:K:236:VAL:HB	3:K:354:VAL:HG21	2.00	0.44
1:A:598:ARG:HG2	1:A:599:PRO:O	2.18	0.44
1:B:245:MET:HE1	1:B:259:LEU:HD13	2.00	0.44
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.81	0.44
1:C:473:VAL:HA	1:C:514:LEU:HD23	2.00	0.44
1:D:573:ILE:CG2	4:D:902:AGS:N6	2.81	0.44
1:D:760:GLU:HG2	1:D:763:ARG:NH2	2.33	0.44
1:E:575:GLN:O	1:E:579:VAL:HG23	2.18	0.44
1:F:168:LEU:HD12	1:F:168:LEU:HA	1.86	0.44
1:F:307:GLY:N	1:F:308:GLU:OE1	2.51	0.44
1:F:649:ILE:HG23	1:F:703:ASP:HA	2.00	0.44
3:I:60:ALA:CB	3:I:77:LEU:HD12	2.47	0.44
3:J:181:ASN:OD1	3:J:183:ALA:HB3	2.18	0.44
1:B:826:GLY:O	1:B:827:GLN:HG2	2.18	0.44
1:C:199:LYS:HE3	1:C:335:GLN:HE21	1.82	0.44
1:C:832:ASP:OD1	1:C:832:ASP:N	2.51	0.44
1:E:699:GLY:O	1:E:712:ARG:NH2	2.51	0.44
1:E:784:GLN:HB2	1:E:833:THR:O	2.18	0.44
1:F:573:ILE:O	4:F:901:AGS:N6	2.50	0.44
3:I:87:ASN:ND2	3:I:94:THR:OG1	2.47	0.44
3:I:181:ASN:OD1	3:I:183:ALA:HB3	2.18	0.44
1:A:364:VAL:HG22	1:A:532:GLU:HA	2.00	0.44
1:B:211:GLY:HA2	4:B:901:AGS:O2A	2.17	0.44
1:E:349:GLY:HA2	1:E:352:ARG:HG2	2.00	0.44
3:I:249:ARG:HG3	3:I:358:THR:HG22	2.00	0.44
1:A:237:ILE:HG12	1:A:274:ILE:HB	2.00	0.43
1:F:347:THR:HA	1:F:350:ILE:HD12	1.99	0.43
1:A:819:LEU:O	1:A:823:LEU:HB2	2.18	0.43
1:F:258:ARG:HG3	1:F:259:LEU:HD22	1.99	0.43
3:I:65:ILE:HG12	3:I:74:VAL:HG13	1.99	0.43
3:J:87:ASN:ND2	3:J:94:THR:OG1	2.47	0.43
3:K:215:LEU:HD13	3:K:367:HIS:HB3	1.99	0.43
1:A:539:ALA:HB1	1:A:550:ALA:O	2.18	0.43
1:A:792:TRP:HE1	1:A:796:ARG:CZ	2.31	0.43
1:A:817:ASP:OD1	1:A:818:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:HG3	1:B:387:LEU:HD11	2.00	0.43
1:C:757:ASN:ND2	1:C:760:GLU:OE2	2.51	0.43
1:E:302:PRO:O	1:E:306:ARG:NH2	2.51	0.43
1:F:310:ARG:NE	1:F:310:ARG:CA	2.81	0.43
3:I:215:LEU:HD13	3:I:367:HIS:HB3	1.99	0.43
1:B:318:ASP:OD1	1:B:321:ARG:NE	2.49	0.43
1:B:422:ARG:HD2	1:C:181:ILE:HG23	2.01	0.43
1:B:808:ARG:NH2	1:C:598:ARG:HD2	2.32	0.43
1:C:513:LYS:HE3	1:C:513:LYS:O	2.19	0.43
1:D:647:ARG:NH2	1:E:703:ASP:O	2.52	0.43
1:E:173:ARG:HE	1:E:224:VAL:HG23	1.82	0.43
3:I:236:VAL:HB	3:I:354:VAL:HG21	2.00	0.43
3:J:60:ALA:CB	3:J:77:LEU:HD12	2.47	0.43
1:A:487:SER:CA	1:A:502:LEU:HD13	2.49	0.43
1:B:634:ILE:HD11	1:B:678:PHE:CE2	2.54	0.43
1:C:508:PRO:O	1:C:512:LYS:HG3	2.19	0.43
1:D:792:TRP:CZ3	1:D:843:ASP:HB2	2.53	0.43
1:E:201:ASN:HB2	1:E:311:LEU:O	2.18	0.43
1:E:636:MET:HB3	1:E:684:ALA:HB2	2.00	0.43
1:F:278:ASP:OD1	1:F:279:GLU:HG2	2.19	0.43
3:J:236:VAL:HB	3:J:354:VAL:HG21	2.00	0.43
3:K:98:VAL:CG2	3:K:153:ILE:HD11	2.48	0.43
3:K:249:ARG:HG3	3:K:358:THR:HG22	2.00	0.43
1:B:553:LEU:HD21	1:B:590:ARG:HB3	2.01	0.43
1:F:365:ARG:HB2	1:F:532:GLU:HB2	2.00	0.43
1:F:761:LEU:HD23	1:F:761:LEU:HA	1.82	0.43
1:F:827:GLN:H	1:F:829:HIS:CE1	2.37	0.43
3:I:181:ASN:N	3:I:184:GLN:OE1	2.45	0.43
3:J:249:ARG:HG3	3:J:358:THR:HG22	2.00	0.43
1:C:281:HIS:NE2	1:C:319:GLU:OE1	2.51	0.43
1:C:411:VAL:O	1:C:412:GLU:HG2	2.19	0.43
1:C:476:LEU:CA	1:C:479:GLN:HB3	2.47	0.43
1:C:487:SER:CA	1:C:502:LEU:HD13	2.49	0.43
1:D:389:ASP:OD1	1:D:390:LYS:N	2.51	0.43
1:F:235:LYS:HA	1:F:235:LYS:HD3	1.70	0.43
1:F:344:VAL:HG22	1:F:387:LEU:HD21	2.00	0.43
1:F:632:VAL:HG12	1:F:676:VAL:HG23	2.01	0.43
1:A:466:GLU:N	1:A:466:GLU:CD	2.70	0.43
1:B:199:LYS:HE3	1:B:332:ARG:O	2.18	0.43
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.84	0.43
1:C:423:LEU:HD22	1:C:445:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LEU:HD23	1:D:277:ILE:HD11	2.01	0.43
1:E:180:VAL:HG13	4:E:901:AGS:C6	2.49	0.43
1:E:802:TYR:CB	1:E:805:ARG:HD2	2.46	0.43
1:F:211:GLY:O	1:F:215:ILE:HG13	2.18	0.43
3:J:365:ILE:HG22	3:J:391:LYS:HE2	2.01	0.43
1:E:783:LEU:HA	1:E:834:VAL:HG22	2.00	0.43
1:F:554:LEU:HB3	1:F:557:GLU:HG2	2.01	0.43
3:I:98:VAL:HG21	3:I:149:ILE:HG22	2.01	0.43
3:K:60:ALA:CB	3:K:77:LEU:HD12	2.47	0.43
1:A:196:ARG:HD2	1:A:198:THR:O	2.18	0.43
1:A:321:ARG:NH1	1:F:659:GLU:O	2.42	0.43
1:C:276:PHE:HA	1:C:312:VAL:O	2.19	0.43
1:C:546:THR:O	1:C:546:THR:OG1	2.36	0.43
1:D:213:THR:HG22	1:D:217:GLU:OE1	2.19	0.43
1:F:703:ASP:OD1	1:F:703:ASP:N	2.51	0.43
3:J:98:VAL:HG21	3:J:149:ILE:HG22	2.01	0.43
3:J:257:LEU:HD11	3:J:262:TRP:HE1	1.84	0.43
3:K:98:VAL:HG21	3:K:149:ILE:HG22	2.01	0.43
3:K:102:ARG:NH2	3:K:118:THR:O	2.45	0.43
1:A:180:VAL:HG21	1:A:218:GLY:HA2	2.00	0.42
1:A:211:GLY:HA2	4:A:901:AGS:O2A	2.18	0.42
1:A:242:LEU:HA	1:A:245:MET:HB3	2.01	0.42
1:A:573:ILE:HD11	1:A:767:ILE:HD12	2.00	0.42
1:B:321:ARG:HA	1:B:325:GLU:HB2	2.00	0.42
1:B:332:ARG:HH21	1:B:333:ARG:NH2	2.17	0.42
1:B:435:ASP:OD1	1:B:436:GLU:N	2.52	0.42
1:B:476:LEU:CG	1:B:510:VAL:HG13	2.49	0.42
1:B:480:LEU:CD1	1:B:507:ILE:HG23	2.49	0.42
1:C:363:GLY:O	1:C:403:ARG:NH1	2.51	0.42
1:C:790:LYS:HE3	1:C:790:LYS:HB2	1.83	0.42
1:D:204:LEU:HD23	1:D:337:VAL:HB	2.01	0.42
3:I:306:SER:OG	3:I:308:SER:O	2.37	0.42
3:J:238:LEU:O	3:J:249:ARG:N	2.52	0.42
1:A:669:ARG:HH22	1:B:325:GLU:CD	2.19	0.42
1:B:358:TYR:CD1	1:C:197:ARG:HD3	2.53	0.42
1:B:487:SER:CA	1:B:502:LEU:HD13	2.49	0.42
1:C:642:LYS:HB3	1:C:642:LYS:HE3	1.90	0.42
3:J:306:SER:OG	3:J:308:SER:O	2.37	0.42
1:B:226:GLY:O	1:B:233:ARG:NH1	2.52	0.42
1:C:211:GLY:HA2	4:C:902:AGS:O2A	2.19	0.42
1:C:321:ARG:HA	1:C:325:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:H	1:C:472:ILE:HG13	1.61	0.42
1:C:677:LEU:HD22	1:C:679:ASP:OD1	2.19	0.42
1:F:343:SER:O	1:F:347:THR:HG23	2.19	0.42
3:I:222:GLN:HG3	3:I:241:ILE:HB	1.94	0.42
1:A:645:VAL:HG22	1:A:688:VAL:HG22	2.00	0.42
1:B:778:GLN:N	1:B:778:GLN:OE1	2.53	0.42
1:C:476:LEU:HD21	1:C:510:VAL:CB	2.47	0.42
1:D:280:LEU:HD23	1:D:313:GLY:HA3	2.00	0.42
1:E:799:ASP:O	1:E:801:VAL:N	2.49	0.42
1:F:300:ILE:HD11	1:F:309:LEU:HD11	2.02	0.42
3:I:229:LEU:HD23	3:I:374:SER:CB	2.50	0.42
1:A:532:GLU:OE1	1:A:532:GLU:CA	2.68	0.42
1:A:545:TRP:O	1:A:547:GLY:N	2.53	0.42
1:A:578:ALA:HA	1:A:751:LEU:HD13	2.01	0.42
1:F:351:LEU:O	1:F:355:LYS:N	2.47	0.42
1:F:387:LEU:HB3	1:F:388:PRO:HD3	2.00	0.42
1:F:678:PHE:HB2	1:F:718:LEU:HG	2.01	0.42
3:I:319:ASP:OD2	3:I:325:LEU:CD2	2.67	0.42
3:K:223:ARG:N	3:K:366:ASP:OD2	2.44	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.77	0.42
1:A:826:GLY:O	1:A:827:GLN:HG2	2.19	0.42
3:K:158:LYS:CB	3:K:197:LEU:HD21	2.50	0.42
1:A:442:LEU:C	1:A:442:LEU:CD2	2.85	0.42
1:A:463:TRP:HB2	1:A:528:MET:HE1	2.02	0.42
1:B:470:ILE:CB	1:B:519:PRO:CG	2.97	0.42
1:D:575:GLN:HE22	1:D:611:VAL:CG1	2.32	0.42
1:D:585:ALA:HB2	1:D:603:PHE:HZ	1.84	0.42
1:E:554:LEU:HD23	1:E:554:LEU:HA	1.80	0.42
1:F:651:ALA:HB3	1:F:657:GLY:O	2.19	0.42
1:F:690:ASP:O	1:F:693:LEU:HB3	2.20	0.42
3:K:70:THR:HG23	3:K:232:GLY:HA3	2.02	0.42
3:K:238:LEU:O	3:K:249:ARG:N	2.52	0.42
3:K:257:LEU:HD11	3:K:262:TRP:HE1	1.84	0.42
3:K:348:ARG:O	3:K:351:PHE:N	2.53	0.42
1:A:660:ALA:HA	1:B:321:ARG:HH22	1.84	0.42
1:B:496:LEU:HD11	3:J:316:ILE:HG23	2.01	0.42
1:B:602:ALA:HA	1:B:716:LEU:O	2.20	0.42
1:D:322:LYS:HE3	1:D:323:HIS:NE2	2.35	0.42
1:E:207:GLU:HB3	1:E:208:PRO:CD	2.48	0.42
1:F:772:LEU:O	1:F:776:LEU:HG	2.19	0.42
1:F:774:LYS:HE2	1:F:774:LYS:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:158:LYS:CB	3:I:197:LEU:HD21	2.50	0.42
3:K:175:THR:HG21	3:K:403:VAL:CG1	2.50	0.42
3:K:229:LEU:HD23	3:K:374:SER:CB	2.50	0.42
1:A:311:LEU:O	1:A:311:LEU:HD23	2.20	0.42
1:A:406:ILE:HD12	1:A:529:LEU:CD1	2.50	0.42
1:A:641:GLU:O	1:A:644:THR:OG1	2.36	0.42
1:B:201:ASN:ND2	1:B:304:LEU:HD22	2.35	0.42
1:B:784:GLN:HB2	1:B:835:PRO:HB3	2.01	0.42
1:C:386:PHE:O	1:C:390:LYS:HG2	2.20	0.42
1:D:378:SER:HB2	1:D:390:LYS:HG2	2.01	0.42
1:E:264:ASP:OD1	1:E:268:ASN:ND2	2.53	0.42
1:E:365:ARG:O	1:E:533:VAL:HG12	2.19	0.42
1:E:834:VAL:HG23	1:E:834:VAL:O	2.19	0.42
1:F:694:GLN:O	1:F:698:GLU:HB3	2.20	0.42
3:I:122:ARG:NH2	3:I:140:ASP:OD2	2.53	0.42
3:J:175:THR:HG21	3:J:403:VAL:CG1	2.50	0.42
3:J:348:ARG:HG3	3:J:387:LEU:HD21	2.02	0.42
1:A:194:LEU:HD21	1:A:274:ILE:HG21	2.01	0.42
1:A:355:LYS:HB2	1:A:371:LEU:HD11	2.01	0.42
1:B:260:LYS:HE2	1:B:260:LYS:HB2	1.75	0.42
1:C:366:ILE:HA	1:C:533:VAL:HG22	2.02	0.42
1:C:480:LEU:CD1	1:C:510:VAL:CG1	2.76	0.42
1:E:264:ASP:O	1:E:268:ASN:ND2	2.53	0.42
1:F:244:SER:HB2	1:F:258:ARG:NH2	2.34	0.42
3:K:238:LEU:HB3	3:K:358:THR:HG21	2.02	0.42
3:K:348:ARG:HG3	3:K:387:LEU:HD21	2.02	0.42
3:K:365:ILE:HG22	3:K:391:LYS:HE2	2.01	0.42
1:A:702:THR:OG1	1:F:647:ARG:NH2	2.53	0.41
1:C:194:LEU:HD11	1:C:310:ARG:HB3	2.01	0.41
1:E:400:SER:OG	1:F:192:GLN:HG2	2.19	0.41
1:E:775:ARG:HA	1:E:775:ARG:HD3	1.82	0.41
3:J:158:LYS:CB	3:J:197:LEU:HD21	2.50	0.41
3:J:282:LEU:HB2	3:J:292:LEU:HD11	2.02	0.41
3:J:348:ARG:O	3:J:351:PHE:N	2.53	0.41
1:B:553:LEU:O	1:B:555:GLU:N	2.48	0.41
1:B:583:SER:O	1:B:583:SER:OG	2.36	0.41
1:C:475:ASP:O	1:C:479:GLN:N	2.53	0.41
1:D:575:GLN:OE1	1:D:575:GLN:CA	2.68	0.41
1:D:837:ASN:ND2	1:D:845:LEU:O	2.53	0.41
1:E:786:SER:C	1:E:790:LYS:HE2	2.40	0.41
4:E:901:AGS:O1A	1:F:332:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:636:MET:HB2	1:F:680:GLU:O	2.20	0.41
1:F:780:ARG:O	1:F:781:LEU:HD23	2.20	0.41
3:I:238:LEU:HB3	3:I:358:THR:HG21	2.02	0.41
3:J:73:VAL:HG21	3:J:400:ASP:HB3	2.01	0.41
3:K:375:THR:HA	3:K:380:VAL:HG21	2.03	0.41
1:A:682:GLU:OE2	1:A:683:LYS:NZ	2.51	0.41
1:B:418:ARG:HG2	1:B:421:ARG:NH2	2.35	0.41
1:C:681:ILE:HG22	1:C:720:SER:HB2	2.02	0.41
4:D:902:AGS:O2B	4:D:902:AGS:O2A	2.38	0.41
1:E:278:ASP:OD1	1:E:278:ASP:N	2.50	0.41
1:F:355:LYS:HB2	1:F:366:ILE:HD11	2.02	0.41
3:I:70:THR:HG23	3:I:232:GLY:HA3	2.02	0.41
3:I:269:TRP:CE3	3:I:270:LEU:HD23	2.56	0.41
3:I:348:ARG:O	3:I:351:PHE:N	2.53	0.41
3:J:398:ASN:O	3:J:401:GLU:N	2.53	0.41
1:A:463:TRP:O	1:A:463:TRP:CG	2.74	0.41
1:D:254:GLU:O	1:D:257:GLU:HG2	2.20	0.41
1:D:358:TYR:CE1	1:E:197:ARG:HD3	2.55	0.41
1:E:400:SER:OG	1:F:192:GLN:O	2.36	0.41
1:F:784:GLN:O	1:F:835:PRO:HA	2.21	0.41
3:I:175:THR:HG21	3:I:403:VAL:CG1	2.50	0.41
3:I:238:LEU:O	3:I:249:ARG:N	2.52	0.41
3:I:257:LEU:HD11	3:I:262:TRP:HE1	1.84	0.41
1:A:496:LEU:HD11	3:I:316:ILE:HG23	2.01	0.41
1:B:316:THR:HG21	1:C:329:ALA:HB2	2.03	0.41
1:D:243:GLY:O	1:D:247:ALA:HB2	2.21	0.41
1:D:300:ILE:O	1:D:300:ILE:CG1	2.68	0.41
1:D:620:LEU:O	1:D:624:LEU:HD23	2.19	0.41
1:D:724:SER:OG	1:D:724:SER:O	2.37	0.41
1:E:260:LYS:HA	1:E:260:LYS:HD2	1.81	0.41
1:F:836:VAL:HG23	1:F:845:LEU:HD23	2.02	0.41
3:J:229:LEU:HD23	3:J:374:SER:CB	2.50	0.41
3:J:238:LEU:HB3	3:J:358:THR:HG21	2.02	0.41
3:K:73:VAL:HG21	3:K:400:ASP:HB3	2.01	0.41
3:K:282:LEU:HB2	3:K:292:LEU:HD11	2.02	0.41
1:B:342:PRO:N	1:B:387:LEU:HD12	2.35	0.41
3:I:73:VAL:HG21	3:I:400:ASP:HB3	2.01	0.41
3:I:365:ILE:HG22	3:I:391:LYS:HE2	2.01	0.41
3:K:122:ARG:NH2	3:K:140:ASP:OD2	2.53	0.41
3:K:398:ASN:O	3:K:401:GLU:N	2.54	0.41
1:A:636:MET:HG3	1:A:681:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:OD2	1:C:335:GLN:NE2	2.52	0.41
1:B:412:GLU:O	1:B:413:ILE:HD13	2.21	0.41
1:C:496:LEU:HD21	3:K:316:ILE:CG2	2.48	0.41
1:E:604:MET:HB2	1:E:718:LEU:O	2.21	0.41
1:E:779:ARG:O	1:E:830:ASP:HB3	2.20	0.41
3:I:65:ILE:HB	3:I:174:ILE:HG12	2.03	0.41
3:I:124:VAL:HG11	3:I:149:ILE:HG21	2.03	0.41
3:I:375:THR:HA	3:I:380:VAL:HG21	2.03	0.41
3:J:65:ILE:HB	3:J:174:ILE:HG12	2.03	0.41
3:J:70:THR:HG23	3:J:232:GLY:HA3	2.02	0.41
3:J:124:VAL:HG11	3:J:149:ILE:HG21	2.03	0.41
3:J:375:THR:HA	3:J:380:VAL:HG21	2.03	0.41
1:A:600:THR:O	1:A:600:THR:OG1	2.37	0.41
1:A:691:VAL:O	1:A:695:VAL:HG23	2.21	0.41
1:C:355:LYS:HE2	1:C:355:LYS:HB3	1.93	0.41
1:D:237:ILE:HA	1:D:274:ILE:O	2.21	0.41
1:D:365:ARG:HB2	1:D:532:GLU:HB2	2.02	0.41
1:D:822:MET:HG3	1:D:827:GLN:NE2	2.35	0.41
1:E:235:LYS:HD2	1:E:272:GLN:HB2	2.03	0.41
1:F:575:GLN:O	1:F:579:VAL:HG22	2.21	0.41
1:F:823:LEU:HD12	1:F:823:LEU:HA	1.87	0.41
3:I:75:SER:O	3:I:408:ALA:HB2	2.21	0.41
3:J:75:SER:O	3:J:408:ALA:HB2	2.21	0.41
3:J:337:GLN:HG2	3:J:379:ALA:HB2	2.03	0.41
1:A:496:LEU:HD21	3:I:316:ILE:HD13	2.03	0.41
1:A:533:VAL:O	1:A:533:VAL:CG2	2.68	0.41
1:A:643:HIS:HB2	1:B:655:TYR:OH	2.21	0.41
1:B:277:ILE:O	1:B:313:GLY:HA2	2.21	0.41
1:B:597:ASN:OD1	1:B:597:ASN:N	2.53	0.41
1:B:675:VAL:HG23	1:B:715:ILE:HB	2.01	0.41
1:C:543:SER:O	1:C:547:GLY:HA2	2.20	0.41
1:C:787:LEU:HD23	1:C:787:LEU:HA	1.88	0.41
1:E:207:GLU:O	1:E:212:LYS:NZ	2.48	0.41
1:E:352:ARG:HE	1:E:352:ARG:HB3	1.68	0.41
1:E:613:LYS:HB2	1:E:613:LYS:HE3	1.84	0.41
1:F:641:GLU:HG3	1:F:643:HIS:CE1	2.56	0.41
3:I:210:ALA:HB2	3:I:224:ILE:HG21	2.03	0.41
3:J:139:ILE:CG2	3:J:144:TYR:CE2	3.04	0.41
3:J:238:LEU:HD12	3:J:354:VAL:HG12	2.03	0.41
3:J:269:TRP:CE3	3:J:270:LEU:HD23	2.56	0.41
3:K:210:ALA:HB2	3:K:224:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:306:SER:OG	3:K:308:SER:O	2.37	0.41
1:B:752:ILE:HD13	1:B:752:ILE:HA	1.93	0.41
1:C:545:TRP:CD1	1:C:546:THR:HG23	2.56	0.41
1:C:820:ALA:O	1:C:824:LEU:HG	2.21	0.41
1:E:824:LEU:HD12	1:F:591:ALA:HB2	2.02	0.41
3:I:65:ILE:HG23	3:I:74:VAL:HG22	2.03	0.41
3:J:174:ILE:H	3:J:199:VAL:HG13	1.86	0.41
3:K:107:LEU:HD13	3:K:111:PRO:O	2.21	0.41
3:K:174:ILE:H	3:K:199:VAL:HG13	1.86	0.41
3:K:269:TRP:CE3	3:K:270:LEU:HD23	2.55	0.41
1:A:500:ALA:HB1	1:A:504:TYR:HD2	1.86	0.40
1:B:374:ALA:HA	1:B:538:ILE:HG21	2.02	0.40
1:C:472:ILE:O	1:C:474:ARG:N	2.54	0.40
1:C:759:GLU:OE1	1:C:759:GLU:N	2.46	0.40
1:E:368:ASP:O	1:E:372:VAL:HG12	2.21	0.40
1:F:311:LEU:O	1:F:311:LEU:CG	2.70	0.40
3:I:282:LEU:HB2	3:I:292:LEU:HD11	2.03	0.40
3:J:65:ILE:HG23	3:J:74:VAL:HG22	2.03	0.40
3:J:209:ALA:CB	3:J:371:VAL:HG11	2.51	0.40
3:K:269:TRP:CZ3	3:K:270:LEU:HD23	2.57	0.40
1:A:322:LYS:HB3	1:A:323:HIS:HD2	1.86	0.40
1:A:327:ASP:O	1:A:329:ALA:N	2.54	0.40
1:A:697:ASP:OD2	1:F:805:ARG:NH1	2.54	0.40
1:B:390:LYS:O	1:B:390:LYS:CG	2.69	0.40
1:D:593:VAL:HG23	1:D:593:VAL:O	2.21	0.40
1:E:213:THR:HG23	4:E:901:AGS:O2B	2.20	0.40
1:F:739:PHE:HB2	1:F:744:ILE:HD11	2.04	0.40
3:I:174:ILE:H	3:I:199:VAL:HG13	1.86	0.40
3:I:348:ARG:HG3	3:I:387:LEU:HD21	2.02	0.40
3:K:337:GLN:HG2	3:K:379:ALA:HB2	2.03	0.40
1:C:246:VAL:HG12	1:C:246:VAL:O	2.20	0.40
1:C:500:ALA:HB1	1:C:504:TYR:HD2	1.86	0.40
1:D:299:MET:C	1:D:301:LYS:H	2.25	0.40
1:E:334:PHE:HD1	1:E:334:PHE:HA	1.80	0.40
1:E:609:THR:OG1	1:E:610:GLY:N	2.54	0.40
3:J:122:ARG:NH2	3:J:140:ASP:OD2	2.53	0.40
3:J:210:ALA:HB2	3:J:224:ILE:HG21	2.03	0.40
3:K:139:ILE:CG2	3:K:144:TYR:CE2	3.04	0.40
1:B:478:GLU:O	1:B:481:GLU:HB2	2.20	0.40
1:B:766:ASP:OD1	1:B:790:LYS:HD3	2.20	0.40
1:D:666:GLU:OE1	1:D:669:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:GLY:H	1:E:537:ASP:CB	2.34	0.40
1:F:183:ARG:O	1:F:187:ILE:HG12	2.21	0.40
1:F:761:LEU:HD12	1:F:798:PHE:HD1	1.86	0.40
3:I:139:ILE:CG2	3:I:144:TYR:CE2	3.04	0.40
3:I:238:LEU:HD12	3:I:354:VAL:HG12	2.03	0.40
3:I:325:LEU:HD23	3:I:325:LEU:HA	1.85	0.40
3:I:398:ASN:O	3:I:401:GLU:N	2.54	0.40
1:A:575:GLN:O	1:A:579:VAL:HG23	2.22	0.40
1:D:184:ASP:OD1	1:D:185:ASN:N	2.54	0.40
1:E:212:LYS:HG3	4:E:901:AGS:PB	2.62	0.40
3:K:75:SER:O	3:K:408:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	668/848 (79%)	590 (88%)	76 (11%)	2 (0%)	41	77
1	B	666/848 (78%)	605 (91%)	60 (9%)	1 (0%)	47	81
1	C	669/848 (79%)	592 (88%)	72 (11%)	5 (1%)	22	63
1	D	556/848 (66%)	480 (86%)	75 (14%)	1 (0%)	47	81
1	E	540/848 (64%)	477 (88%)	62 (12%)	1 (0%)	47	81
1	F	538/848 (63%)	472 (88%)	65 (12%)	1 (0%)	47	81
3	I	355/625 (57%)	318 (90%)	34 (10%)	3 (1%)	19	60
3	J	355/625 (57%)	318 (90%)	33 (9%)	4 (1%)	14	52
3	K	355/625 (57%)	317 (89%)	34 (10%)	4 (1%)	14	52
All	All	4702/6963 (68%)	4169 (89%)	511 (11%)	22 (0%)	32	69

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLU
1	B	388	PRO
1	C	516	ALA
3	I	315	TYR
3	I	322	LYS
3	J	217	LYS
3	J	315	TYR
3	K	221	GLU
3	K	315	TYR
3	K	322	LYS
1	C	547	GLY
1	C	473	VAL
1	C	478	GLU
1	F	235	LYS
1	A	465	ASN
1	E	566	ASP
3	J	324	PRO
3	J	138	GLU
3	K	138	GLU
1	C	472	ILE
1	D	302	PRO
3	I	324	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	549/682 (80%)	537 (98%)	12 (2%)	52 71
1	B	547/682 (80%)	544 (100%)	3 (0%)	88 93
1	C	548/682 (80%)	539 (98%)	9 (2%)	62 79
1	D	455/682 (67%)	449 (99%)	6 (1%)	69 81
1	E	448/682 (66%)	444 (99%)	4 (1%)	78 87
1	F	448/682 (66%)	445 (99%)	3 (1%)	84 90
3	I	291/500 (58%)	288 (99%)	3 (1%)	76 86
3	J	291/500 (58%)	289 (99%)	2 (1%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	K	291/500 (58%)	289 (99%)	2 (1%)	84 90
All	All	3868/5592 (69%)	3824 (99%)	44 (1%)	74 84

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	ARG
1	A	444	LYS
1	A	459	LEU
1	A	464	GLN
1	A	466	GLU
1	A	527	VAL
1	A	529	LEU
1	A	530	LYS
1	A	533	VAL
1	A	712	ARG
1	A	738	THR
1	A	780	ARG
1	B	388	PRO
1	B	461	THR
1	B	467	LYS
1	C	189	ARG
1	C	264	ASP
1	C	472	ILE
1	C	473	VAL
1	C	474	ARG
1	C	476	LEU
1	C	477	LYS
1	C	509	GLU
1	C	513	LYS
1	D	300	ILE
1	D	303	MET
1	D	333	ARG
1	D	576	LYS
1	D	605	PHE
1	D	809	ARG
1	E	252	ARG
1	E	275	THR
1	E	552	ARG
1	E	802	TYR
1	F	176	LYS
1	F	311	LEU

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Mol	Chain	Res	Type
1	F	738	THR
3	I	142	LYS
3	I	317	THR
3	I	318	VAL
3	J	142	LYS
3	J	317	THR
3	K	142	LYS
3	K	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	A	281	HIS
1	A	323	HIS
1	A	361	HIS
1	A	464	GLN
1	A	705	HIS
1	A	784	GLN
1	B	221	GLN
1	B	272	GLN
1	B	361	HIS
1	B	479	GLN
1	B	705	HIS
1	B	812	GLN
1	C	221	GLN
1	C	323	HIS
1	C	520	GLN
1	C	643	HIS
1	C	685	HIS
1	C	730	GLN
1	C	757	ASN
1	C	818	GLN
1	C	827	GLN
1	D	643	HIS
1	D	685	HIS
1	D	784	GLN
1	D	827	GLN
1	E	201	ASN
1	E	272	GLN
1	E	281	HIS
1	E	362	HIS

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Mol	Chain	Res	Type
1	E	685	HIS
1	E	721	ASN
1	E	730	GLN
1	E	784	GLN
1	E	818	GLN
1	F	268	ASN
1	F	685	HIS
3	I	114	ASN
3	I	290	GLN
3	I	341	GLN
3	I	394	ASN
3	J	114	ASN
3	J	290	GLN
3	J	341	GLN
3	J	394	ASN
3	K	114	ASN
3	K	181	ASN
3	K	290	GLN
3	K	341	GLN
3	K	394	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AGS	D	902	-	26,33,33	0.69	1 (3%)	26,52,52	1.18	2 (7%)
4	AGS	B	901	-	26,33,33	0.73	1 (3%)	26,52,52	1.32	2 (7%)
4	AGS	C	902	-	26,33,33	0.74	1 (3%)	26,52,52	1.24	2 (7%)
4	AGS	C	901	-	26,33,33	0.73	0	26,52,52	1.21	2 (7%)
4	AGS	B	902	-	26,33,33	0.73	1 (3%)	26,52,52	1.27	2 (7%)
4	AGS	E	901	-	26,33,33	1.89	4 (15%)	26,52,52	1.58	4 (15%)
5	ADP	F	902	-	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
4	AGS	D	901	-	26,33,33	0.73	0	26,52,52	1.18	2 (7%)
4	AGS	A	901	-	26,33,33	0.71	0	26,52,52	1.30	2 (7%)
4	AGS	F	901	-	26,33,33	0.72	1 (3%)	26,52,52	1.13	2 (7%)
4	AGS	A	902	-	26,33,33	0.75	1 (3%)	26,52,52	1.29	2 (7%)
5	ADP	E	902	-	24,29,29	0.78	0	29,45,45	1.01	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	D	902	-	-	3/17/38/38	0/3/3/3
4	AGS	B	901	-	-	4/17/38/38	0/3/3/3
4	AGS	C	902	-	-	2/17/38/38	0/3/3/3
4	AGS	C	901	-	-	4/17/38/38	0/3/3/3
4	AGS	B	902	-	-	6/17/38/38	0/3/3/3
4	AGS	E	901	-	-	3/17/38/38	0/3/3/3
5	ADP	F	902	-	-	1/12/32/32	0/3/3/3
4	AGS	D	901	-	-	6/17/38/38	0/3/3/3
4	AGS	A	901	-	-	6/17/38/38	0/3/3/3
4	AGS	F	901	-	-	7/17/38/38	0/3/3/3
4	AGS	A	902	-	-	5/17/38/38	0/3/3/3
5	ADP	E	902	-	-	5/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	901	AGS	PG-S1G	7.95	2.07	1.90
4	E	901	AGS	C5-C4	2.50	1.47	1.40
5	F	902	ADP	C5-C4	2.45	1.47	1.40
4	A	902	AGS	PG-S1G	2.11	1.95	1.90
4	C	902	AGS	PG-S1G	2.10	1.95	1.90
4	F	901	AGS	PG-S1G	2.09	1.95	1.90
4	D	902	AGS	PG-S1G	2.06	1.95	1.90
4	B	901	AGS	PG-S1G	2.03	1.95	1.90
4	E	901	AGS	PG-O3G	-2.02	1.48	1.54
4	B	902	AGS	PG-S1G	2.02	1.95	1.90
4	E	901	AGS	PG-O2G	2.02	1.61	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	AGS	PA-O3A-PB	-5.56	113.74	132.83
4	A	901	AGS	PA-O3A-PB	-5.43	114.19	132.83
4	A	902	AGS	PA-O3A-PB	-5.27	114.75	132.83
4	C	902	AGS	PA-O3A-PB	-5.09	115.36	132.83
4	B	902	AGS	PA-O3A-PB	-5.03	115.56	132.83
4	D	901	AGS	PA-O3A-PB	-4.87	116.11	132.83
4	C	901	AGS	PA-O3A-PB	-4.83	116.27	132.83
4	D	902	AGS	PA-O3A-PB	-4.42	117.66	132.83
4	F	901	AGS	PA-O3A-PB	-4.39	117.77	132.83
5	F	902	ADP	PA-O3A-PB	-3.74	120.01	132.83
4	E	901	AGS	PA-O3A-PB	-3.58	120.53	132.83
4	E	901	AGS	C3'-C2'-C1'	3.43	106.14	100.98
5	F	902	ADP	C3'-C2'-C1'	3.27	105.90	100.98
4	E	901	AGS	N3-C2-N1	-3.18	123.70	128.68
5	F	902	ADP	N3-C2-N1	-3.14	123.77	128.68
5	E	902	ADP	PA-O3A-PB	-2.96	122.68	132.83
4	E	901	AGS	C4-C5-N7	-2.70	106.58	109.40
4	D	902	AGS	C5-C6-N6	2.50	124.15	120.35
5	F	902	ADP	C4-C5-N7	-2.48	106.81	109.40
4	B	901	AGS	C5-C6-N6	2.29	123.83	120.35
4	C	902	AGS	C5-C6-N6	2.28	123.82	120.35
4	C	901	AGS	C5-C6-N6	2.26	123.79	120.35
4	A	901	AGS	C5-C6-N6	2.26	123.78	120.35
4	F	901	AGS	C5-C6-N6	2.26	123.78	120.35
4	D	901	AGS	C5-C6-N6	2.24	123.76	120.35
4	A	902	AGS	C5-C6-N6	2.23	123.74	120.35
4	B	902	AGS	C5-C6-N6	2.19	123.69	120.35
5	E	902	ADP	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	AGS	PB-O3B-PG-O2G
4	A	901	AGS	PB-O3B-PG-O3G
4	A	901	AGS	C5'-O5'-PA-O1A
4	A	901	AGS	C5'-O5'-PA-O2A
4	A	902	AGS	C5'-O5'-PA-O1A
4	A	902	AGS	C5'-O5'-PA-O2A
4	B	901	AGS	PB-O3B-PG-O2G
4	B	901	AGS	PB-O3B-PG-O3G
4	B	902	AGS	PB-O3B-PG-O2G
4	B	902	AGS	PB-O3B-PG-O3G
4	B	902	AGS	C5'-O5'-PA-O1A
4	C	901	AGS	PB-O3B-PG-O2G
4	C	901	AGS	PB-O3B-PG-O3G
4	D	901	AGS	PB-O3B-PG-O2G
4	D	901	AGS	PB-O3B-PG-O3G
4	D	901	AGS	C5'-O5'-PA-O2A
4	D	902	AGS	PB-O3B-PG-O2G
4	D	902	AGS	PB-O3B-PG-O3G
4	D	902	AGS	C5'-O5'-PA-O1A
4	F	901	AGS	PB-O3B-PG-O2G
4	F	901	AGS	PB-O3B-PG-O3G
4	F	901	AGS	C5'-O5'-PA-O3A
4	F	901	AGS	O4'-C4'-C5'-O5'
5	E	902	ADP	C5'-O5'-PA-O2A
4	B	901	AGS	O4'-C4'-C5'-O5'
4	B	902	AGS	C3'-C4'-C5'-O5'
4	C	902	AGS	O4'-C4'-C5'-O5'
4	F	901	AGS	C3'-C4'-C5'-O5'
4	B	902	AGS	O4'-C4'-C5'-O5'
4	D	901	AGS	O4'-C4'-C5'-O5'
5	E	902	ADP	O4'-C4'-C5'-O5'
4	D	901	AGS	C5'-O5'-PA-O3A
5	E	902	ADP	C5'-O5'-PA-O3A
4	B	901	AGS	C3'-C4'-C5'-O5'
4	D	901	AGS	C5'-O5'-PA-O1A
4	F	901	AGS	C5'-O5'-PA-O1A
4	F	901	AGS	C5'-O5'-PA-O2A
5	E	902	ADP	C5'-O5'-PA-O1A
4	C	902	AGS	C3'-C4'-C5'-O5'
4	A	902	AGS	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	C	901	AGS	PB-O3A-PA-O2A
5	E	902	ADP	C3'-C4'-C5'-O5'
4	A	901	AGS	C5'-O5'-PA-O3A
4	A	902	AGS	C5'-O5'-PA-O3A
4	B	902	AGS	C5'-O5'-PA-O3A
4	A	901	AGS	O4'-C4'-C5'-O5'
4	E	901	AGS	O4'-C4'-C5'-O5'
5	F	902	ADP	O4'-C4'-C5'-O5'
4	A	902	AGS	PA-O3A-PB-O1B
4	C	901	AGS	PB-O3A-PA-O1A
4	E	901	AGS	PA-O3A-PB-O1B
4	E	901	AGS	PA-O3A-PB-O2B

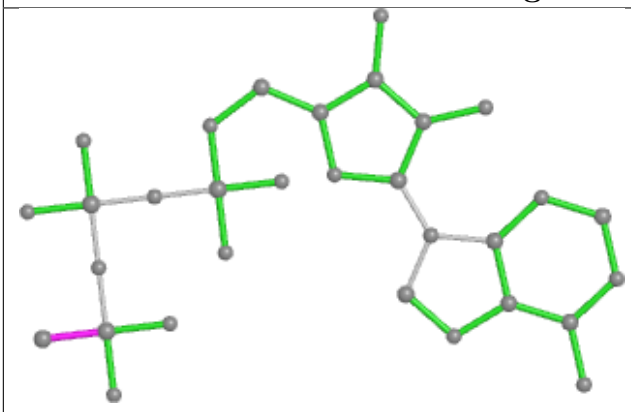
There are no ring outliers.

12 monomers are involved in 57 short contacts:

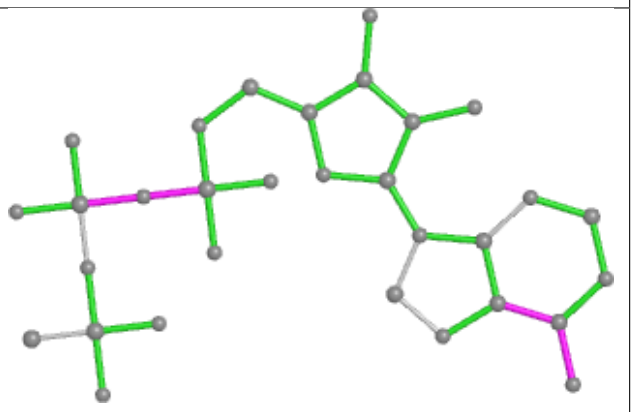
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	902	AGS	7	0
4	B	901	AGS	3	0
4	C	902	AGS	4	0
4	C	901	AGS	6	0
4	B	902	AGS	4	0
4	E	901	AGS	14	0
5	F	902	ADP	2	0
4	D	901	AGS	4	0
4	A	901	AGS	3	0
4	F	901	AGS	3	0
4	A	902	AGS	4	0
5	E	902	ADP	3	0

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

Ligand AGS D 902



Bond lengths



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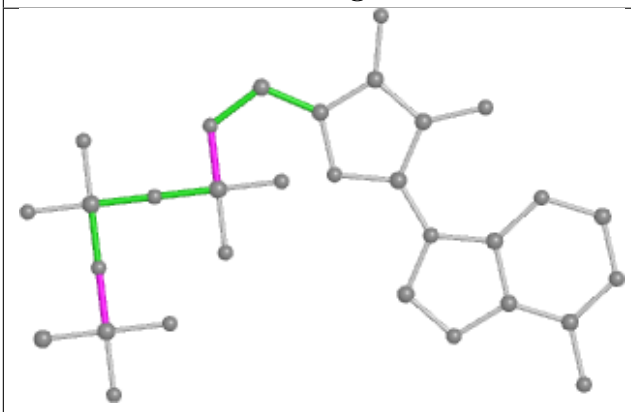

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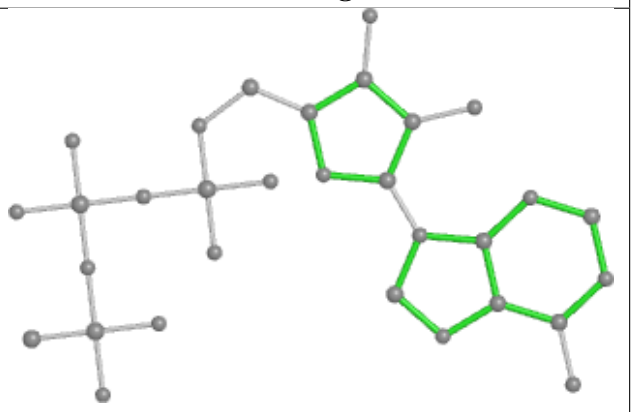
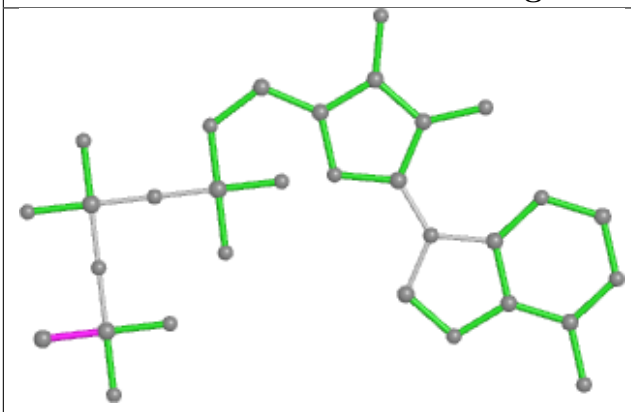


Rings

Ligand AGS B 901



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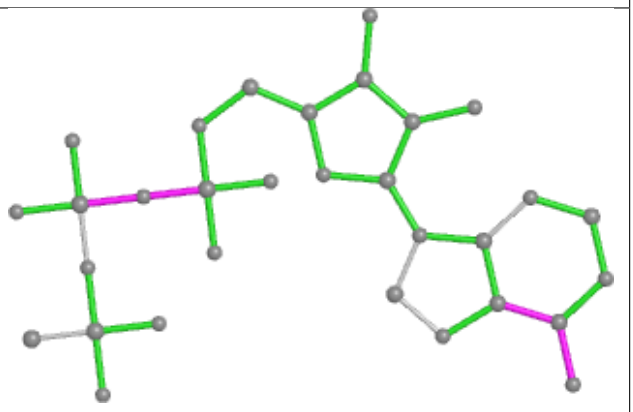

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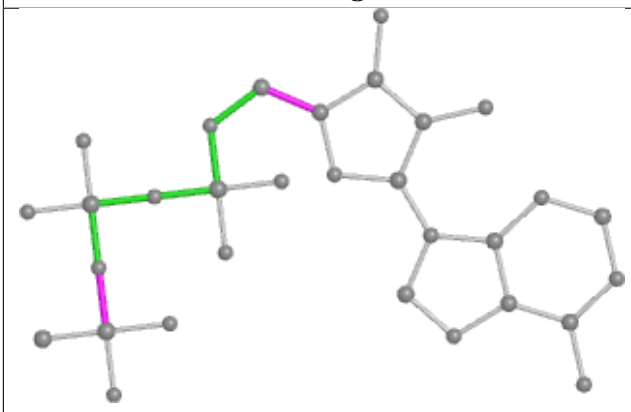

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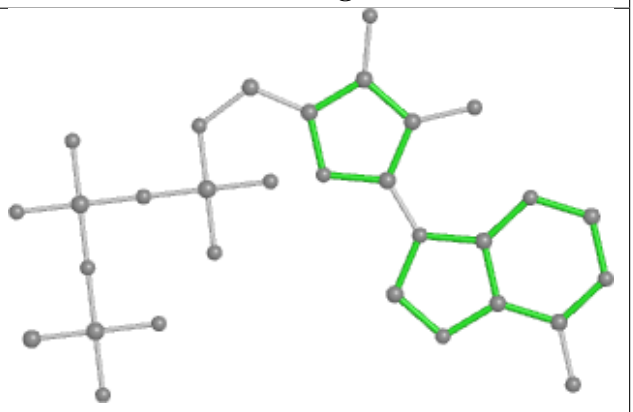
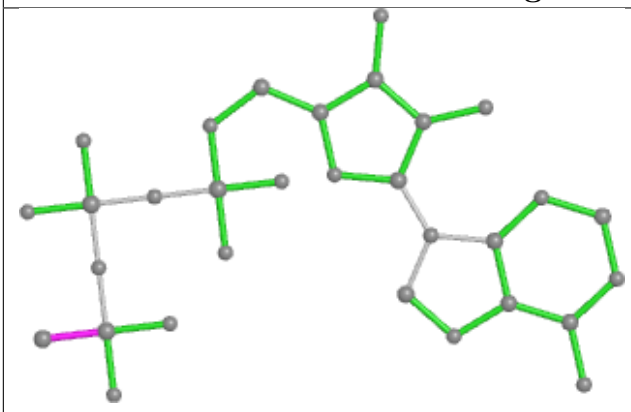


Rings

Ligand AGS C 902



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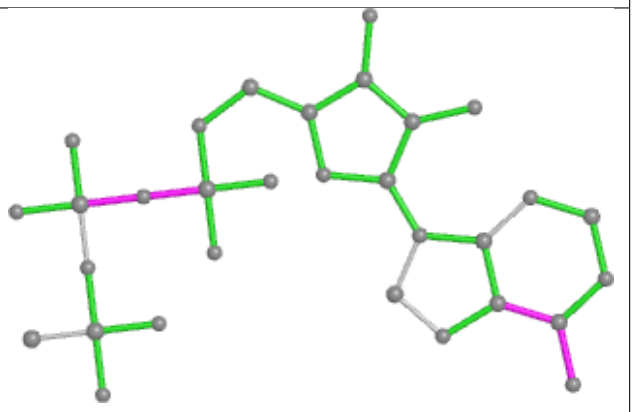

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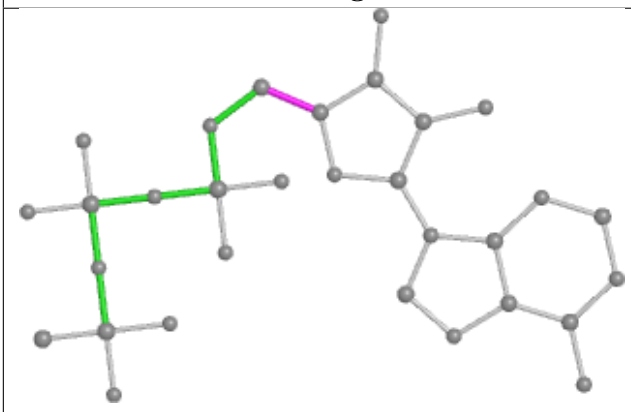

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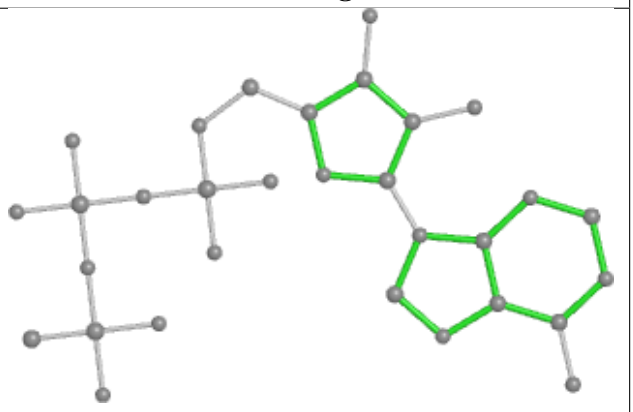
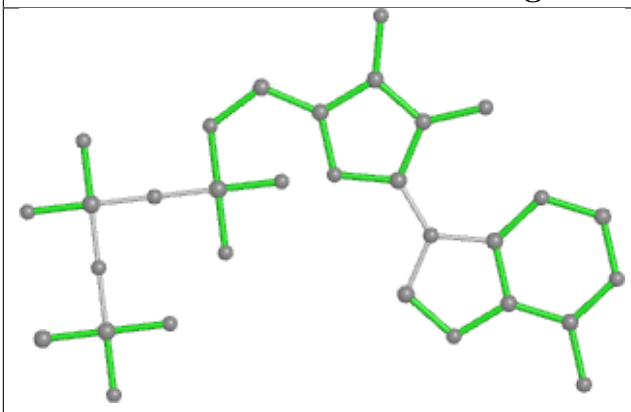


Rings

Ligand AGS C 901



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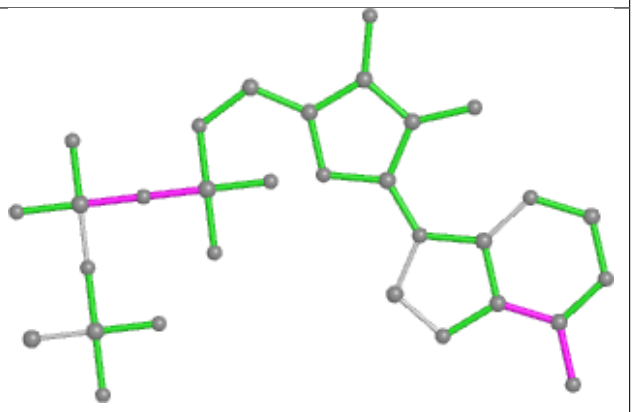

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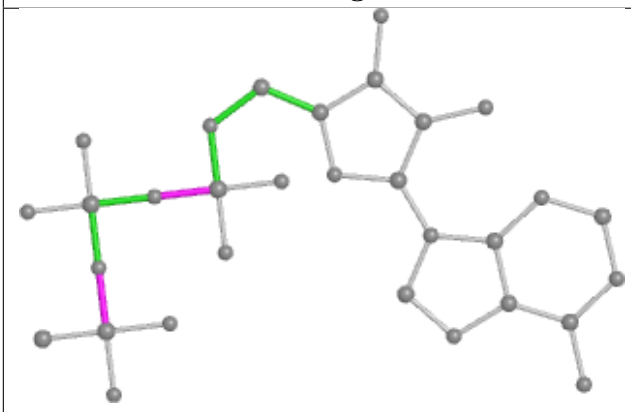

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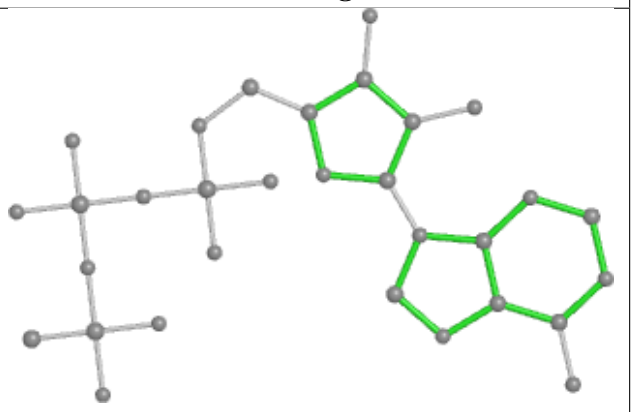
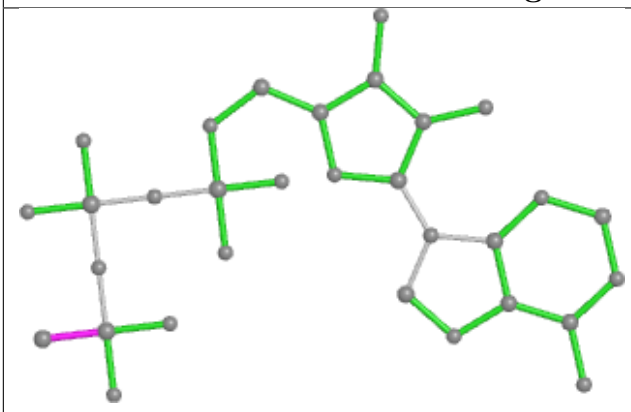


Rings

Ligand AGS B 902



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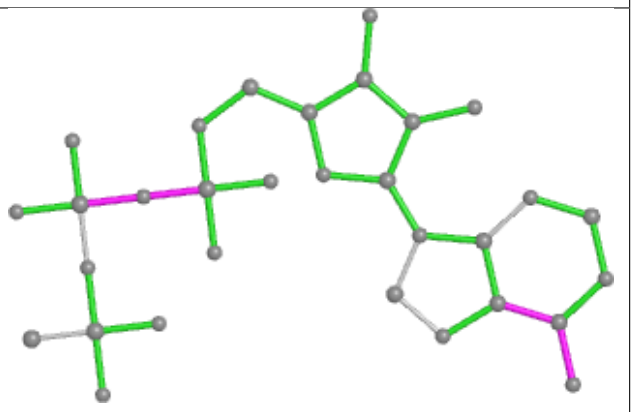

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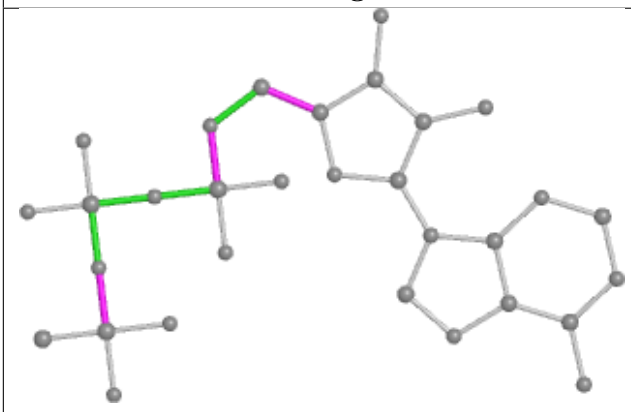

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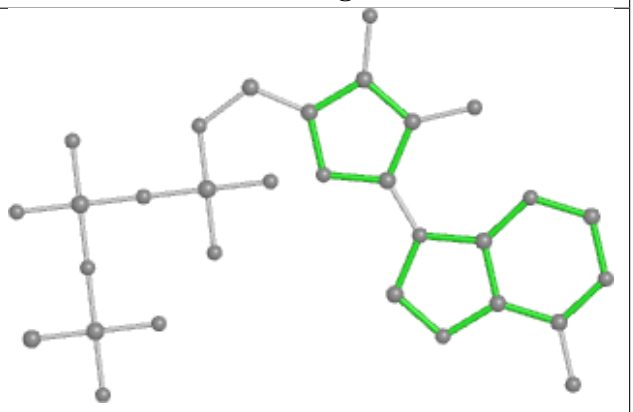
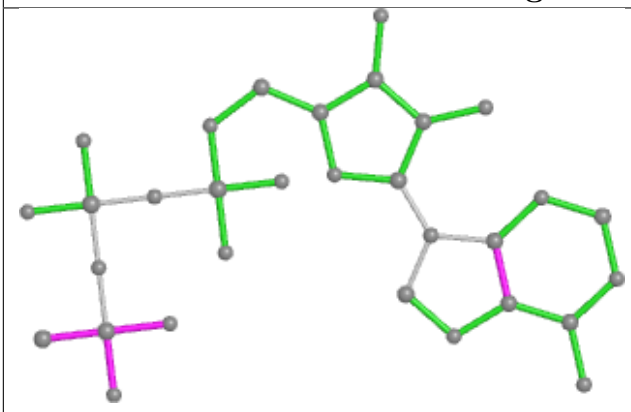


Rings

Ligand AGS E 901



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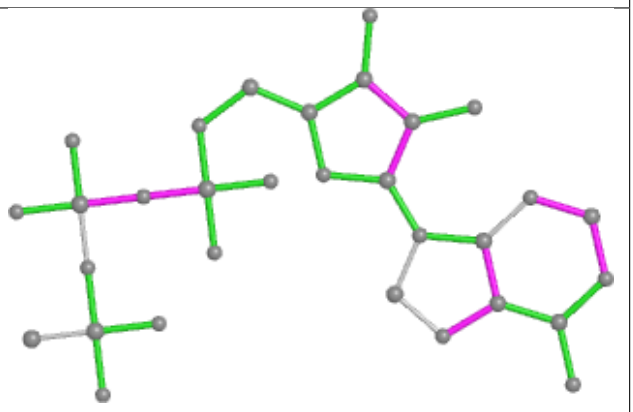

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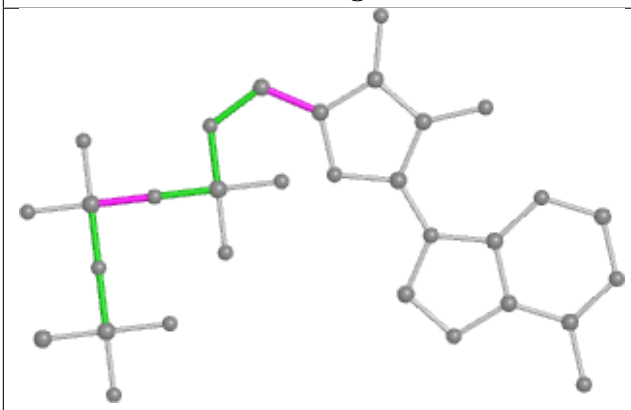

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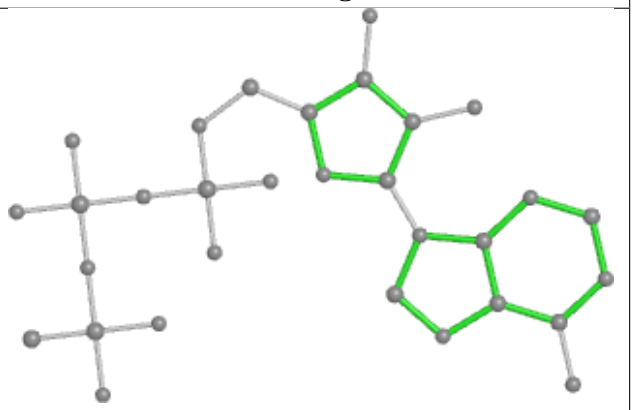
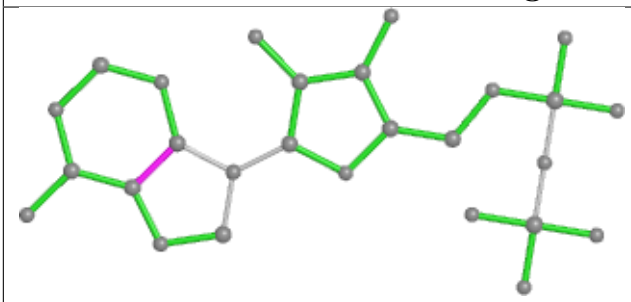


Rings

Ligand ADP F 902



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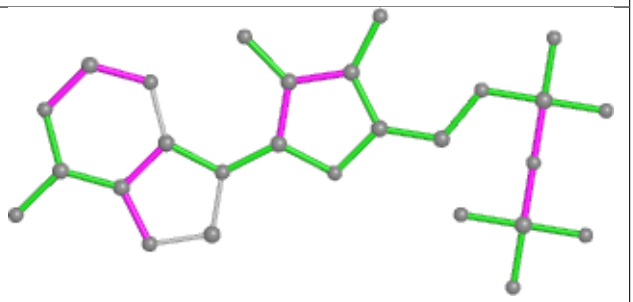

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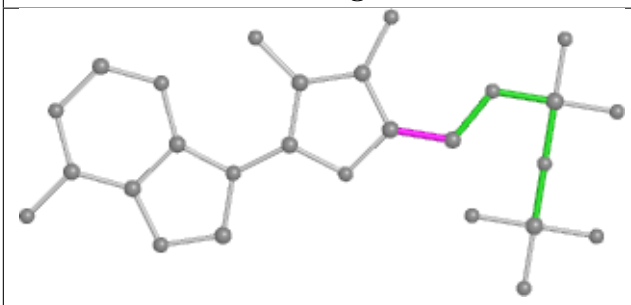

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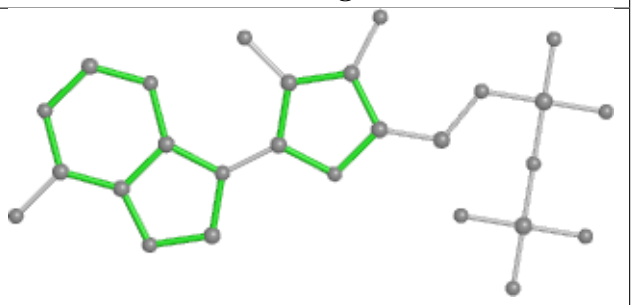
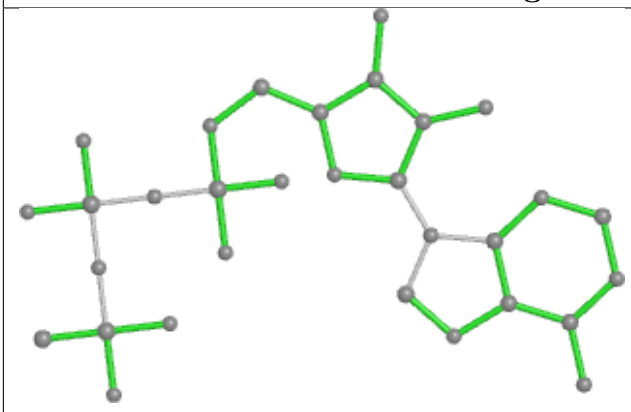


Rings

Ligand AGS D 901



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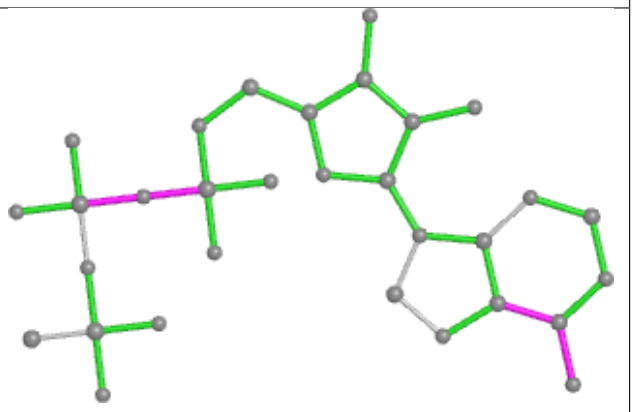

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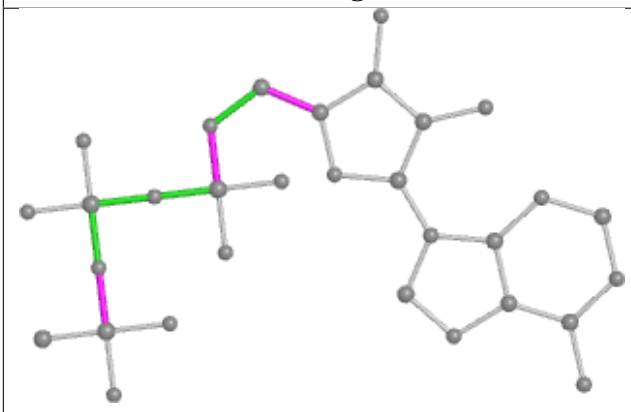

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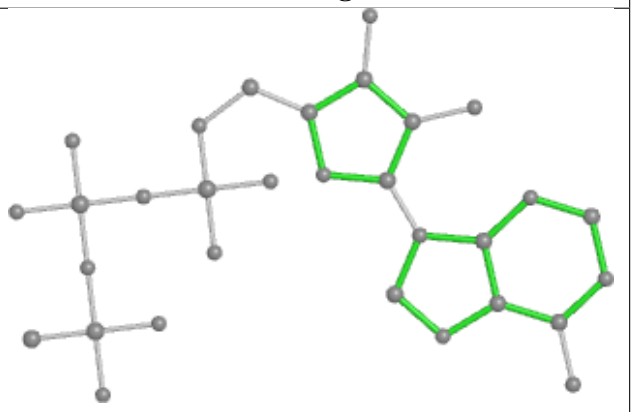
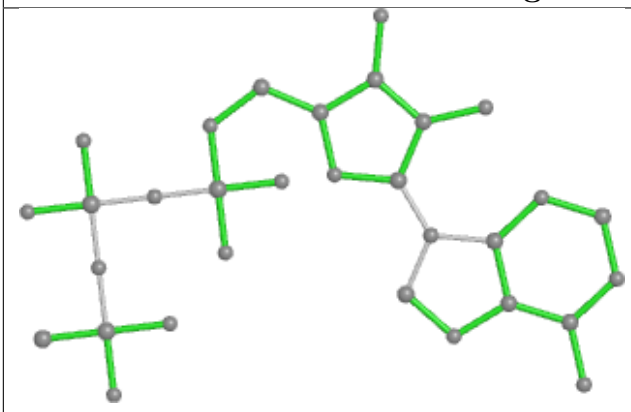


Rings

Ligand AGS A 901



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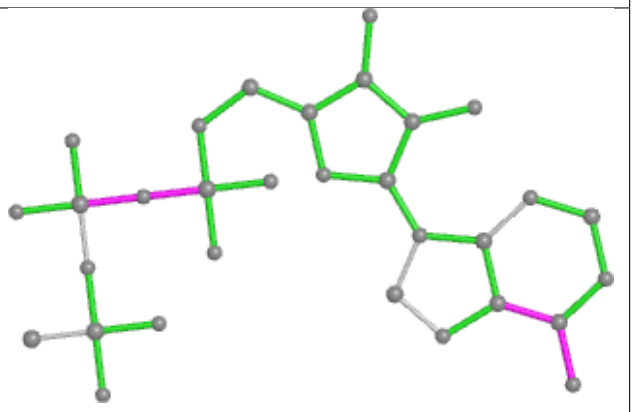

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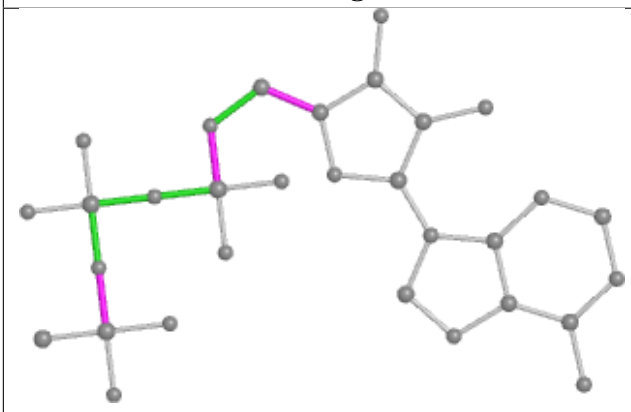

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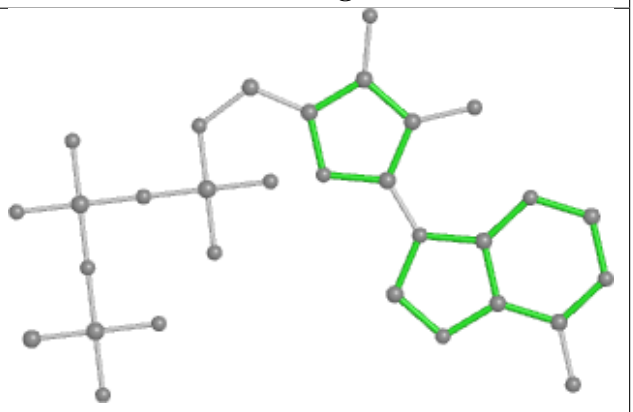
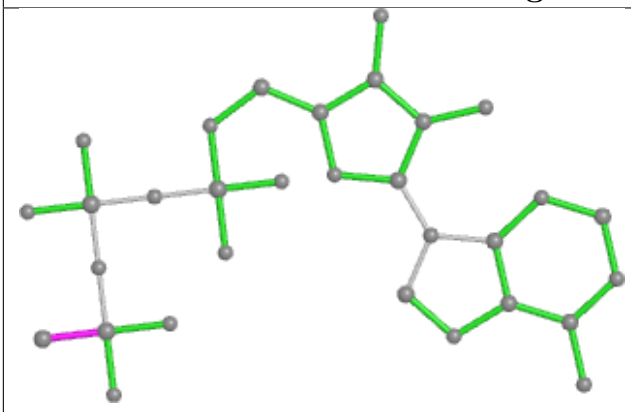


Rings

Ligand AGS F 901



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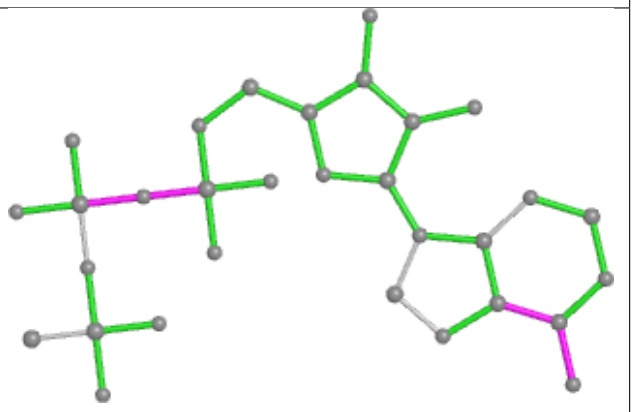

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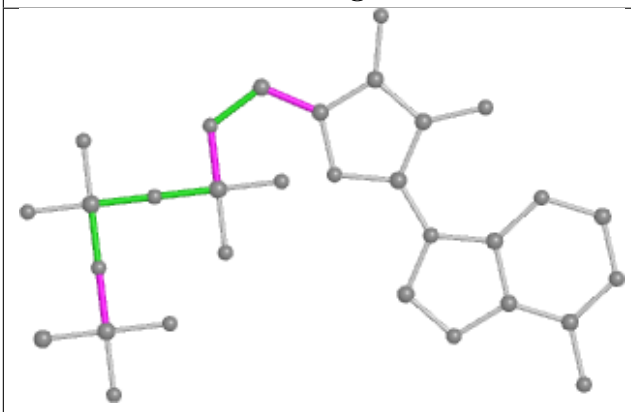

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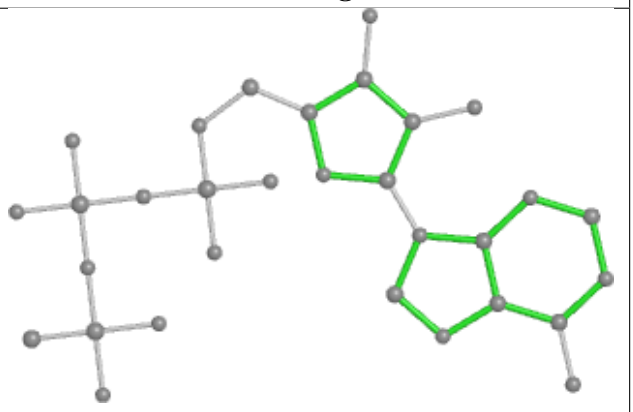
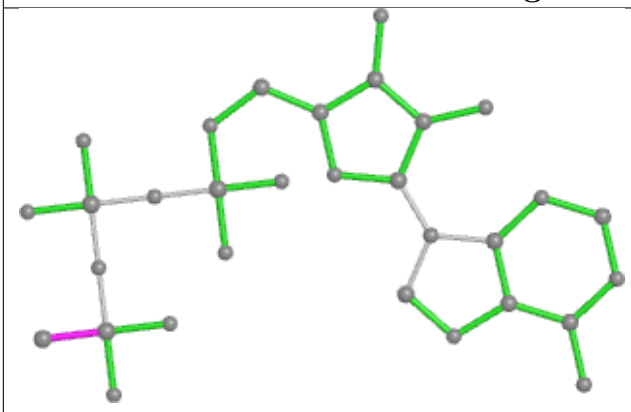
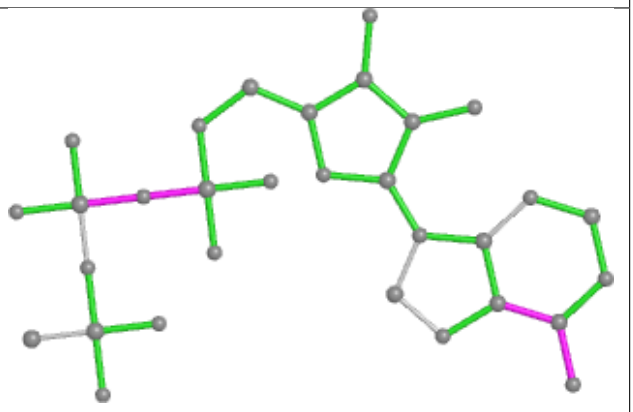


Rings

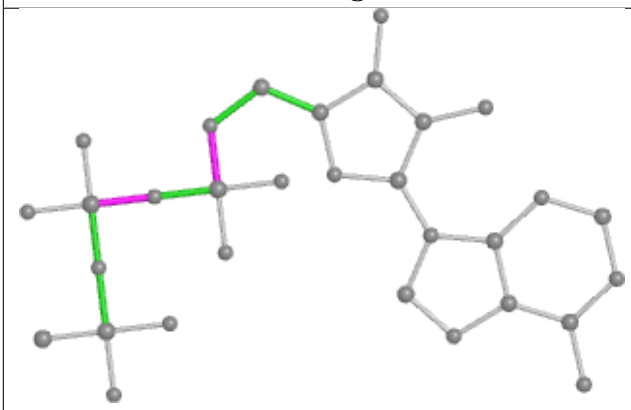
Ligand AGS A 902



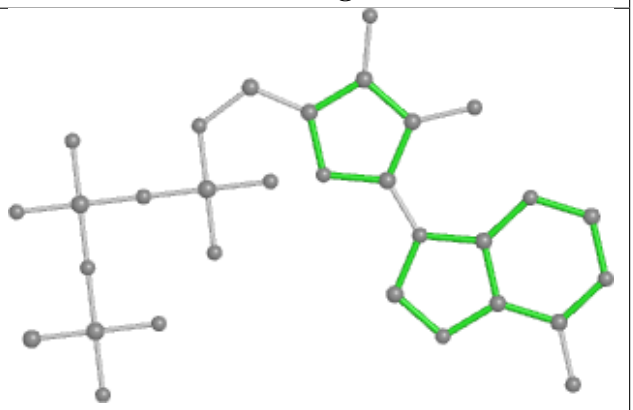
Bond lengths



Bond angles

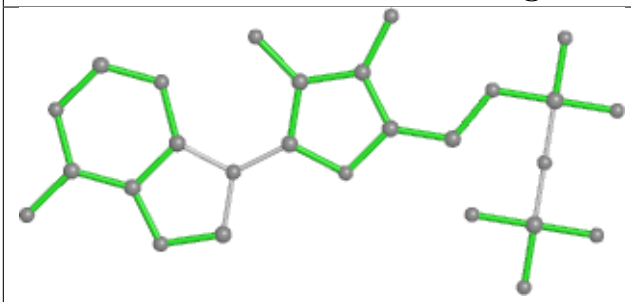


Torsions

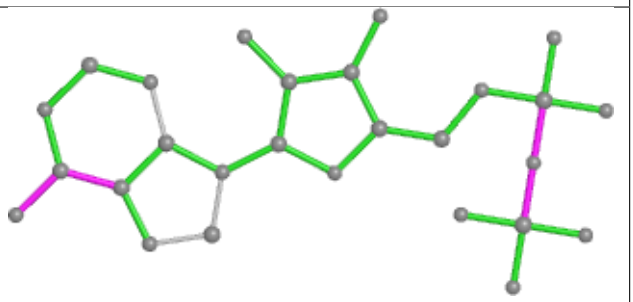


Rings

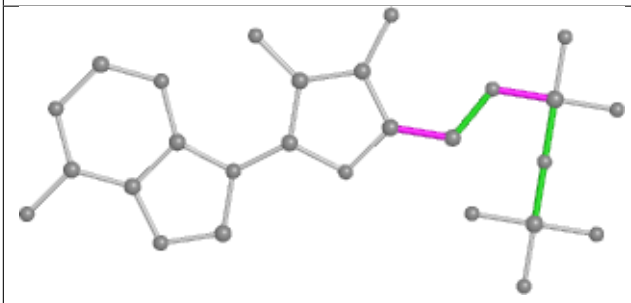
Ligand ADP E 902



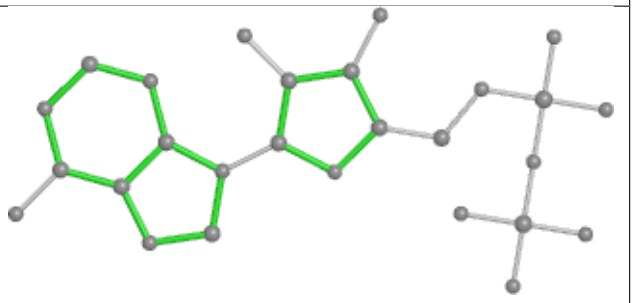
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

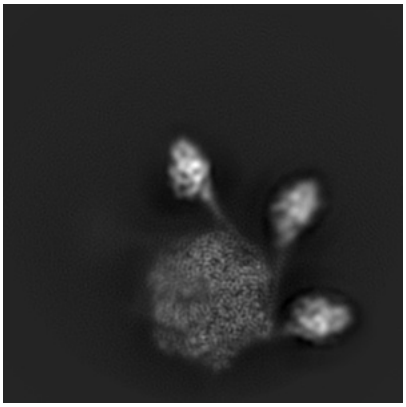
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23206. These allow visual inspection of the internal detail of the map and identification of artifacts.

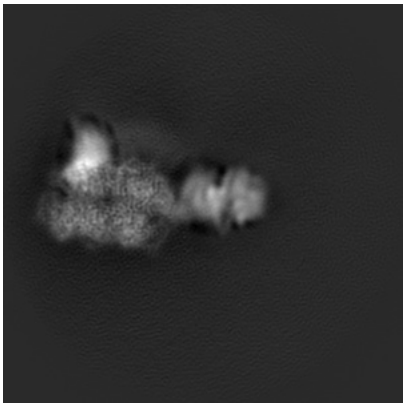
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

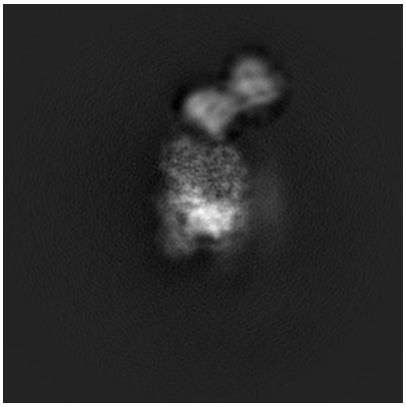
6.1.1 Primary map



X



Y

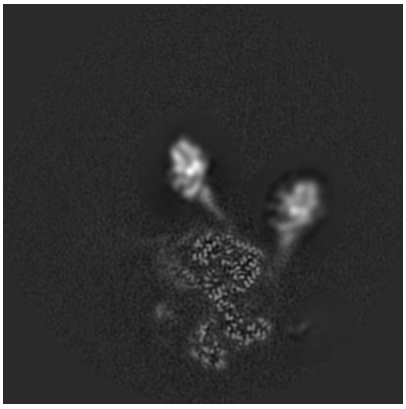


Z

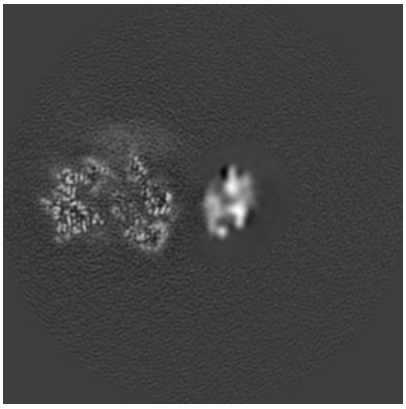
The images above show the map projected in three orthogonal directions.

6.2 Central slices

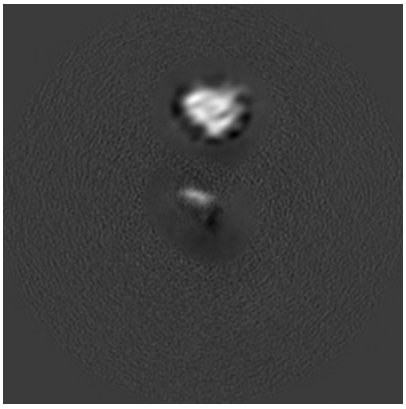
6.2.1 Primary map



X Index: 180



Y Index: 180

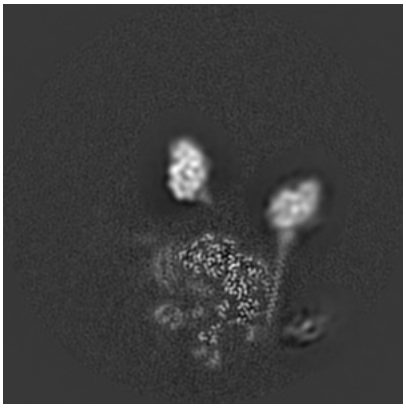


Z Index: 180

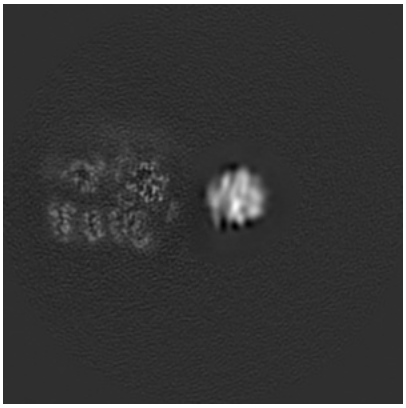
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

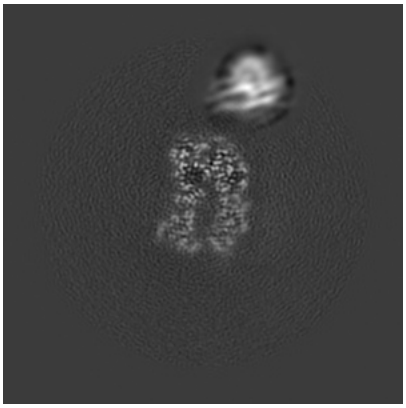
6.3.1 Primary map



X Index: 189



Y Index: 169



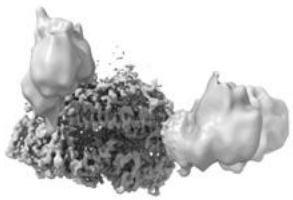
Z Index: 75

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

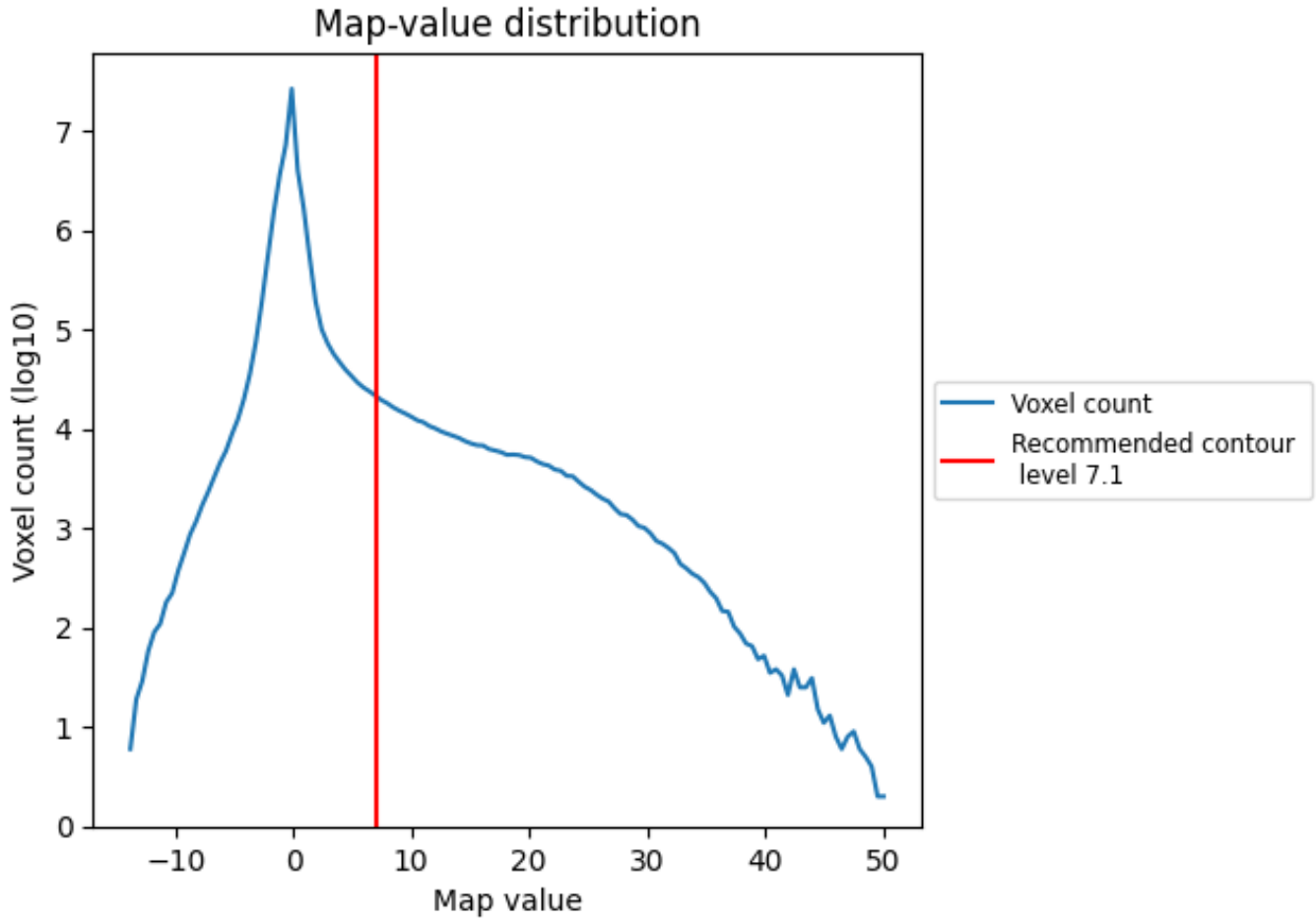
6.5 Mask visualisation (i)

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

7 Map analysis

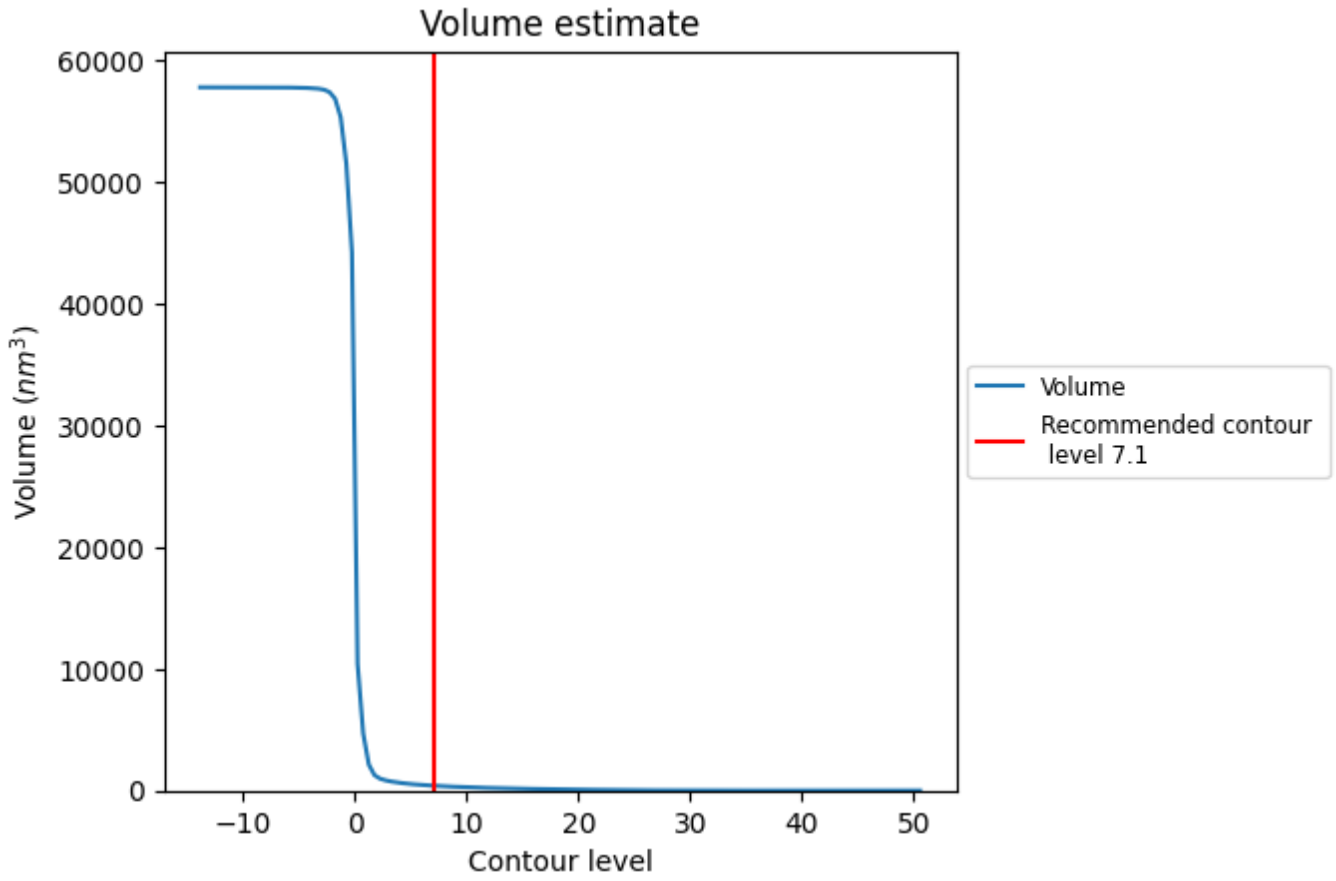
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

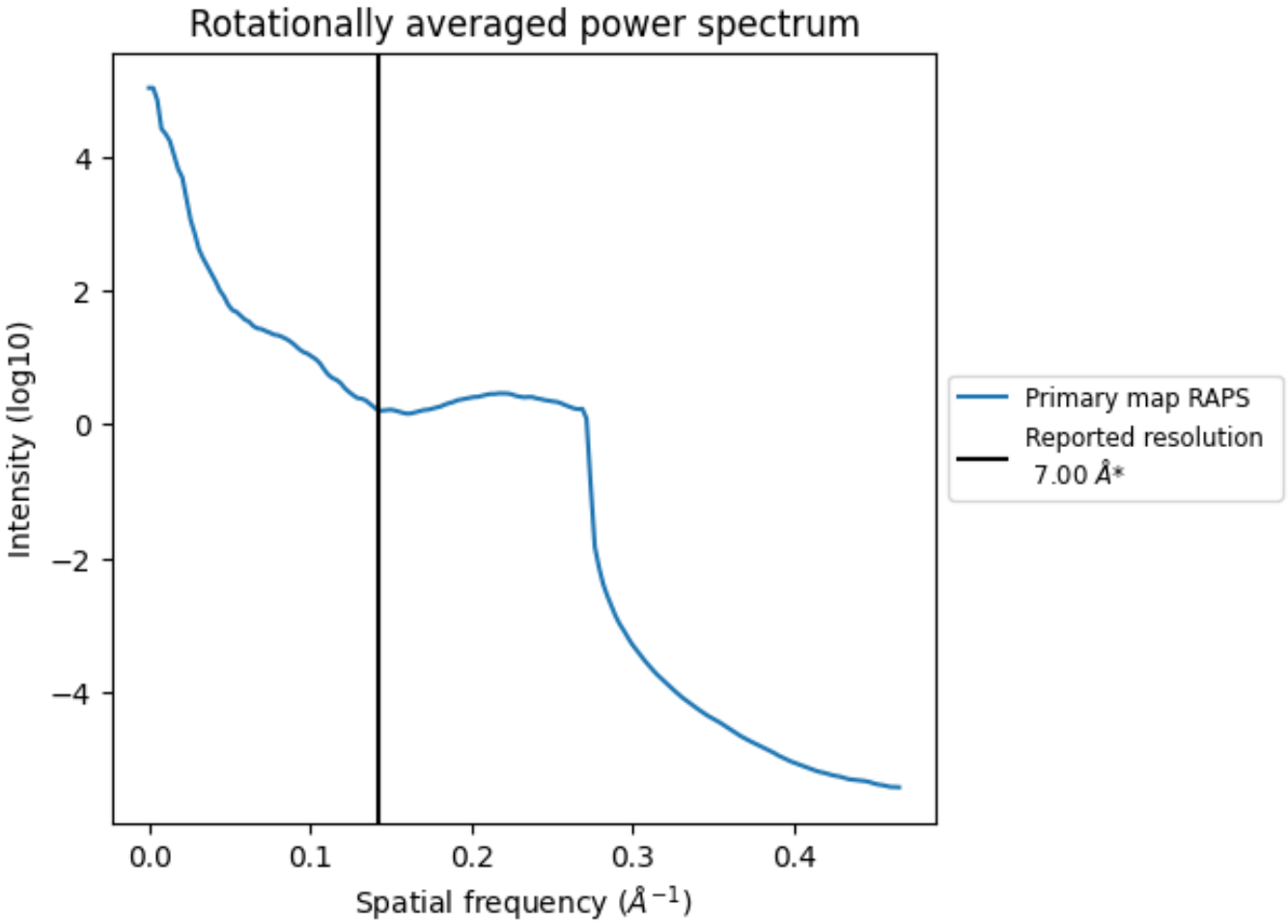
7.2 Volume estimate



The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 359 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

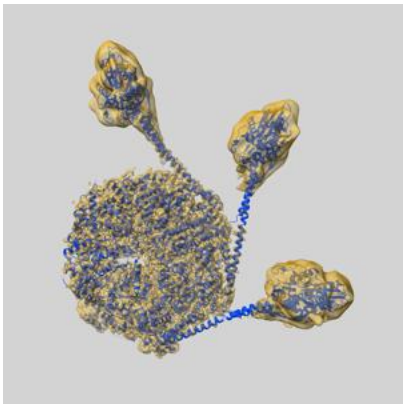
8 Fourier-Shell correlation (i)

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

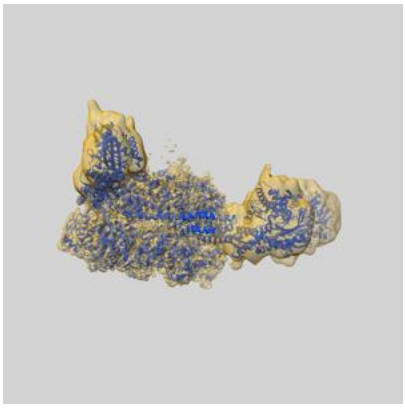
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23206 and PDB model 7L6N. Per-residue inclusion information can be found in section 3 on page 7.

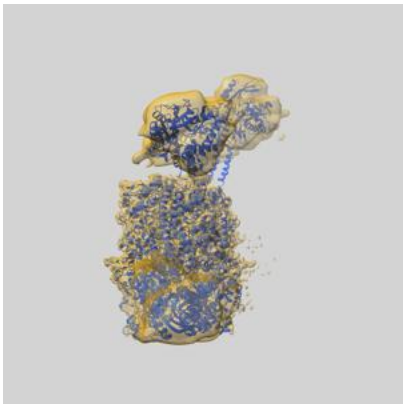
9.1 Map-model overlay



X



Y



Z

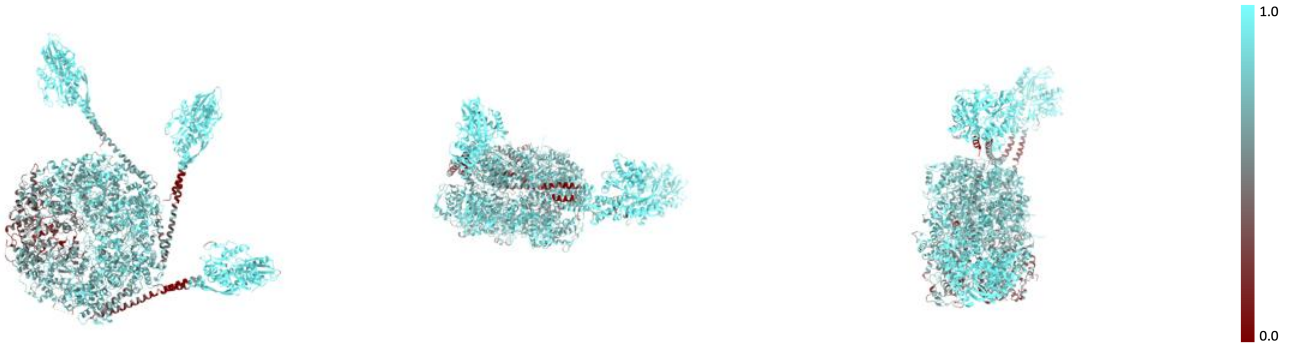
The images above show the 3D surface view of the map at the recommended contour level 7.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

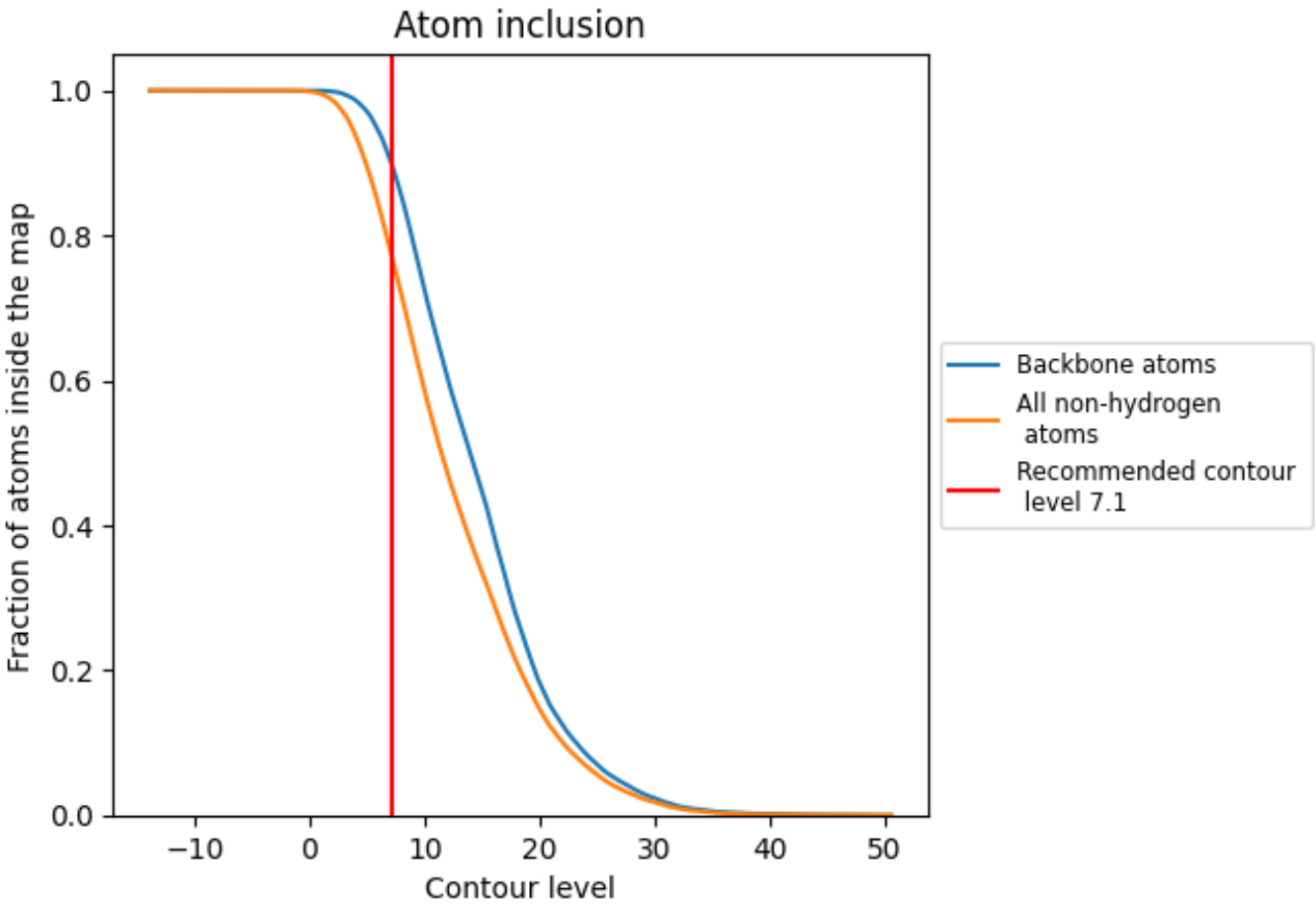
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% 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 (7.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7759	0.3550
A	0.8015	0.4420
B	0.7818	0.4530
C	0.7609	0.4530
D	0.7997	0.4560
E	0.6274	0.3510
F	0.5037	0.3330
I	0.9864	0.1440
J	0.9641	0.1230
K	0.9656	0.1140
N	0.8538	0.4860