Full wwPDB EM Validation Report (i)

Jul 7, 2024 – 12:07 pm BST

PDB ID	:	7PXC
EMDB ID	:	EMD-13697
Title	:	Substrate-engaged mycobacterial Proteasome-associated ATPase in complex with open-gate 20S CP - composite map (state A)
Authors	:	Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.
Deposited on	:	2021-10-08
Resolution	:	3.84 Å(reported)
Based on initial model	:	5KWA

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 (i) 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 (1)) were used in the production of this report:

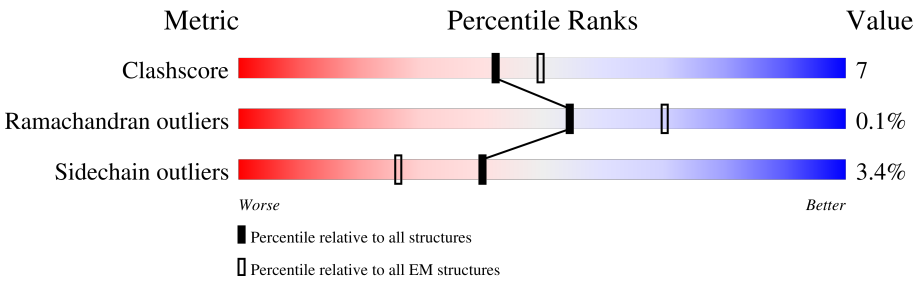
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.84 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	0	248	68% 16% • 13%
1	2	248	72% 13% • 13%
1	4	248	69% 15% • 13%
1	6	248	72% 13% • 13%
1	8	248	70% 14% • 13%
1	I	248	19% 63% 20% • 14%
1	K	248	18% 67% 19% • 12%
1	O	248	18% 69% 16% • 13%

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Mol	Chain	Length	Quality of chain
1	Q	248	17% 67% 16% 13%
1	T	248	18% 66% 18% 14%
1	X	248	19% 69% 16% 14%
1	Z	248	20% 65% 20% 13%
1	d	248	82% 13%
1	f	248	82% 5% 13%
2	1	609	99%
2	A	609	21% 58% 18% 23%
2	B	609	13% 60% 18% 22%
2	C	609	24% 59% 18% 23%
2	D	609	40% 58% 16% 25%
2	E	609	11% 60% 18% 21%
2	F	609	13% 61% 18% 21%
3	G	66	15% 24% 74%
4	H	291	71% 24%
4	J	291	66% 10% 23%
4	L	291	67% 9% 24%
4	M	291	69% 7% 24%
4	N	291	69% 7% 24%
4	P	291	68% 9% 23%
4	R	291	66% 10% 24%
4	S	291	69% 6% 24%
4	U	291	71% 9% 20%
4	V	291	71% 5% 23%
4	W	291	74% 6% 20%

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Mol	Chain	Length	Quality of chain
4	Y	291	68% 8% 23%
4	a	291	76% • 23%
4	b	291	74% • 23%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 68808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	215	1658	1039	303	313	3	0	0
1	2	215	1658	1039	303	313	3	0	0
1	4	215	1658	1039	303	313	3	0	0
1	6	215	1658	1039	303	313	3	0	0
1	8	215	1658	1039	303	313	3	0	0
1	I	214	1650	1033	302	312	3	0	0
1	K	217	1668	1044	305	316	3	0	0
1	O	215	1658	1039	303	313	3	0	0
1	Q	215	1658	1039	303	313	3	0	0
1	T	214	1650	1033	302	312	3	0	0
1	X	214	1650	1033	302	312	3	0	0
1	Z	215	1658	1039	303	313	3	0	0
1	d	215	1658	1039	303	313	3	0	0
1	f	215	1658	1039	303	313	3	0	0

- Molecule 2 is a protein called Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	5	42	28	6	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	468	3665	2318	630	706	11	0	0
2	B	473	3701	2338	635	717	11	0	0
2	C	471	3685	2326	634	714	11	0	0
2	D	457	3584	2270	613	690	11	0	0
2	E	483	3775	2378	651	735	11	0	0
2	F	483	3773	2377	651	734	11	0	0

- Molecule 3 is a protein called Prokaryotic ubiquitin-like protein Pup.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	17	112	62	23	26	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP P9WHN5
G	0	SER	-	expression tag	UNP P9WHN5

- Molecule 4 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	222	1636	1026	282	323	5	0	0
4	J	223	1640	1028	283	324	5	0	0
4	L	222	1636	1026	282	323	5	0	0
4	M	222	1636	1026	282	323	5	0	0
4	N	222	1636	1026	282	323	5	0	0
4	P	223	1640	1028	283	324	5	0	0
4	R	222	1636	1026	282	323	5	0	0

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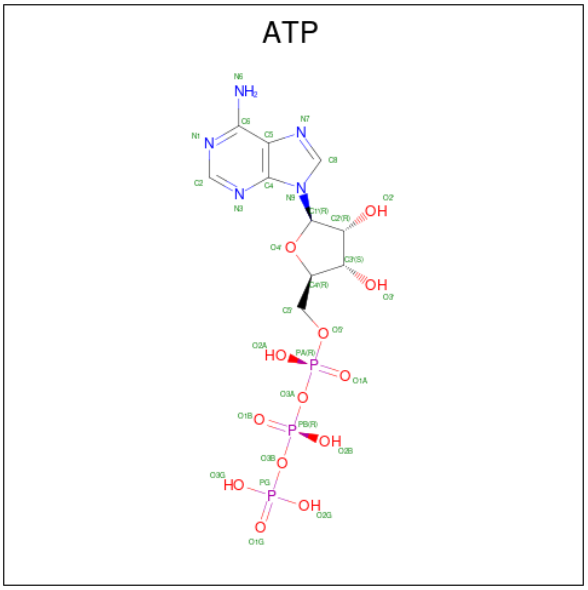
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	222	1636	1026	282	323	5	0	0
			Total	C	N	O	S		
4	U	234	1715	1072	295	343	5	0	0
			Total	C	N	O	S		
4	V	223	1640	1028	283	324	5	0	0
			Total	C	N	O	S		
4	W	234	1715	1072	295	343	5	0	0
			Total	C	N	O	S		
4	Y	223	1640	1028	283	324	5	0	0
			Total	C	N	O	S		
4	a	223	1640	1028	283	324	5	0	0
			Total	C	N	O	S		
4	b	223	1640	1028	283	324	5	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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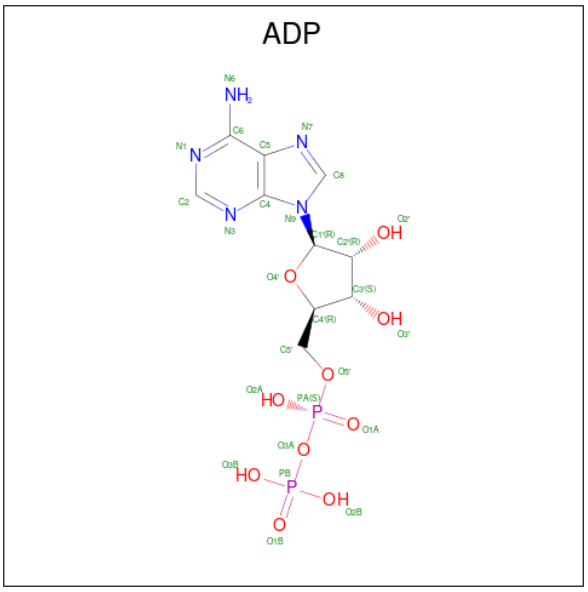
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	F	1	31	10	5	13	3	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	B	1	1	1	0
6	C	1	1	1	0
6	E	1	1	1	0
6	F	1	1	1	0

- Molecule 7 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).



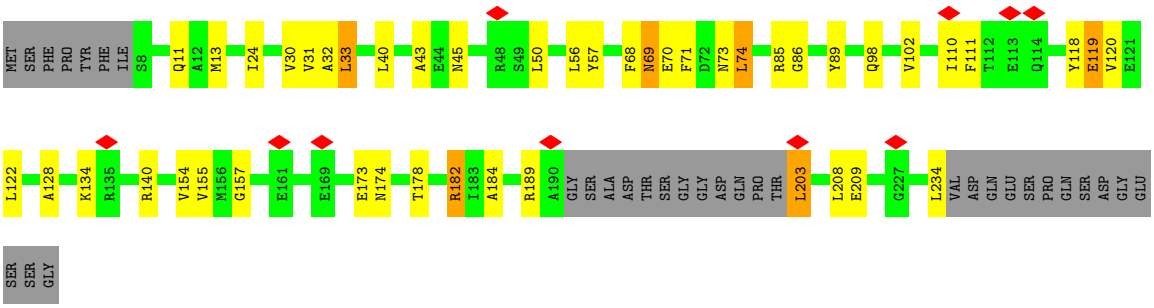
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	D	1	27	10	5	10	2	0

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.

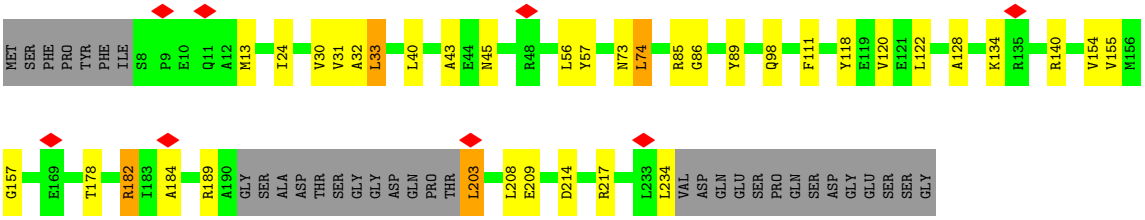
- Molecule 1: Proteasome subunit alpha

Chain 0:



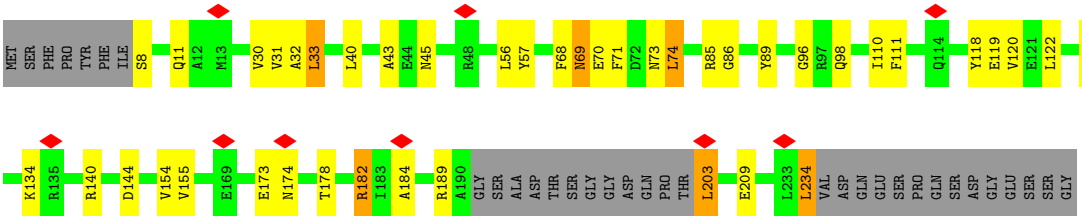
- Molecule 1: Proteasome subunit alpha

Chain 2:



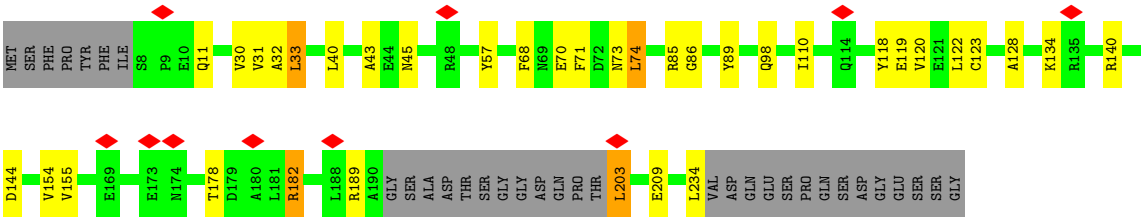
- Molecule 1: Proteasome subunit alpha

Chain 4:



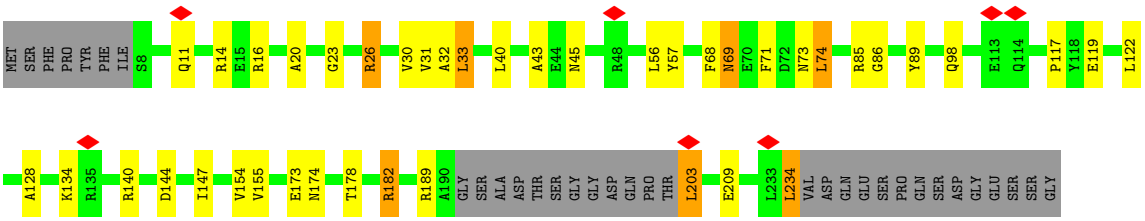
- Molecule 1: Proteasome subunit alpha

Chain 6:



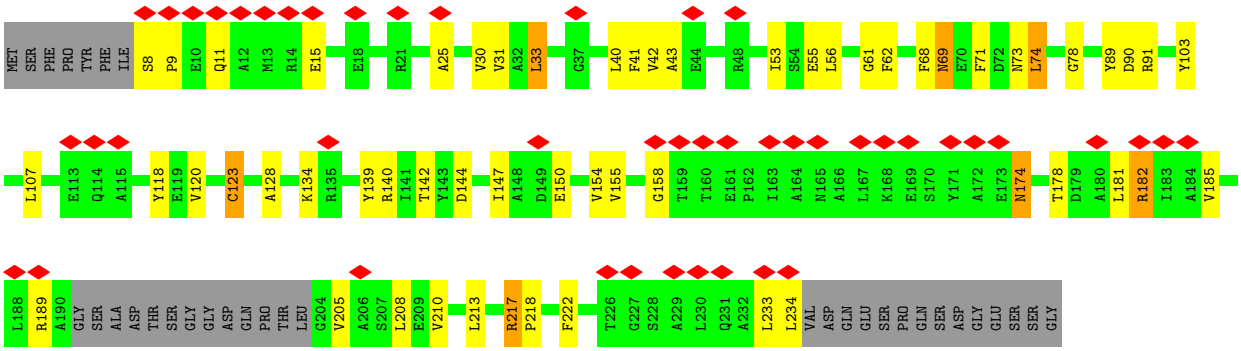
• Molecule 1: Proteasome subunit alpha

Chain 8:



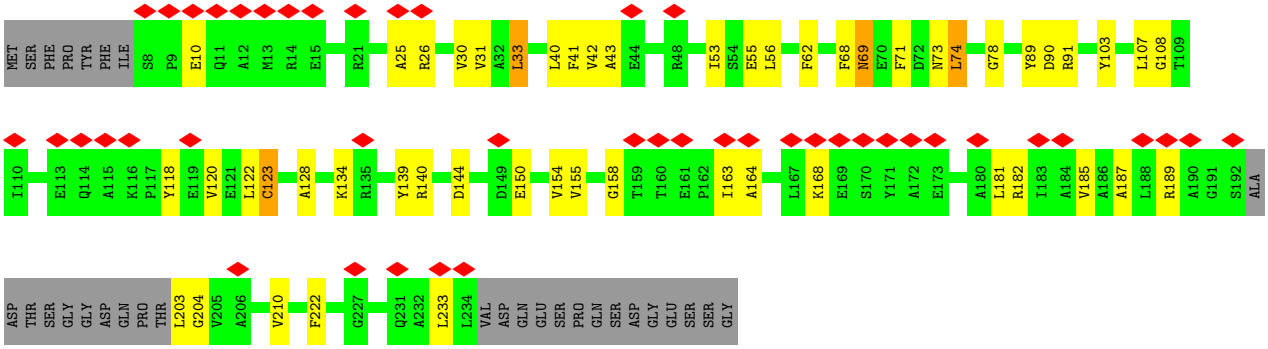
• Molecule 1: Proteasome subunit alpha

Chain I:



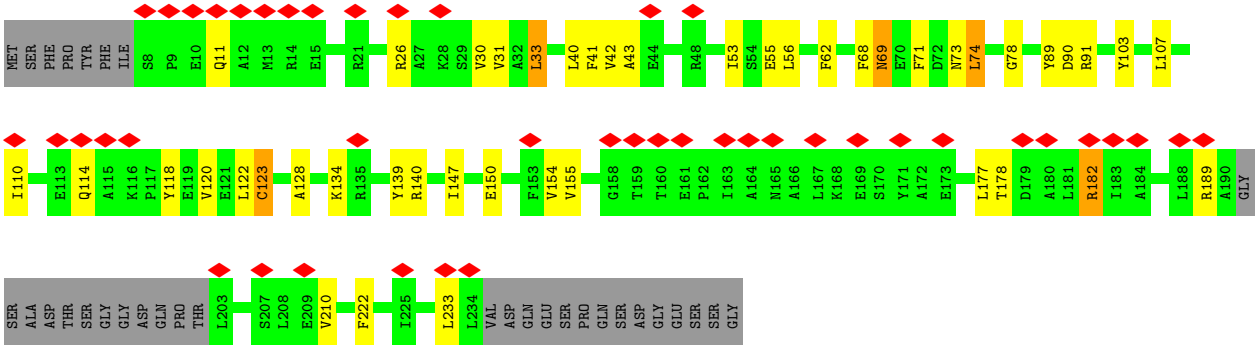
• Molecule 1: Proteasome subunit alpha

Chain K:



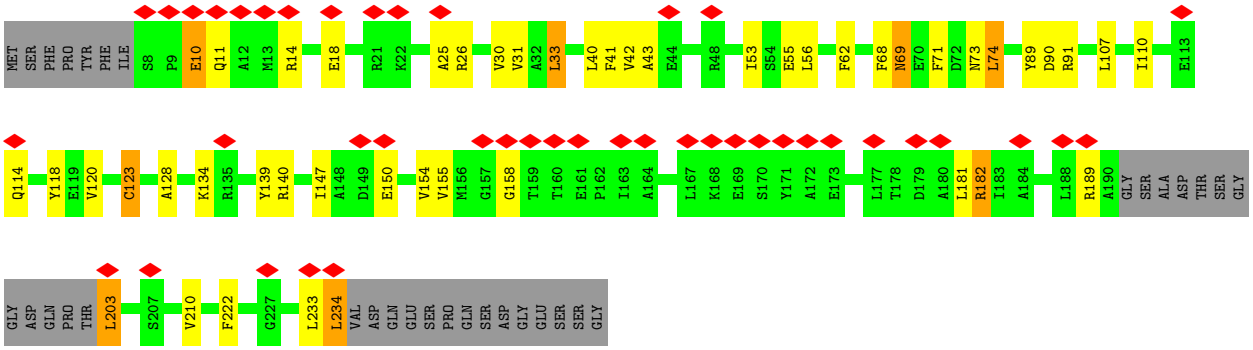
- Molecule 1: Proteasome subunit alpha

Chain O:



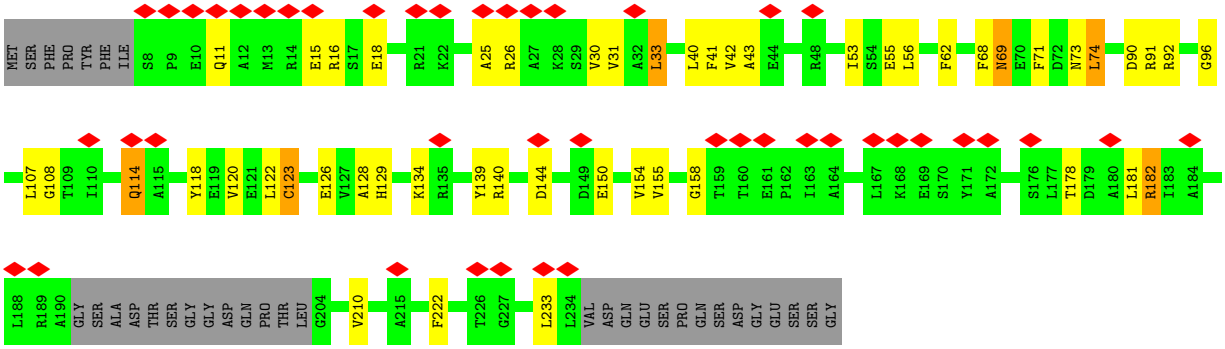
- Molecule 1: Proteasome subunit alpha

Chain Q:



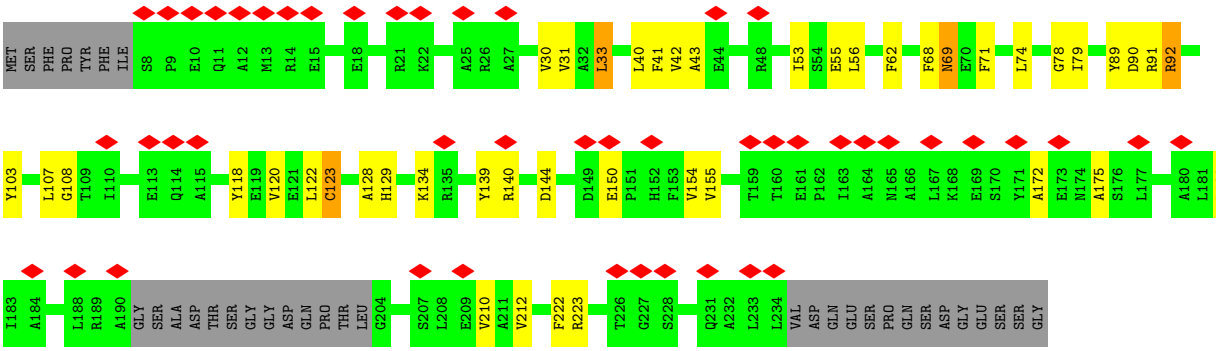
- Molecule 1: Proteasome subunit alpha

Chain T:



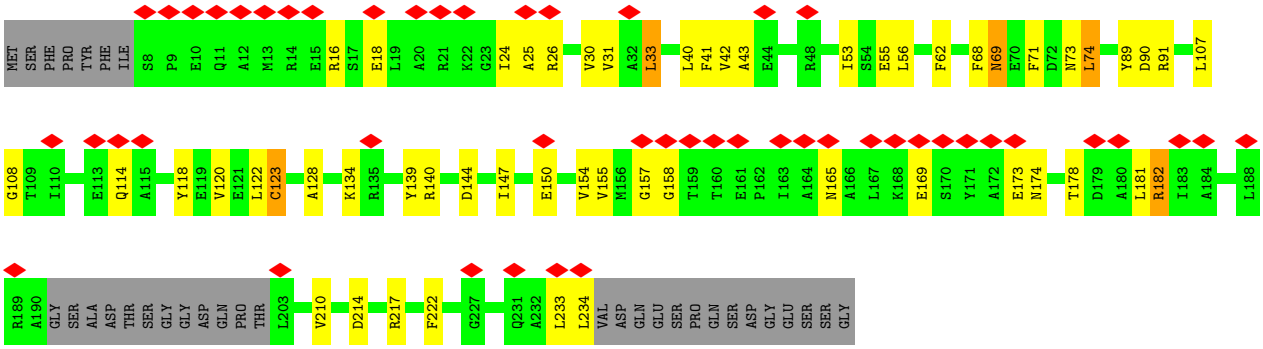
- Molecule 1: Proteasome subunit alpha

Chain X:



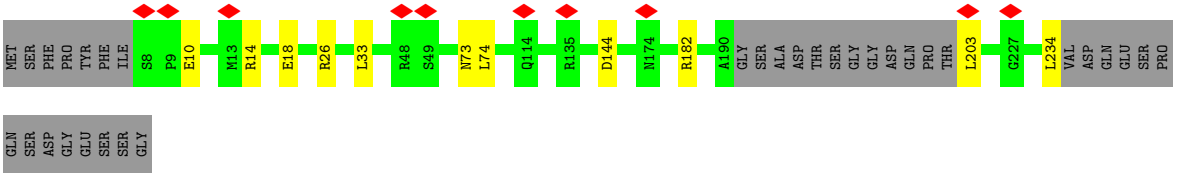
• Molecule 1: Proteasome subunit alpha

Chain Z:



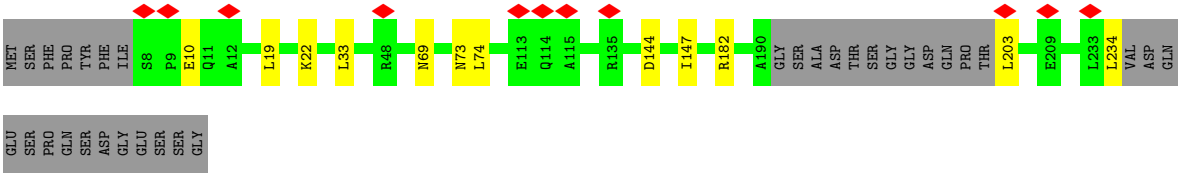
• Molecule 1: Proteasome subunit alpha

Chain d:



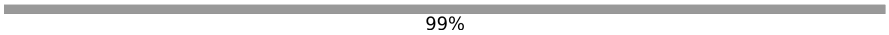
• Molecule 1: Proteasome subunit alpha

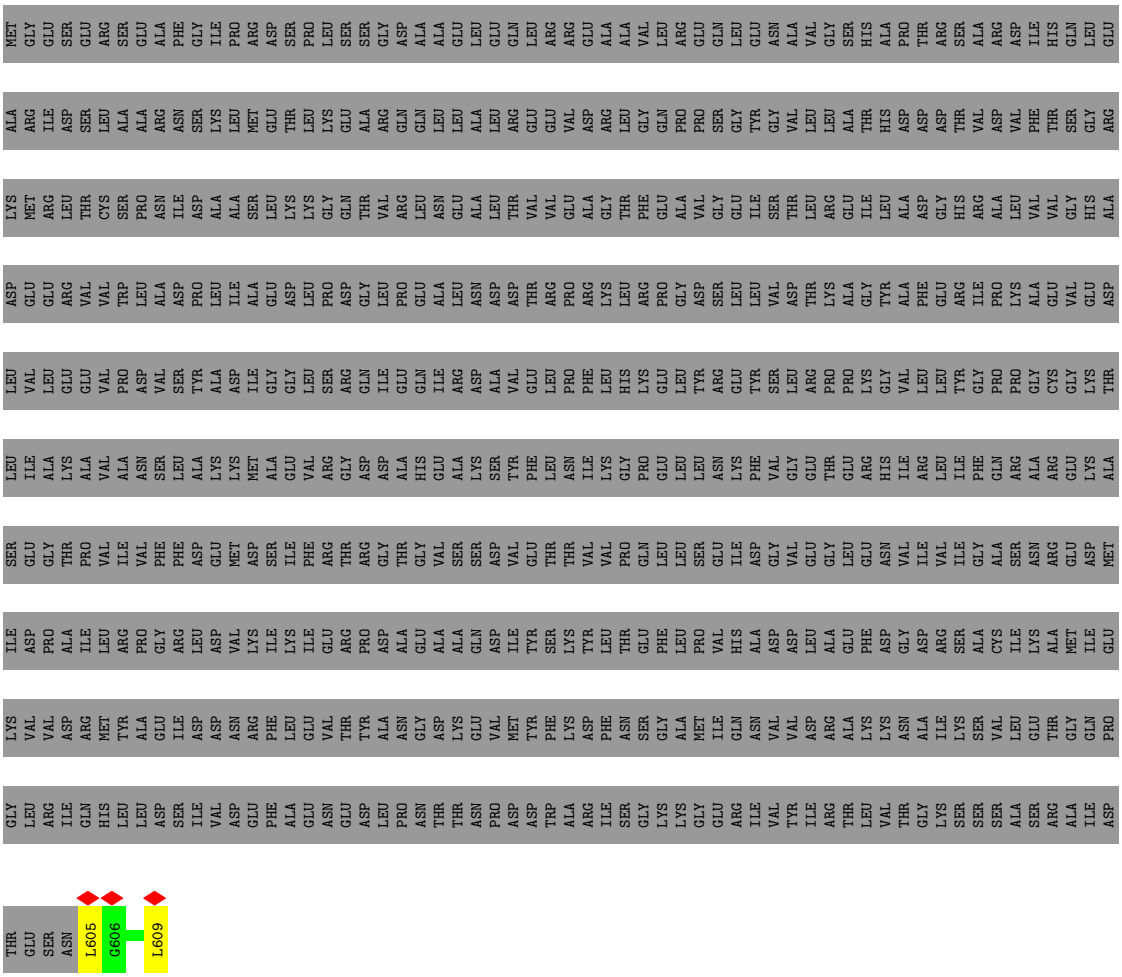
Chain f:



• Molecule 2: Proteasome-associated ATPase

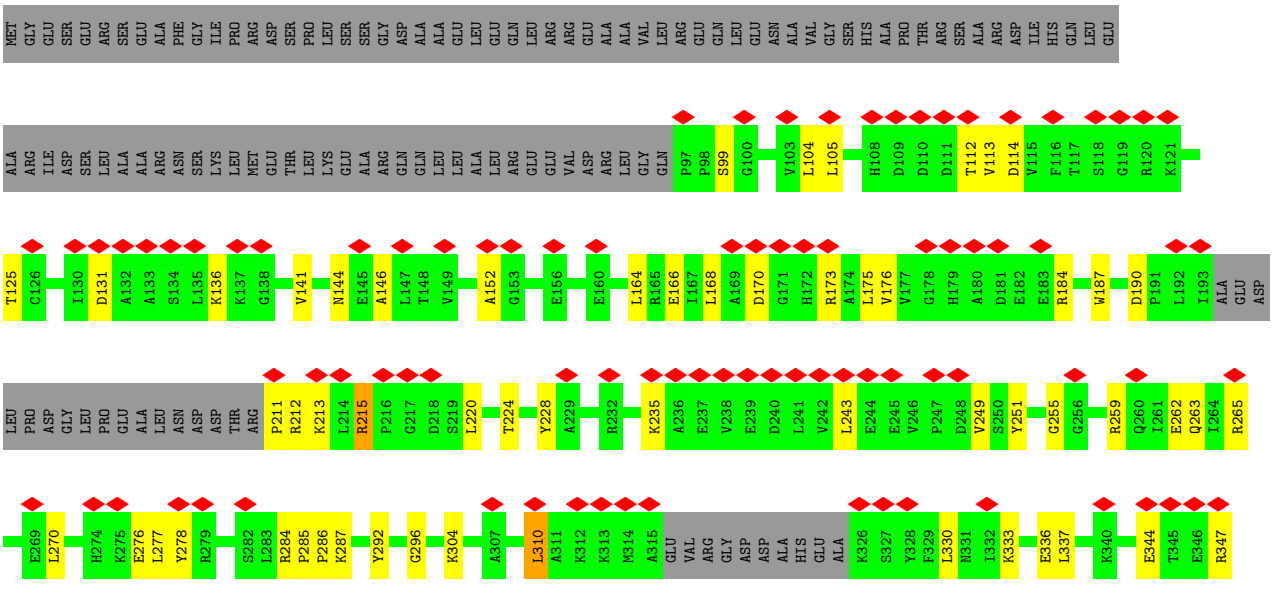
Chain 1:

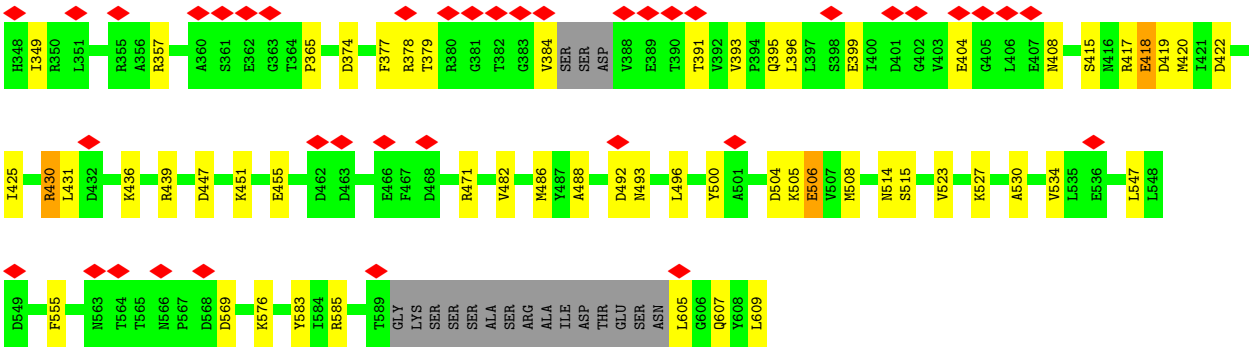




• Molecule 2: Proteasome-associated ATPase

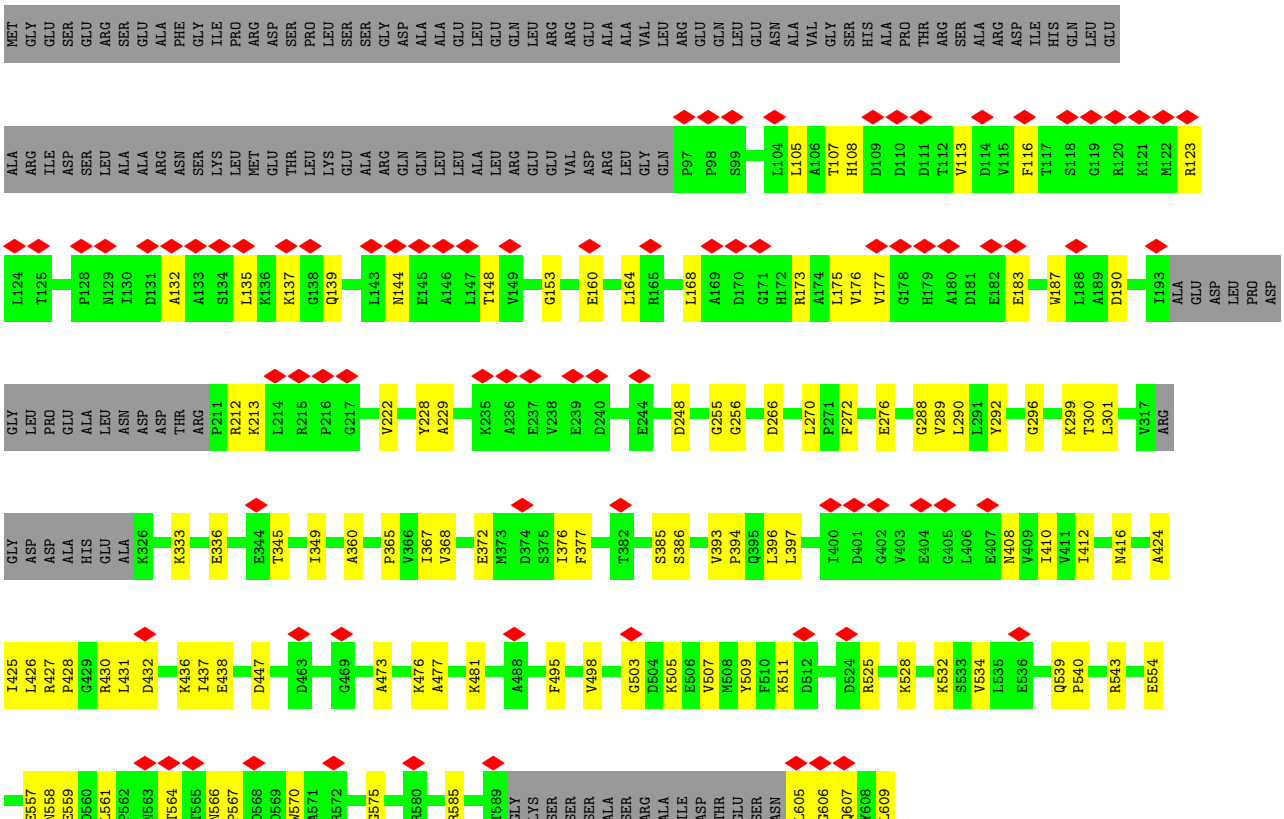
Chain A: 21% 58% 18% • 23%





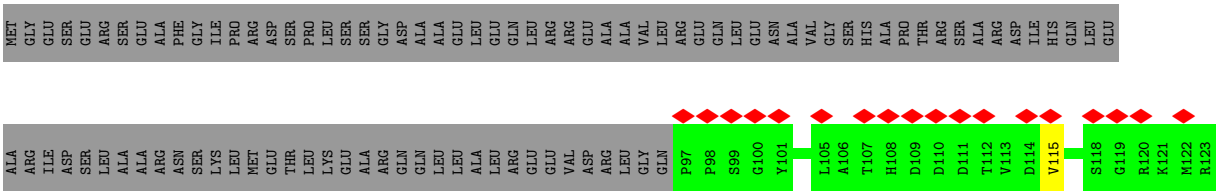
• Molecule 2: Proteasome-associated ATPase

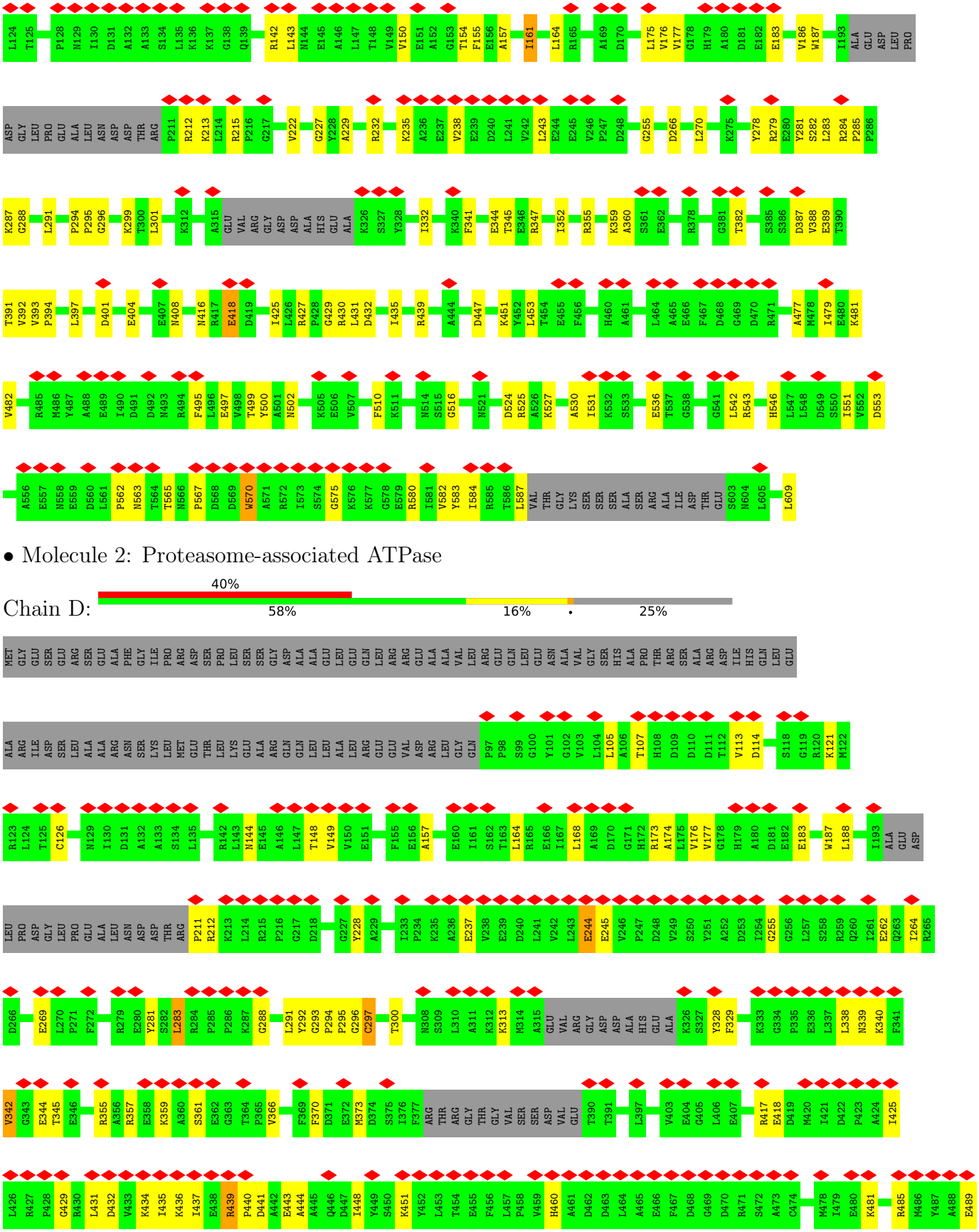
Chain B:



• Molecule 2: Proteasome-associated ATPase

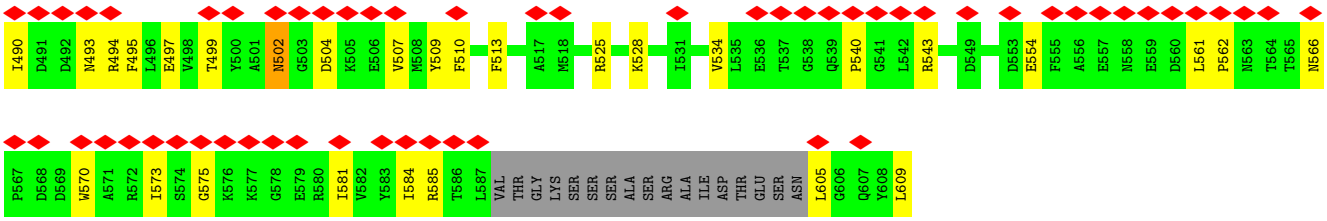
Chain C:





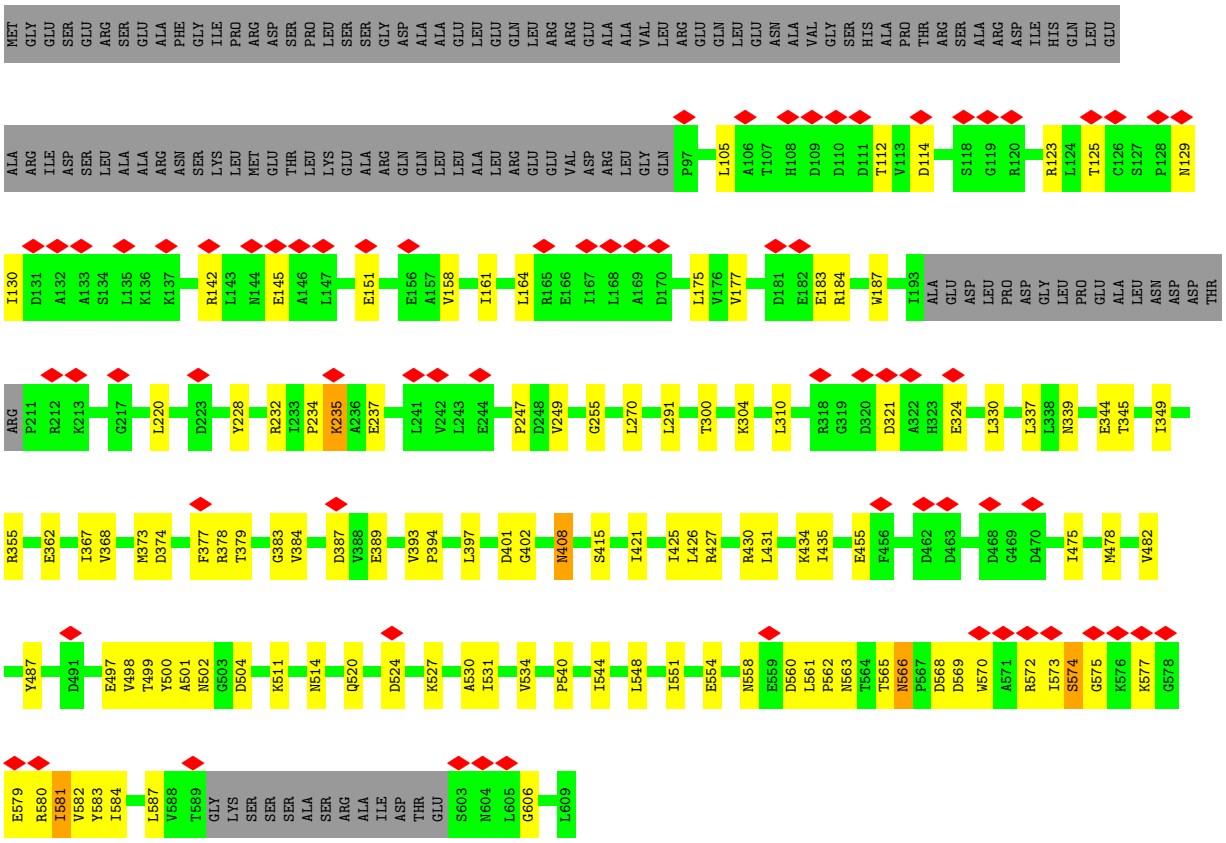
- Molecule 2: Proteasome-associated ATPase

Chain D:



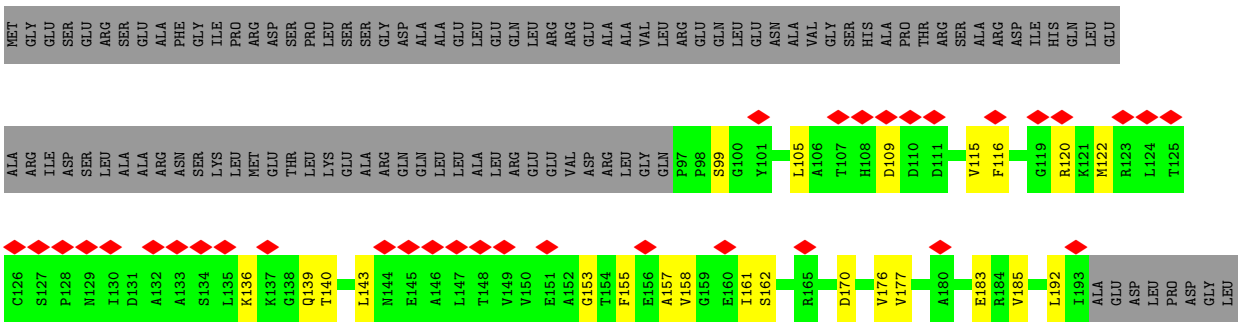
• Molecule 2: Proteasome-associated ATPase

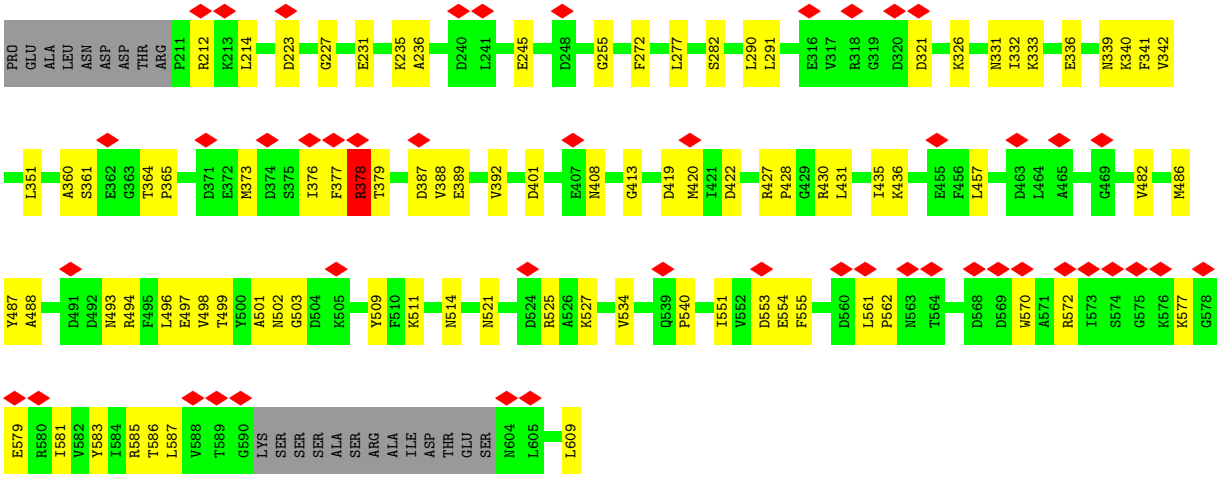
Chain E:



• Molecule 2: Proteasome-associated ATPase

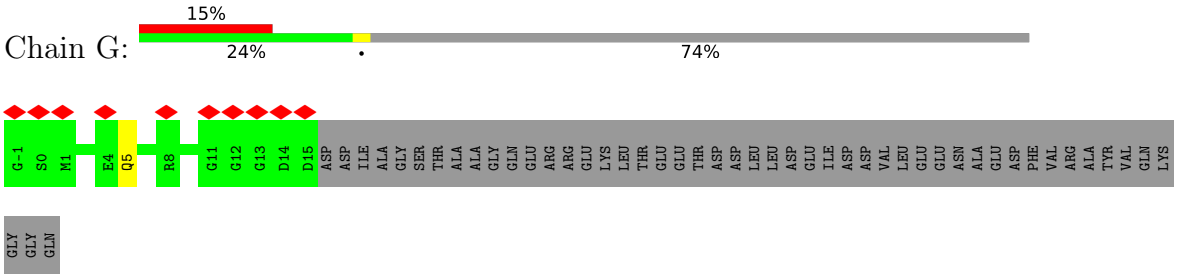
Chain F:





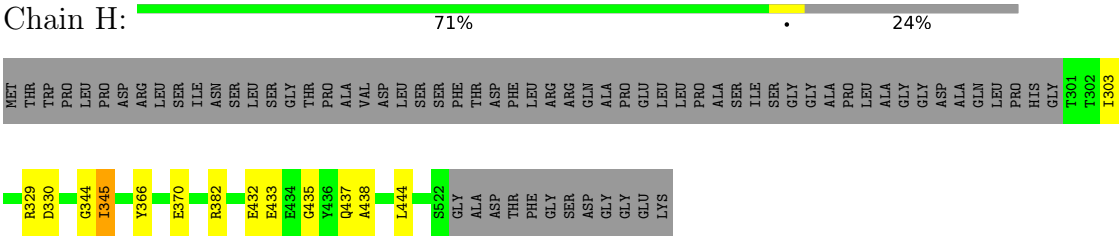
• Molecule 3: Prokaryotic ubiquitin-like protein Pup

Chain G:



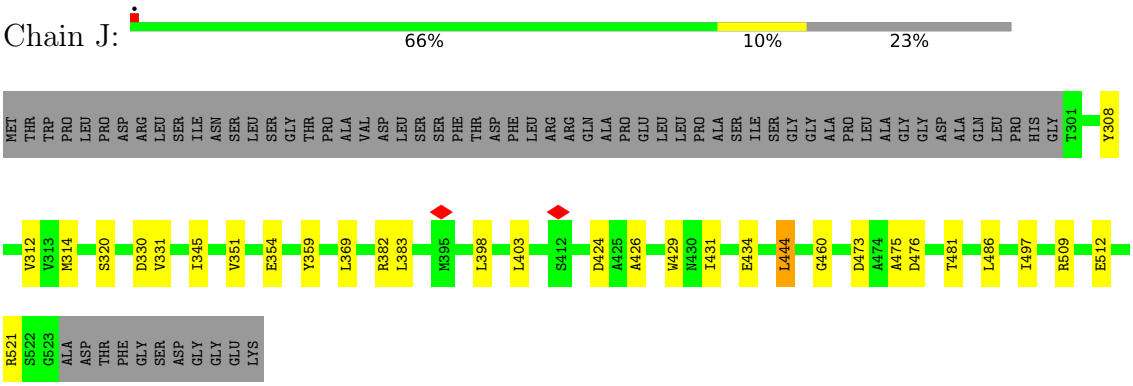
• Molecule 4: Proteasome subunit beta

Chain H:



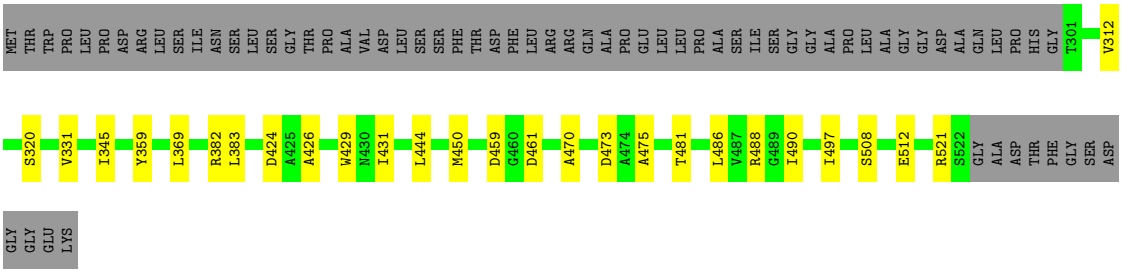
• Molecule 4: Proteasome subunit beta

Chain J:



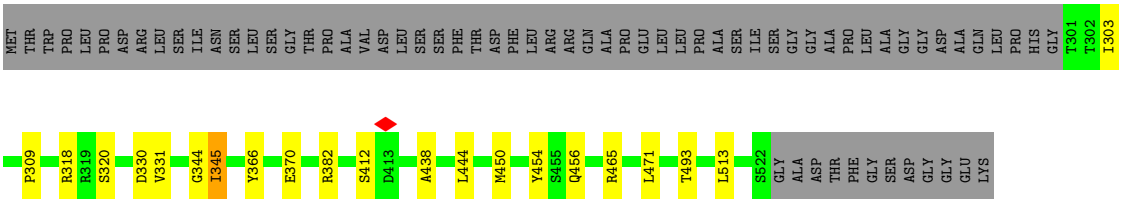
• Molecule 4: Proteasome subunit beta

Chain L:



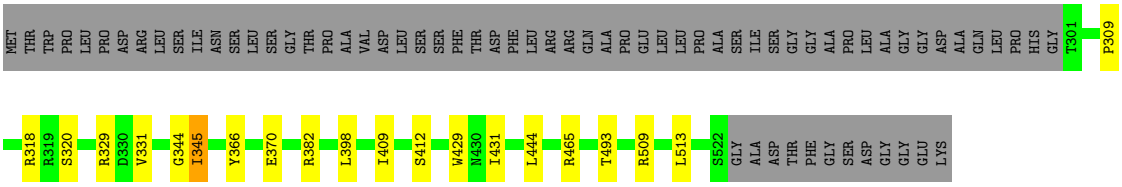
• Molecule 4: Proteasome subunit beta

Chain M:



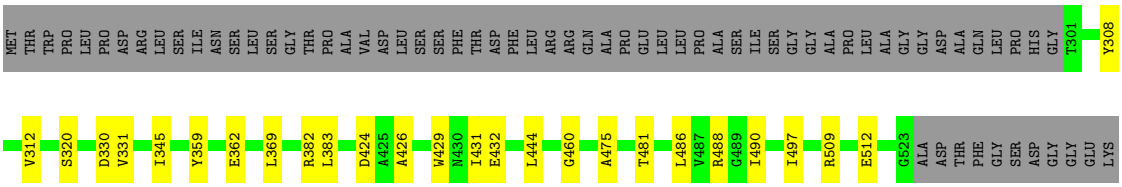
• Molecule 4: Proteasome subunit beta

Chain N:



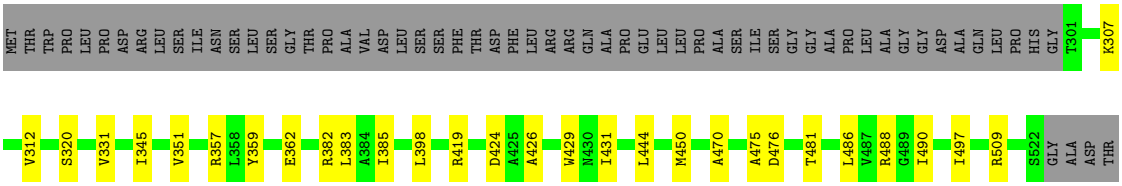
• Molecule 4: Proteasome subunit beta

Chain P:



• Molecule 4: Proteasome subunit beta

Chain R:



PHE GLY SER ASP GLY GLY GLU LYS

- Molecule 4: Proteasome subunit beta

Chain S:

MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY T301 P309

R318 R329 D330 D338 T341 G344 I345 Y366 E370 R382 M395 S412 D413 W429 M430 I431 L444 M450 Y454 R465 L471 T493 L513 S522 GLY ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS

- Molecule 4: Proteasome subunit beta

Chain U:

MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY T301 V312

V313 M314 S320 D330 V331 Y359 L363 L369 R382 L383 L403 D424 A425 A426 W429 N430 I431 E432 E433 L444 D459 G460 D461 A475 D476 T481 L486 V487 R488 G489 I490 I497 A524 D525 T526 F527 G528 S529 D530 G531 G532 E533 K534

- Molecule 4: Proteasome subunit beta

Chain V:

MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY T301 T302 I303

P309 Y335 D338 T341 G344 I345 V353 E362 Y366 E370 R382 E432 Q437 A438 L444 R509 G523 ALA ASP THR PHE GLY SER ASP GLY GLY GLU LYS

- Molecule 4: Proteasome subunit beta

Chain W:

MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY T301 T302 I303

P309 D330 G344 I345 E354 Y366 E370 I380 N381 R382 V421 A438 L444 M450 Y454 R465 L471 L513 G523 A524 D525 T526 F527 G528 S529 D530 G531 G532 E533 K534

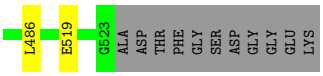
- Molecule 4: Proteasome subunit beta

Chain Y:

MET THR TRP PRO LEU PRO ASP ARG LEU SER ILE ASN SER LEU SER GLY THR PRO ALA VAL ASP LEU SER SER PHE THR ASP PHE LEU ARG ARG GLN ALA PRO GLU LEU LEU PRO ALA SER ILE SER GLY GLY ALA PRO LEU ALA GLY GLY ASP ALA GLN LEU PRO HIS GLY T301 V312

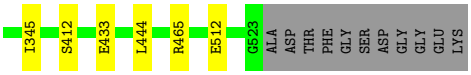
- Molecule 4: Proteasome subunit beta

Chain a:



- Molecule 4: Proteasome subunit beta

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48054	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0216	Depositor
Map size (Å)	430.144, 430.144, 430.144	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.222, 1.222, 1.222	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 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	0	0.42	0/1683	0.57	0/2274
1	2	0.41	0/1683	0.57	0/2274
1	4	0.41	0/1683	0.57	0/2274
1	6	0.42	0/1683	0.56	0/2274
1	8	0.43	0/1683	0.58	0/2274
1	I	0.36	0/1675	0.53	0/2263
1	K	0.35	0/1693	0.51	0/2287
1	O	0.35	0/1683	0.53	0/2274
1	Q	0.37	0/1683	0.53	0/2274
1	T	0.36	0/1675	0.52	0/2263
1	X	0.35	0/1675	0.52	0/2263
1	Z	0.38	0/1683	0.54	0/2274
1	d	0.42	0/1683	0.59	0/2274
1	f	0.46	0/1683	0.59	0/2274
2	1	0.57	0/42	0.55	0/54
2	A	0.27	0/3724	0.43	0/5033
2	B	0.27	0/3761	0.42	0/5085
2	C	0.30	0/3745	0.44	0/5062
2	D	0.34	0/3643	0.47	0/4923
2	E	0.30	0/3837	0.44	0/5189
2	F	0.29	0/3835	0.43	0/5186
3	G	0.23	0/111	0.44	0/143
4	H	0.38	0/1660	0.58	0/2251
4	J	0.39	0/1664	0.58	0/2256
4	L	0.40	0/1660	0.59	0/2251
4	M	0.38	0/1660	0.57	0/2251
4	N	0.39	0/1660	0.58	0/2251
4	P	0.39	0/1664	0.59	0/2256
4	R	0.39	0/1660	0.58	0/2251
4	S	0.38	0/1660	0.58	0/2251
4	U	0.40	0/1740	0.58	0/2357
4	V	0.39	0/1664	0.58	0/2256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	W	0.38	0/1740	0.56	0/2357
4	Y	0.39	0/1664	0.60	0/2256
4	a	0.40	0/1664	0.59	0/2256
4	b	0.38	0/1664	0.57	0/2256
All	All	0.36	0/69670	0.53	0/94247

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	378	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1658	0	1659	46	0
1	2	1658	0	1659	28	0
1	4	1658	0	1659	51	0
1	6	1658	0	1659	19	0
1	8	1658	0	1659	27	0
1	I	1650	0	1648	35	0
1	K	1668	0	1667	29	0
1	O	1658	0	1659	24	0
1	Q	1658	0	1659	27	0
1	T	1650	0	1648	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1650	0	1648	26	0
1	Z	1658	0	1659	31	0
1	d	1658	0	1659	0	0
1	f	1658	0	1659	0	0
2	1	42	0	41	22	0
2	A	3665	0	3691	79	0
2	B	3701	0	3721	75	0
2	C	3685	0	3700	65	0
2	D	3584	0	3605	86	0
2	E	3775	0	3779	83	0
2	F	3773	0	3777	86	0
3	G	112	0	102	2	0
4	H	1636	0	1625	8	0
4	J	1640	0	1628	17	0
4	L	1636	0	1625	14	0
4	M	1636	0	1625	11	0
4	N	1636	0	1625	10	0
4	P	1640	0	1628	13	0
4	R	1636	0	1625	16	0
4	S	1636	0	1625	12	0
4	U	1715	0	1690	16	0
4	V	1640	0	1628	8	0
4	W	1715	0	1690	9	0
4	Y	1640	0	1628	13	0
4	a	1640	0	1628	0	0
4	b	1640	0	1628	0	0
5	A	31	0	12	3	0
5	B	31	0	12	4	0
5	C	31	0	12	4	0
5	E	31	0	12	5	0
5	F	31	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	D	27	0	12	1	0
All	All	68808	0	68587	911	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 7.

All (911) 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)
2:1:605:LEU:CD2	1:4:144:ASP:HB2	1.53	1.39
2:1:605:LEU:HD23	1:4:144:ASP:CB	1.68	1.22
1:2:13:MET:SD	2:A:605:LEU:HG	1.84	1.15
2:1:605:LEU:CD2	1:4:144:ASP:CB	2.22	1.13
2:1:605:LEU:HD23	1:4:144:ASP:HB2	1.13	1.10
2:1:605:LEU:HD21	1:4:111:PHE:CD2	1.88	1.09
1:2:111:PHE:HE2	2:A:605:LEU:HD23	1.13	1.07
2:1:605:LEU:HD22	1:4:144:ASP:HB2	1.39	1.05
1:0:111:PHE:HE2	2:D:605:LEU:HD23	1.18	1.04
1:2:111:PHE:CE2	2:A:605:LEU:HD23	1.93	1.03
1:0:13:MET:CE	2:D:605:LEU:HG	1.93	0.98
2:E:500:TYR:HA	2:E:581:ILE:HA	1.44	0.98
1:0:13:MET:HE2	2:D:605:LEU:HG	1.48	0.96
1:0:111:PHE:CE2	2:D:605:LEU:HD23	2.00	0.95
1:0:13:MET:HE1	2:D:605:LEU:CD2	1.99	0.93
1:0:13:MET:HE1	2:D:605:LEU:HD21	1.51	0.92
2:1:605:LEU:HD22	1:4:144:ASP:O	1.71	0.90
2:1:605:LEU:CD2	1:4:144:ASP:CA	2.54	0.85
1:0:13:MET:HE1	2:D:605:LEU:CG	2.07	0.84
1:X:42:VAL:HG22	1:X:210:VAL:HG22	1.62	0.82
2:C:284:ARG:HE	2:C:285:PRO:HD2	1.44	0.82
1:I:185:VAL:HG21	1:I:234:LEU:HD11	1.59	0.82
2:1:605:LEU:CD2	1:4:111:PHE:CD2	2.62	0.82
2:C:563:ASN:HB3	2:C:567:PRO:HG3	1.62	0.82
1:2:111:PHE:HE2	2:A:605:LEU:CD2	1.94	0.80
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.64	0.80
2:A:430:ARG:HE	2:A:430:ARG:H	1.30	0.80
1:0:13:MET:CE	2:D:605:LEU:CG	2.61	0.79
4:J:509:ARG:NH1	4:J:512:GLU:OE1	2.14	0.79
1:0:13:MET:CE	2:D:605:LEU:CD2	2.60	0.79
1:K:140:ARG:NH1	1:K:154:VAL:HG13	1.99	0.78
2:E:377:PHE:HB3	2:E:421:ILE:HA	1.66	0.78
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.65	0.77
1:8:14:ARG:HG3	2:F:503:GLY:HA3	1.65	0.77
1:Z:31:VAL:HG12	1:Z:155:VAL:HG22	1.66	0.77
1:I:140:ARG:NH1	1:I:154:VAL:HG13	2.00	0.77
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.67	0.77
1:T:140:ARG:NH1	1:T:154:VAL:HG13	2.00	0.77
1:2:111:PHE:CE2	2:A:605:LEU:CD2	2.67	0.76
2:1:605:LEU:HD22	1:4:144:ASP:CA	2.15	0.76
1:Z:140:ARG:NH1	1:Z:154:VAL:HG13	2.00	0.76
1:I:42:VAL:HG22	1:I:210:VAL:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:140:ARG:NH1	1:X:154:VAL:HG13	2.01	0.75
1:O:140:ARG:NH1	1:O:154:VAL:HG13	2.00	0.75
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.67	0.75
1:T:31:VAL:HG12	1:T:155:VAL:HG22	1.69	0.75
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.69	0.75
1:X:31:VAL:HG12	1:X:155:VAL:HG22	1.68	0.75
1:Q:140:ARG:NH1	1:Q:154:VAL:HG13	2.02	0.74
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.69	0.74
1:O:42:VAL:HG22	1:O:210:VAL:HG22	1.68	0.74
2:1:605:LEU:HD21	1:4:111:PHE:CG	2.22	0.74
1:T:42:VAL:HG22	1:T:210:VAL:HG22	1.68	0.74
1:0:13:MET:HE1	2:D:605:LEU:HG	1.70	0.73
4:V:362:GLU:OE2	4:V:382:ARG:HD3	1.89	0.72
2:1:605:LEU:HD22	1:4:144:ASP:CB	2.04	0.71
1:Z:42:VAL:HG22	1:Z:210:VAL:HG22	1.71	0.71
2:B:561:LEU:HD13	2:E:426:LEU:HD13	1.72	0.71
2:A:243:LEU:HD21	2:A:330:LEU:HA	1.71	0.71
2:F:378:ARG:HB2	2:F:389:GLU:HB3	1.73	0.71
1:0:111:PHE:CE2	2:D:605:LEU:CD2	2.73	0.70
5:B:701:ATP:O1B	2:E:427:ARG:NH1	2.24	0.70
1:0:111:PHE:HE2	2:D:605:LEU:CD2	1.99	0.70
2:E:482:VAL:HG13	2:E:551:ILE:HD11	1.74	0.69
1:X:74:LEU:HD23	1:X:122:LEU:HD11	1.75	0.69
2:F:482:VAL:HG13	2:F:551:ILE:HD11	1.74	0.68
2:B:397:LEU:HD21	2:B:425:ILE:HG12	1.75	0.68
2:B:567:PRO:HA	2:B:570:TRP:HD1	1.59	0.68
2:1:605:LEU:HD22	1:4:144:ASP:C	2.14	0.67
2:B:554:GLU:OE2	2:B:558:ASN:ND2	2.27	0.67
2:1:605:LEU:HD23	1:4:144:ASP:HB3	1.70	0.67
5:E:701:ATP:O1B	2:F:427:ARG:NH2	2.28	0.67
2:C:401:ASP:OD2	2:C:427:ARG:NH1	2.28	0.67
2:D:534:VAL:HG22	2:D:540:PRO:HA	1.77	0.67
2:C:482:VAL:HG13	2:C:551:ILE:HD11	1.76	0.66
1:8:144:ASP:HB3	2:E:606:GLY:H	1.61	0.66
2:D:355:ARG:HE	2:D:359:LYS:HZ3	1.43	0.66
2:E:501:ALA:HB3	2:E:579:GLU:HB3	1.77	0.66
2:E:175:LEU:HD11	2:E:183:GLU:HB3	1.77	0.66
2:E:554:GLU:O	2:E:558:ASN:ND2	2.28	0.65
1:I:8:SER:HB3	1:I:9:PRO:HD3	1.79	0.65
1:0:68:PHE:HB3	2:A:607:GLN:HG3	1.79	0.64
1:2:74:LEU:HD23	1:2:122:LEU:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:181:LEU:HD22	1:Z:233:LEU:HD23	1.79	0.64
2:D:328:TYR:HB2	2:D:366:VAL:HG22	1.78	0.64
4:R:362:GLU:OE2	4:R:382:ARG:HD3	1.98	0.64
2:F:177:VAL:HG12	2:F:183:GLU:HG2	1.80	0.64
1:6:74:LEU:HD23	1:6:122:LEU:HD11	1.79	0.64
2:A:173:ARG:HH11	2:D:157:ALA:HB1	1.62	0.63
1:0:85:ARG:HH12	1:0:98:GLN:NE2	1.96	0.63
2:D:359:LYS:HB3	2:D:366:VAL:HG21	1.78	0.63
2:C:401:ASP:HB2	2:C:430:ARG:HH11	1.61	0.63
2:E:339:ASN:HD22	2:E:344:GLU:HG2	1.64	0.63
2:F:290:LEU:HB2	2:F:431:LEU:HD23	1.80	0.63
2:B:385:SER:HB2	2:E:387:ASP:H	1.62	0.63
1:8:140:ARG:NH1	1:8:154:VAL:HG13	2.13	0.63
1:0:13:MET:CE	2:D:605:LEU:HD21	2.27	0.63
2:D:292:TYR:CE2	2:D:436:LYS:HG2	2.34	0.63
1:I:217:ARG:HG3	1:I:218:PRO:HD2	1.81	0.63
1:0:74:LEU:HD23	1:0:122:LEU:HD11	1.80	0.62
2:B:139:GLN:NE2	2:B:153:GLY:O	2.31	0.62
2:A:287:LYS:HE3	2:A:430:ARG:HA	1.80	0.62
1:4:140:ARG:NH1	1:4:154:VAL:HG13	2.14	0.62
1:6:140:ARG:NH1	1:6:154:VAL:HG13	2.15	0.62
4:U:429:TRP:HZ3	4:U:431:ILE:HG13	1.65	0.62
2:1:605:LEU:CD2	1:4:144:ASP:HA	2.30	0.62
2:C:255:GLY:H	5:C:701:ATP:HN61	1.48	0.62
2:E:498:VAL:HG13	2:E:581:ILE:HD12	1.80	0.61
2:E:499:THR:HB	2:E:583:TYR:HB3	1.81	0.61
2:A:164:LEU:HA	2:A:176:VAL:HG12	1.82	0.61
2:C:164:LEU:HA	2:C:176:VAL:HG12	1.82	0.61
2:D:439:ARG:HG3	2:D:440:PRO:HD2	1.82	0.61
4:R:382:ARG:HH21	4:R:385:ILE:HD13	1.64	0.61
2:E:255:GLY:O	5:E:701:ATP:N6	2.31	0.61
4:P:362:GLU:OE2	4:P:382:ARG:HD3	2.00	0.61
2:B:212:ARG:HE	2:B:213:LYS:H	1.48	0.61
1:I:74:LEU:HD21	1:I:107:LEU:HD21	1.82	0.61
1:0:68:PHE:HD2	2:A:607:GLN:HE21	1.49	0.61
1:T:92:ARG:HH12	1:T:129:HIS:CG	2.19	0.61
1:4:74:LEU:HD23	1:4:122:LEU:HD11	1.83	0.60
1:Z:182:ARG:NH1	1:Z:234:LEU:O	2.34	0.60
2:F:377:PHE:O	2:F:378:ARG:HB2	2.01	0.60
2:B:164:LEU:HA	2:B:176:VAL:HG12	1.83	0.60
2:E:330:LEU:HD12	2:E:368:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:333:LYS:HB2	2:A:336:GLU:HG3	1.84	0.60
1:X:128:ALA:HB2	1:X:134:LYS:HB3	1.83	0.60
1:0:140:ARG:NH1	1:0:154:VAL:HG13	2.17	0.60
2:B:137:LYS:N	2:B:190:ASP:OD1	2.34	0.60
1:8:74:LEU:HD23	1:8:122:LEU:HD11	1.83	0.59
2:A:249:VAL:HG21	2:A:304:LYS:HG3	1.84	0.59
1:2:140:ARG:NH1	1:2:154:VAL:HG13	2.17	0.59
2:E:112:THR:HG22	2:E:125:THR:HG22	1.84	0.59
2:F:255:GLY:O	5:F:701:ATP:N6	2.35	0.59
1:2:85:ARG:HH12	1:2:98:GLN:NE2	1.99	0.59
2:B:266:ASP:HA	2:B:270:LEU:HD13	1.85	0.59
2:B:248:ASP:N	2:B:248:ASP:OD1	2.35	0.59
1:2:31:VAL:HG12	1:2:155:VAL:HG22	1.84	0.59
5:A:701:ATP:O2G	2:B:430:ARG:NH2	2.36	0.59
2:B:532:LYS:HE2	2:E:270:LEU:HD22	1.85	0.59
1:Z:128:ALA:HB2	1:Z:134:LYS:HB3	1.84	0.59
1:4:45:ASN:ND2	1:4:209:GLU:OE1	2.35	0.59
2:B:296:GLY:HA3	2:E:427:ARG:HD2	1.84	0.59
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.84	0.59
4:R:382:ARG:NH2	4:R:385:ILE:HD13	2.18	0.59
1:T:74:LEU:HD21	1:T:107:LEU:HD21	1.85	0.59
2:A:251:TYR:HD2	2:A:265:ARG:HH21	1.52	0.58
1:4:189:ARG:NH1	1:4:203:LEU:N	2.52	0.58
1:8:85:ARG:HH12	1:8:98:GLN:NE2	2.01	0.58
2:B:333:LYS:HB2	2:B:336:GLU:HB2	1.86	0.58
1:2:45:ASN:ND2	1:2:209:GLU:OE1	2.36	0.58
2:A:259:ARG:NH2	2:A:262:GLU:OE1	2.31	0.58
2:B:175:LEU:HD11	2:B:183:GLU:HB2	1.85	0.58
2:E:520:GLN:NE2	2:E:524:ASP:OD2	2.36	0.58
2:E:247:PRO:HG2	2:E:304:LYS:HB2	1.86	0.58
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.85	0.58
1:X:30:VAL:HG13	1:X:43:ALA:HB2	1.84	0.58
2:E:563:ASN:HB2	2:F:419:ASP:HB2	1.84	0.58
1:0:189:ARG:NH1	1:0:203:LEU:N	2.52	0.57
1:6:128:ALA:HB2	1:6:134:LYS:HB3	1.86	0.57
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.85	0.57
1:6:31:VAL:HG12	1:6:155:VAL:HG22	1.85	0.57
2:C:279:ARG:NH2	2:C:283:LEU:O	2.36	0.57
4:U:424:ASP:OD1	4:U:426:ALA:N	2.35	0.57
1:6:45:ASN:ND2	1:6:209:GLU:OE1	2.37	0.57
2:A:112:THR:HG22	2:A:125:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:339:ASN:HB3	2:D:344:GLU:HB3	1.86	0.57
1:4:31:VAL:HG12	1:4:155:VAL:HG22	1.85	0.57
2:B:255:GLY:O	5:B:701:ATP:N6	2.36	0.57
2:F:115:VAL:HG21	2:F:143:LEU:HD21	1.86	0.57
4:L:429:TRP:HZ3	4:L:431:ILE:HG13	1.70	0.57
1:6:189:ARG:NH1	1:6:203:LEU:N	2.52	0.57
2:D:490:ILE:O	2:D:494:ARG:NH1	2.38	0.57
2:A:213:LYS:O	2:A:215:ARG:NH1	2.37	0.57
2:C:295:PRO:HG3	2:C:416:ASN:HD22	1.69	0.57
1:Q:74:LEU:HD21	1:Q:107:LEU:HD21	1.86	0.57
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.86	0.57
1:Z:30:VAL:HG13	1:Z:43:ALA:HB2	1.86	0.57
1:O:74:LEU:HD21	1:O:107:LEU:HD21	1.86	0.57
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.85	0.57
2:C:389:GLU:HA	2:C:392:VAL:HG12	1.87	0.57
1:2:24:ILE:HG22	1:2:157:GLY:HA2	1.86	0.57
1:2:189:ARG:NH1	1:2:203:LEU:N	2.53	0.57
2:A:365:PRO:HA	2:A:408:ASN:HD22	1.69	0.57
2:D:291:LEU:HD23	2:D:435:ILE:HB	1.87	0.57
2:E:377:PHE:CG	2:E:421:ILE:HG23	2.40	0.57
2:A:378:ARG:O	2:A:422:ASP:N	2.37	0.56
1:8:31:VAL:HG12	1:8:155:VAL:HG22	1.87	0.56
2:B:299:LYS:HG2	2:B:437:ILE:HD13	1.86	0.56
2:B:377:PHE:HD2	2:B:425:ILE:HD13	1.70	0.56
4:Y:320:SER:HB3	4:Y:331:VAL:HG21	1.88	0.56
1:Z:74:LEU:HD21	1:Z:107:LEU:HD21	1.87	0.56
2:A:439:ARG:NH2	2:A:569:ASP:OD2	2.38	0.56
4:J:429:TRP:HZ3	4:J:431:ILE:HG13	1.70	0.56
4:U:320:SER:HB3	4:U:331:VAL:HG21	1.88	0.56
2:A:284:ARG:NH1	2:A:404:GLU:OE2	2.39	0.56
2:D:338:LEU:HG	2:D:340:LYS:HG3	1.87	0.56
1:8:189:ARG:NH1	1:8:203:LEU:N	2.53	0.56
1:K:140:ARG:HH11	1:K:154:VAL:HG13	1.69	0.56
1:X:74:LEU:HD21	1:X:107:LEU:HD21	1.88	0.56
4:Y:424:ASP:OD1	4:Y:426:ALA:N	2.37	0.56
1:8:128:ALA:HB2	1:8:134:LYS:HB3	1.87	0.56
2:D:497:GLU:HG3	2:D:585:ARG:HB3	1.88	0.56
1:K:74:LEU:HD21	1:K:107:LEU:HD21	1.88	0.56
4:S:465:ARG:HG3	4:S:513:LEU:HD22	1.87	0.56
2:1:605:LEU:HG	1:4:111:PHE:CE2	2.40	0.56
1:0:31:VAL:HG12	1:0:155:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.87	0.56
1:T:16:ARG:NH2	1:T:114:GLN:O	2.27	0.56
2:E:569:ASP:HB3	2:E:572:ARG:HH21	1.70	0.55
1:Q:189:ARG:NH1	1:Q:203:LEU:N	2.54	0.55
2:1:605:LEU:CG	1:4:111:PHE:CD2	2.89	0.55
1:4:85:ARG:HH12	1:4:98:GLN:NE2	2.05	0.55
2:F:255:GLY:H	5:F:701:ATP:HN61	1.55	0.55
2:F:534:VAL:HG22	2:F:540:PRO:HA	1.87	0.55
4:J:320:SER:HB3	4:J:331:VAL:HG21	1.87	0.55
4:U:432:GLU:OE2	4:U:433:GLU:N	2.39	0.55
2:A:349:ILE:HG21	2:A:396:LEU:HD21	1.89	0.55
2:C:525:ARG:HD3	2:C:553:ASP:HB3	1.88	0.55
4:L:320:SER:HB3	4:L:331:VAL:HG21	1.88	0.55
1:4:128:ALA:HB2	1:4:134:LYS:HB3	1.89	0.55
1:6:68:PHE:HA	1:6:71:PHE:CE2	2.41	0.55
2:A:486:MET:HG3	2:A:555:PHE:HZ	1.71	0.55
2:D:417:ARG:HH22	2:D:575:GLY:HA3	1.72	0.55
4:Y:429:TRP:HZ3	4:Y:431:ILE:HG13	1.72	0.55
2:F:436:LYS:HE2	2:F:572:ARG:HH21	1.71	0.55
2:B:539:GLN:OE1	2:B:543:ARG:NH2	2.39	0.55
1:I:174:ASN:N	1:I:174:ASN:HD22	2.05	0.55
2:E:574:SER:HB2	2:E:580:ARG:HA	1.88	0.55
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.42	0.55
2:A:168:LEU:HD12	2:A:173:ARG:HB2	1.88	0.54
2:C:291:LEU:HD13	2:C:435:ILE:HB	1.89	0.54
2:C:301:LEU:HD11	5:C:701:ATP:H2'	1.89	0.54
2:F:120:ARG:NH1	2:F:122:MET:SD	2.81	0.54
2:B:107:THR:HA	2:B:113:VAL:HG12	1.90	0.54
2:C:157:ALA:HB1	2:D:173:ARG:HH11	1.72	0.54
2:D:168:LEU:HD12	2:D:173:ARG:HB2	1.89	0.54
2:F:509:TYR:HB2	2:F:511:LYS:HG2	1.88	0.54
1:T:140:ARG:HH11	1:T:154:VAL:HG13	1.73	0.54
1:0:45:ASN:ND2	1:0:209:GLU:OE1	2.40	0.54
2:B:160:GLU:OE2	2:E:184:ARG:NH2	2.40	0.54
4:P:320:SER:HB3	4:P:331:VAL:HG21	1.89	0.54
1:2:128:ALA:HB2	1:2:134:LYS:HB3	1.89	0.54
2:D:187:TRP:HB2	2:D:228:TYR:CE1	2.42	0.54
1:O:150:GLU:HG3	1:O:154:VAL:HG22	1.90	0.54
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.89	0.54
1:8:45:ASN:ND2	1:8:209:GLU:OE1	2.41	0.54
2:D:187:TRP:HB2	2:D:228:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:VAL:HG13	2:C:394:PRO:HD3	1.89	0.54
2:E:300:THR:OG1	5:E:701:ATP:O2B	2.25	0.54
2:F:496:LEU:HD11	2:F:562:PRO:HB3	1.89	0.54
1:T:181:LEU:HD23	1:T:233:LEU:HB3	1.89	0.54
1:0:128:ALA:HB2	1:0:134:LYS:HB3	1.88	0.54
2:A:500:TYR:HE2	2:A:506:GLU:HB2	1.73	0.54
1:O:177:LEU:HG	1:O:233:LEU:HD21	1.90	0.54
2:A:530:ALA:O	2:A:534:VAL:HG13	2.09	0.53
2:D:340:LYS:H	2:D:340:LYS:HD2	1.72	0.53
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.43	0.53
2:E:187:TRP:HB2	2:E:228:TYR:CE1	2.43	0.53
2:E:249:VAL:HG11	2:E:304:LYS:HG3	1.90	0.53
1:K:89:TYR:CE1	4:R:382:ARG:HD2	2.43	0.53
1:Z:140:ARG:HH11	1:Z:154:VAL:HG13	1.70	0.53
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.89	0.53
2:F:497:GLU:HG2	2:F:585:ARG:HH21	1.74	0.53
4:J:424:ASP:OD1	4:J:426:ALA:N	2.41	0.53
2:D:561:LEU:HB2	2:D:562:PRO:HD3	1.91	0.53
2:E:158:VAL:HA	2:F:185:VAL:HG23	1.91	0.53
1:O:69:ASN:HD22	1:O:69:ASN:H	1.56	0.53
1:T:92:ARG:NH1	1:T:129:HIS:CG	2.77	0.53
2:D:211:PRO:N	2:D:212:ARG:HA	2.23	0.53
2:D:288:GLY:HA3	2:D:431:LEU:HA	1.90	0.53
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.44	0.53
2:F:140:THR:HG23	2:F:155:PHE:HB2	1.91	0.53
1:O:110:ILE:HA	1:O:114:GLN:HG3	1.91	0.53
1:X:140:ARG:HH11	1:X:154:VAL:HG13	1.74	0.53
1:8:89:TYR:CD1	4:N:382:ARG:HD3	2.44	0.53
2:F:494:ARG:HB3	2:F:587:LEU:HD12	1.90	0.53
2:A:211:PRO:N	2:A:212:ARG:HA	2.24	0.52
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.44	0.52
1:T:30:VAL:HG13	1:T:43:ALA:HB2	1.89	0.52
1:4:68:PHE:HB3	2:B:607:GLN:HG3	1.91	0.52
2:A:576:LYS:O	2:D:566:ASN:ND2	2.38	0.52
2:A:136:LYS:HB3	2:A:190:ASP:HB2	1.91	0.52
2:A:523:VAL:HG12	2:A:527:LYS:HE2	1.91	0.52
2:E:455:GLU:HA	2:E:475:ILE:HD12	1.89	0.52
2:E:487:TYR:OH	2:E:514:ASN:ND2	2.39	0.52
2:F:162:SER:HB3	2:F:176:VAL:HB	1.91	0.52
1:I:8:SER:CB	1:I:9:PRO:HD3	2.39	0.52
2:D:489:GLU:N	2:D:489:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.90	0.52
2:F:502:ASN:HD21	2:F:577:LYS:HE3	1.75	0.52
1:I:140:ARG:HH11	1:I:154:VAL:HG13	1.71	0.52
1:I:178:THR:HG22	1:I:182:ARG:HE	1.74	0.52
1:I:182:ARG:HH11	1:I:234:LEU:HD23	1.75	0.52
1:Q:18:GLU:OE2	1:Q:18:GLU:HA	2.10	0.52
2:D:436:LYS:HD3	2:D:437:ILE:H	1.74	0.52
2:D:105:LEU:HD11	2:D:121:LYS:HD2	1.91	0.52
1:T:11:GLN:O	1:T:15:GLU:HG2	2.10	0.52
1:K:150:GLU:HG3	1:K:154:VAL:HG22	1.92	0.52
2:B:288:GLY:HA3	2:B:431:LEU:HA	1.91	0.52
2:F:373:MET:HA	2:F:376:ILE:HB	1.91	0.52
2:C:404:GLU:OE2	2:F:331:ASN:ND2	2.43	0.51
2:D:107:THR:HA	2:D:113:VAL:HG12	1.92	0.51
1:Z:150:GLU:HG3	1:Z:154:VAL:HG22	1.92	0.51
1:Z:165:ASN:O	1:Z:169:GLU:HG2	2.09	0.51
1:4:68:PHE:HA	1:4:71:PHE:CE2	2.45	0.51
2:E:384:VAL:HB	2:F:387:ASP:HB2	1.91	0.51
2:A:276:GLU:HG3	2:A:277:LEU:HD12	1.92	0.51
2:A:384:VAL:HG12	2:B:386:SER:HA	1.92	0.51
2:C:243:LEU:HD23	2:C:243:LEU:H	1.75	0.51
2:E:502:ASN:HD22	2:E:579:GLU:HB2	1.74	0.51
2:B:386:SER:OG	3:G:5:GLN:N	2.43	0.51
1:I:123:CYS:HA	1:I:139:TYR:O	2.11	0.51
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.92	0.51
4:R:359:TYR:CE1	4:R:383:LEU:HB2	2.45	0.51
1:Z:90:ASP:OD1	1:Z:91:ARG:N	2.44	0.51
2:B:177:VAL:HG12	2:B:183:GLU:HB3	1.93	0.51
2:D:429:GLY:N	2:D:432:ASP:OD1	2.43	0.51
1:I:69:ASN:H	1:I:69:ASN:HD22	1.58	0.51
1:I:150:GLU:HG3	1:I:154:VAL:HG22	1.93	0.51
1:Z:68:PHE:HA	1:Z:71:PHE:CE2	2.46	0.51
2:F:361:SER:HB3	2:F:364:THR:HB	1.92	0.51
2:F:488:ALA:O	2:F:493:ASN:ND2	2.44	0.51
2:B:424:ALA:O	2:B:430:ARG:NH1	2.44	0.51
1:K:90:ASP:OD1	1:K:91:ARG:N	2.44	0.51
2:A:585:ARG:NH1	2:B:575:GLY:O	2.44	0.51
2:B:255:GLY:H	5:B:701:ATP:HN61	1.57	0.51
2:C:177:VAL:HG22	2:C:183:GLU:HG2	1.93	0.51
2:E:321:ASP:HB2	2:E:324:GLU:HG2	1.93	0.51
1:I:11:GLN:O	1:I:15:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:429:TRP:HZ3	4:P:431:ILE:HG13	1.77	0.51
1:0:68:PHE:HA	1:0:71:PHE:CE2	2.46	0.50
1:6:85:ARG:HH12	1:6:98:GLN:NE2	2.08	0.50
2:C:186:VAL:HA	2:F:158:VAL:HG12	1.92	0.50
2:C:222:VAL:HG12	2:C:229:ALA:HA	1.93	0.50
4:N:329:ARG:NH2	4:U:476:ASP:O	2.44	0.50
1:Q:123:CYS:HA	1:Q:139:TYR:O	2.11	0.50
2:A:170:ASP:OD2	2:A:173:ARG:NE	2.43	0.50
2:D:292:TYR:O	2:D:436:LYS:HA	2.11	0.50
4:R:320:SER:HB3	4:R:331:VAL:HG21	1.92	0.50
2:E:255:GLY:H	5:E:701:ATP:HN61	1.59	0.50
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.92	0.50
1:Z:118:TYR:HB3	1:Z:120:VAL:HG22	1.93	0.50
1:K:69:ASN:H	1:K:69:ASN:HD22	1.57	0.50
4:L:424:ASP:OD1	4:L:426:ALA:N	2.41	0.50
2:C:497:GLU:HB2	2:C:587:LEU:HD11	1.93	0.50
2:E:534:VAL:HG22	2:E:540:PRO:HA	1.93	0.50
1:T:150:GLU:HG3	1:T:154:VAL:HG22	1.94	0.50
2:E:475:ILE:HA	2:E:478:MET:HE2	1.93	0.50
2:F:136:LYS:N	2:F:139:GLN:OE1	2.37	0.50
2:B:427:ARG:HD2	2:B:428:PRO:O	2.12	0.50
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.59	0.50
1:Z:25:ALA:O	1:Z:158:GLY:HA2	2.11	0.50
1:Z:178:THR:HG22	1:Z:182:ARG:HE	1.77	0.50
1:2:13:MET:SD	2:A:605:LEU:CG	2.78	0.50
1:4:89:TYR:CD1	4:M:382:ARG:HD3	2.46	0.50
4:P:312:VAL:HG12	4:P:497:ILE:HB	1.92	0.50
1:X:41:PHE:HB3	1:X:53:ILE:HD13	1.94	0.50
1:2:89:TYR:CD1	4:S:382:ARG:HD3	2.47	0.49
4:R:424:ASP:OD1	4:R:426:ALA:N	2.45	0.49
1:T:69:ASN:HD22	1:T:69:ASN:H	1.59	0.49
2:B:144:ASN:ND2	2:B:148:THR:O	2.45	0.49
2:F:388:VAL:O	2:F:392:VAL:HG22	2.13	0.49
1:0:89:TYR:CD1	4:W:382:ARG:HD3	2.47	0.49
1:6:89:TYR:CD1	4:H:382:ARG:HD3	2.47	0.49
2:A:488:ALA:O	2:A:493:ASN:ND2	2.46	0.49
2:B:393:VAL:HG12	2:B:394:PRO:HD3	1.93	0.49
2:C:294:PRO:O	2:C:299:LYS:NZ	2.45	0.49
2:E:112:THR:OG1	2:E:123:ARG:NH1	2.40	0.49
5:E:701:ATP:O2G	2:F:430:ARG:NH1	2.40	0.49
1:I:142:THR:OG1	1:I:144:ASP:OD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:92:ARG:NH1	1:X:129:HIS:CD2	2.80	0.49
2:A:496:LEU:HB2	2:A:508:MET:HB2	1.95	0.49
2:B:105:LEU:HD11	2:B:116:PHE:HB2	1.94	0.49
2:D:255:GLY:H	7:D:701:ADP:HN62	1.60	0.49
2:D:495:PHE:HB2	2:D:510:PHE:HE1	1.76	0.49
4:J:312:VAL:HG12	4:J:497:ILE:HB	1.94	0.49
1:X:68:PHE:HA	1:X:71:PHE:CE2	2.48	0.49
2:A:357:ARG:NH1	2:A:399:GLU:OE2	2.38	0.49
2:C:531:ILE:HD11	2:D:283:LEU:HD21	1.95	0.49
1:K:68:PHE:HA	1:K:71:PHE:CE2	2.47	0.49
1:O:123:CYS:HA	1:O:139:TYR:O	2.13	0.49
2:D:436:LYS:HD3	2:D:437:ILE:N	2.28	0.49
1:I:55:GLU:HB2	1:I:222:PHE:CG	2.47	0.49
2:F:235:LYS:HG2	2:F:351:LEU:HD13	1.95	0.49
2:F:361:SER:O	2:F:408:ASN:ND2	2.40	0.49
1:4:70:GLU:HB3	1:4:118:TYR:CD2	2.48	0.49
2:A:104:LEU:HD11	2:A:113:VAL:HB	1.94	0.49
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.95	0.49
1:T:18:GLU:OE2	1:T:18:GLU:HA	2.12	0.49
2:F:339:ASN:OD1	2:F:340:LYS:N	2.46	0.49
4:M:465:ARG:HG3	4:M:513:LEU:HD22	1.94	0.49
2:A:164:LEU:HB2	2:A:220:LEU:HD13	1.93	0.49
1:T:55:GLU:HB2	1:T:222:PHE:CG	2.48	0.49
1:4:33:LEU:HD12	1:4:40:LEU:HB3	1.94	0.48
2:B:290:LEU:HD22	2:B:426:LEU:HD22	1.95	0.48
4:U:459:ASP:OD1	4:U:461:ASP:N	2.44	0.48
1:2:33:LEU:HD12	1:2:40:LEU:HB3	1.94	0.48
2:D:164:LEU:HA	2:D:176:VAL:HG12	1.94	0.48
2:E:129:ASN:OD1	2:E:130:ILE:N	2.47	0.48
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.75	0.48
1:6:110:ILE:HG21	1:6:118:TYR:CD1	2.47	0.48
2:A:391:THR:O	2:A:395:GLN:NE2	2.41	0.48
2:B:289:VAL:HB	2:B:412:ILE:HG12	1.95	0.48
1:8:33:LEU:HD12	1:8:40:LEU:HB3	1.93	0.48
1:8:69:ASN:HD22	1:8:69:ASN:H	1.61	0.48
2:B:427:ARG:HH11	2:B:430:ARG:NH2	2.10	0.48
2:D:481:LYS:O	2:D:485:ARG:HG2	2.13	0.48
2:E:566:ASN:O	2:E:566:ASN:ND2	2.46	0.48
4:R:312:VAL:HG12	4:R:497:ILE:HB	1.94	0.48
1:T:178:THR:HG22	1:T:182:ARG:HE	1.76	0.48
1:Z:214:ASP:OD2	1:Z:217:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:TYR:CZ	2:B:436:LYS:HB2	2.49	0.48
2:D:144:ASN:HD21	2:D:148:THR:HB	1.78	0.48
1:6:33:LEU:HD12	1:6:40:LEU:HB3	1.94	0.48
4:L:382:ARG:HD3	1:X:89:TYR:CD1	2.48	0.48
1:0:50:LEU:HB3	2:A:609:LEU:HD11	1.95	0.48
1:0:68:PHE:CD1	2:A:609:LEU:HD12	2.49	0.48
2:B:416:ASN:HD22	2:B:566:ASN:HD21	1.61	0.48
4:L:459:ASP:OD1	4:L:461:ASP:N	2.44	0.48
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.96	0.48
4:W:465:ARG:HG3	4:W:513:LEU:HD22	1.95	0.48
2:B:272:PHE:CZ	2:B:365:PRO:HB3	2.48	0.48
2:C:175:LEU:HD23	2:F:236:ALA:HB2	1.95	0.48
2:F:457:LEU:HD21	2:F:527:LYS:HE2	1.95	0.48
1:I:182:ARG:HD2	1:I:234:LEU:HD23	1.94	0.48
4:P:359:TYR:CE1	4:P:383:LEU:HB2	2.48	0.48
1:0:178:THR:HG22	1:0:182:ARG:HE	1.79	0.48
2:B:509:TYR:HB2	2:B:511:LYS:HG2	1.96	0.48
2:F:109:ASP:N	2:F:109:ASP:OD1	2.47	0.48
2:C:142:ARG:HE	2:C:150:VAL:HG23	1.79	0.48
2:C:389:GLU:O	2:C:393:VAL:HG12	2.13	0.48
2:F:291:LEU:HD23	2:F:435:ILE:HB	1.96	0.48
4:L:359:TYR:CE1	4:L:383:LEU:HB2	2.49	0.48
2:D:494:ARG:HD3	2:D:507:VAL:HG11	1.94	0.47
2:E:362:GLU:OE1	2:E:408:ASN:ND2	2.47	0.47
2:F:377:PHE:HB3	2:F:392:VAL:HG23	1.96	0.47
1:Q:90:ASP:OD1	1:Q:91:ARG:N	2.47	0.47
4:U:312:VAL:HG12	4:U:497:ILE:HB	1.96	0.47
1:X:92:ARG:HD3	1:X:129:HIS:CE1	2.49	0.47
1:X:123:CYS:HA	1:X:139:TYR:O	2.14	0.47
1:Z:69:ASN:H	1:Z:69:ASN:HD22	1.61	0.47
1:4:110:ILE:HG21	1:4:118:TYR:CD1	2.49	0.47
2:E:310:LEU:HD22	2:E:367:ILE:HD12	1.96	0.47
2:E:561:LEU:N	2:E:562:PRO:HD3	2.30	0.47
2:F:212:ARG:NH2	2:F:360:ALA:O	2.47	0.47
1:O:55:GLU:HB2	1:O:222:PHE:CG	2.49	0.47
1:0:24:ILE:HG22	1:0:157:GLY:HA2	1.95	0.47
2:A:482:VAL:HG11	2:A:547:LEU:HD13	1.95	0.47
2:B:349:ILE:HD12	2:B:396:LEU:HD21	1.95	0.47
2:F:498:VAL:HG13	2:F:581:ILE:HG23	1.96	0.47
4:R:475:ALA:HA	4:R:481:THR:HB	1.95	0.47
4:R:476:ASP:O	4:S:329:ARG:NH2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:TYR:CD1	4:U:382:ARG:HD3	2.49	0.47
4:P:424:ASP:OD1	4:P:426:ALA:N	2.46	0.47
2:B:367:ILE:HD13	2:B:410:ILE:HB	1.94	0.47
2:B:436:LYS:HE2	2:B:438:GLU:HG2	1.97	0.47
2:C:447:ASP:O	2:C:451:LYS:HG2	2.14	0.47
1:Q:140:ARG:HH11	1:Q:154:VAL:HG13	1.75	0.47
4:R:429:TRP:HZ3	4:R:431:ILE:HG13	1.79	0.47
4:Y:312:VAL:HG12	4:Y:497:ILE:HB	1.97	0.47
4:L:312:VAL:HG12	4:L:497:ILE:HB	1.96	0.47
1:0:33:LEU:HD21	1:0:184:ALA:HB2	1.96	0.47
1:8:182:ARG:NH1	1:8:234:LEU:O	2.48	0.47
2:B:187:TRP:HB2	2:B:228:TYR:CE1	2.50	0.47
2:E:378:ARG:NE	2:E:389:GLU:HG2	2.29	0.47
2:E:408:ASN:OD1	2:E:408:ASN:N	2.47	0.47
2:F:525:ARG:NH1	2:F:553:ASP:OD2	2.48	0.47
1:I:185:VAL:O	1:I:189:ARG:HG3	2.14	0.47
4:J:382:ARG:HD3	1:O:89:TYR:CD1	2.50	0.47
1:Q:33:LEU:HD12	1:Q:40:LEU:HB3	1.96	0.47
1:Z:123:CYS:HA	1:Z:139:TYR:O	2.15	0.47
1:2:111:PHE:CD2	2:A:605:LEU:CD2	2.98	0.47
1:2:178:THR:HG22	1:2:182:ARG:HE	1.80	0.47
2:D:460:HIS:CE1	2:D:543:ARG:HH11	2.33	0.47
1:K:123:CYS:HA	1:K:139:TYR:O	2.14	0.47
1:Z:55:GLU:HB2	1:Z:222:PHE:CG	2.50	0.47
4:H:344:GLY:C	4:H:345:ILE:HG12	2.35	0.47
1:T:90:ASP:OD1	1:T:91:ARG:N	2.47	0.47
1:0:33:LEU:HD12	1:0:40:LEU:HB3	1.95	0.47
1:K:55:GLU:HB2	1:K:222:PHE:CG	2.50	0.47
4:N:465:ARG:HG3	4:N:513:LEU:HD22	1.97	0.47
2:A:344:GLU:HA	2:A:347:ARG:HB3	1.96	0.46
2:C:187:TRP:HE1	2:F:157:ALA:HA	1.80	0.46
2:D:264:ILE:HD11	2:D:291:LEU:HD21	1.97	0.46
2:D:417:ARG:HH12	2:D:575:GLY:HA3	1.80	0.46
1:Q:110:ILE:HA	1:Q:114:GLN:HG3	1.96	0.46
2:F:521:ASN:ND2	2:F:554:GLU:OE1	2.49	0.46
1:T:123:CYS:HA	1:T:139:TYR:O	2.15	0.46
2:1:605:LEU:HD11	1:4:111:PHE:HD2	1.79	0.46
2:F:502:ASN:HB3	2:F:579:GLU:HG3	1.96	0.46
4:L:475:ALA:HA	4:L:481:THR:HB	1.96	0.46
4:Y:459:ASP:OD1	4:Y:461:ASP:N	2.48	0.46
1:8:14:ARG:HA	1:8:14:ARG:HD3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:131:ASP:OD1	2:A:131:ASP:N	2.40	0.46
2:D:441:ASP:OD2	2:D:443:GLU:HB3	2.15	0.46
2:E:560:ASP:OD1	2:E:560:ASP:N	2.47	0.46
1:X:212:VAL:HG21	1:X:223:ARG:HH21	1.80	0.46
1:0:70:GLU:HB3	1:0:118:TYR:CD2	2.50	0.46
1:K:185:VAL:O	1:K:189:ARG:HB2	2.15	0.46
1:Z:33:LEU:HD12	1:Z:40:LEU:HB3	1.97	0.46
1:2:33:LEU:HD21	1:2:184:ALA:HB2	1.97	0.46
2:B:609:LEU:HD23	2:B:609:LEU:HA	1.78	0.46
2:C:227:GLY:HA3	2:F:158:VAL:HG11	1.97	0.46
2:D:144:ASN:ND2	2:D:148:THR:O	2.48	0.46
2:F:342:VAL:HG21	3:G:5:GLN:HG2	1.98	0.46
2:F:401:ASP:OD2	2:F:427:ARG:NH2	2.43	0.46
2:F:496:LEU:HD23	2:F:586:THR:HA	1.97	0.46
4:L:429:TRP:CZ3	4:L:431:ILE:HG13	2.51	0.46
4:N:344:GLY:C	4:N:345:ILE:HG12	2.36	0.46
2:B:473:ALA:HA	2:B:476:LYS:HE2	1.97	0.46
2:F:192:LEU:HD12	2:F:214:LEU:HD11	1.96	0.46
1:Z:18:GLU:OE2	1:Z:18:GLU:HA	2.16	0.46
1:2:57:TYR:OH	1:2:86:GLY:HA3	2.15	0.46
1:6:118:TYR:HB3	1:6:120:VAL:HG22	1.98	0.46
2:C:287:LYS:NZ	2:C:401:ASP:OD1	2.43	0.46
4:H:366:TYR:CZ	4:H:370:GLU:HG3	2.51	0.46
1:4:57:TYR:OH	1:4:86:GLY:HA3	2.16	0.46
1:8:178:THR:HG22	1:8:182:ARG:HE	1.80	0.46
2:B:372:GLU:HB3	2:E:394:PRO:HB3	1.96	0.46
2:C:296:GLY:N	5:C:701:ATP:O3G	2.48	0.46
4:J:444:LEU:HD12	4:J:444:LEU:HA	1.80	0.46
1:4:56:LEU:HD23	1:4:56:LEU:HA	1.73	0.46
1:6:57:TYR:OH	1:6:86:GLY:HA3	2.16	0.46
1:6:70:GLU:HB3	1:6:118:TYR:CD2	2.51	0.46
2:A:292:TYR:CZ	2:A:436:LYS:HB2	2.50	0.46
2:C:294:PRO:HG2	2:C:439:ARG:HG3	1.97	0.46
4:J:359:TYR:CE1	4:J:383:LEU:HB2	2.51	0.46
4:L:508:SER:O	4:L:512:GLU:HG3	2.16	0.46
1:X:55:GLU:HB2	1:X:222:PHE:CG	2.51	0.46
1:6:178:THR:HG22	1:6:182:ARG:HE	1.80	0.45
2:A:296:GLY:HA3	2:B:427:ARG:HD3	1.98	0.45
2:B:132:ALA:HA	2:B:135:LEU:HD23	1.97	0.45
2:C:213:LYS:HB3	2:C:215:ARG:HH12	1.81	0.45
4:J:429:TRP:CZ3	4:J:431:ILE:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:CYS:HA	2:D:149:VAL:HG13	1.97	0.45
2:D:173:ARG:HG2	2:D:187:TRP:CD1	2.52	0.45
2:E:232:ARG:HG2	2:E:234:PRO:HD3	1.99	0.45
2:E:431:LEU:O	2:E:434:LYS:NZ	2.31	0.45
1:O:90:ASP:OD1	1:O:91:ARG:N	2.50	0.45
1:0:30:VAL:HG13	1:0:43:ALA:HB2	1.97	0.45
1:4:8:SER:HB3	1:4:11:GLN:HB2	1.98	0.45
2:E:105:LEU:HB2	2:E:114:ASP:HB2	1.99	0.45
2:E:401:ASP:OD1	2:E:430:ARG:NE	2.49	0.45
2:F:99:SER:HB2	2:F:143:LEU:O	2.16	0.45
1:Q:11:GLN:HG2	1:Q:14:ARG:HH22	1.81	0.45
4:S:429:TRP:HZ3	4:S:431:ILE:HG13	1.82	0.45
2:1:605:LEU:HD21	1:4:144:ASP:HA	1.98	0.45
1:8:56:LEU:HD23	1:8:56:LEU:HA	1.71	0.45
2:C:495:PHE:HB2	2:C:510:PHE:CD1	2.51	0.45
2:F:192:LEU:HD21	2:F:231:GLU:HA	1.97	0.45
1:T:25:ALA:O	1:T:158:GLY:HA2	2.16	0.45
2:B:495:PHE:HE1	2:B:559:GLU:HA	1.82	0.45
2:D:245:GLU:HG2	2:D:329:PHE:HB3	1.99	0.45
2:D:281:TYR:CD2	2:D:283:LEU:HD22	2.51	0.45
2:E:378:ARG:HE	2:E:389:GLU:HG2	1.81	0.45
2:F:170:ASP:OD1	2:F:170:ASP:N	2.48	0.45
2:F:487:TYR:OH	2:F:514:ASN:ND2	2.46	0.45
2:F:570:TRP:CD1	2:F:581:ILE:HD12	2.51	0.45
4:U:475:ALA:HA	4:U:481:THR:HB	1.96	0.45
4:W:513:LEU:HD23	4:W:513:LEU:HA	1.84	0.45
4:Y:475:ALA:HA	4:Y:481:THR:HB	1.98	0.45
1:4:33:LEU:HD21	1:4:184:ALA:HB2	1.98	0.45
1:8:69:ASN:HD22	1:8:69:ASN:N	2.15	0.45
2:E:425:ILE:HD12	2:E:430:ARG:HD3	1.99	0.45
4:P:509:ARG:HA	4:P:512:GLU:OE2	2.17	0.45
1:X:69:ASN:HD22	1:X:69:ASN:H	1.63	0.45
2:F:223:ASP:O	2:F:227:GLY:N	2.44	0.45
4:N:398:LEU:N	4:N:398:LEU:HD12	2.32	0.45
1:O:69:ASN:HD22	1:O:69:ASN:N	2.15	0.45
1:0:118:TYR:HB3	1:0:120:VAL:HG22	1.99	0.45
1:8:57:TYR:OH	1:8:86:GLY:HA3	2.17	0.45
2:A:374:ASP:OD2	2:A:417:ARG:HB2	2.16	0.45
2:C:387:ASP:OD1	2:C:388:VAL:N	2.48	0.45
2:F:272:PHE:CZ	2:F:365:PRO:HB3	2.52	0.45
1:X:150:GLU:HG3	1:X:154:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:516:GLY:HA3	5:C:701:ATP:N3	2.31	0.45
1:X:33:LEU:HD12	1:X:40:LEU:HB3	1.99	0.45
1:X:172:ALA:HB3	1:X:175:ALA:HB2	1.98	0.45
1:2:30:VAL:HG13	1:2:43:ALA:HB2	1.98	0.44
1:4:118:TYR:HB3	1:4:120:VAL:HG22	1.99	0.44
1:4:178:THR:HG22	1:4:182:ARG:HE	1.82	0.44
1:8:68:PHE:HA	1:8:71:PHE:CE2	2.52	0.44
2:A:374:ASP:OD1	2:A:415:SER:OG	2.29	0.44
2:B:432:ASP:N	2:B:432:ASP:OD1	2.50	0.44
2:D:425:ILE:HD11	2:D:431:LEU:HD13	1.99	0.44
2:F:376:ILE:HD12	2:F:376:ILE:HA	1.86	0.44
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.99	0.44
1:I:56:LEU:HG	1:I:62:PHE:HB2	1.99	0.44
1:K:33:LEU:HD12	1:K:40:LEU:HB3	1.99	0.44
1:O:41:PHE:HB3	1:O:53:ILE:HD13	1.99	0.44
1:T:69:ASN:HD22	1:T:69:ASN:N	2.15	0.44
4:R:307:LYS:NZ	4:R:419:ARG:HA	2.32	0.44
4:V:366:TYR:CZ	4:V:370:GLU:HG3	2.52	0.44
1:0:57:TYR:OH	1:0:86:GLY:HA3	2.16	0.44
2:C:527:LYS:O	2:C:531:ILE:HG13	2.17	0.44
2:C:567:PRO:HD2	2:C:570:TRP:HB2	1.98	0.44
2:D:573:ILE:HG23	2:D:581:ILE:HD12	1.99	0.44
2:E:374:ASP:OD1	2:E:415:SER:OG	2.30	0.44
2:F:497:GLU:HB3	2:F:587:LEU:HD21	1.98	0.44
1:I:90:ASP:OD1	1:I:91:ARG:N	2.50	0.44
4:P:308:TYR:CD2	4:P:460:GLY:HA2	2.51	0.44
1:Q:10:GLU:HG3	1:Q:11:GLN:N	2.32	0.44
1:Q:118:TYR:HB3	1:Q:120:VAL:HG22	2.00	0.44
4:U:429:TRP:CZ3	4:U:431:ILE:HG13	2.48	0.44
1:0:140:ARG:HH11	1:0:154:VAL:HG13	1.83	0.44
1:K:69:ASN:HD22	1:K:69:ASN:N	2.16	0.44
2:F:105:LEU:HD11	2:F:116:PHE:HB2	1.99	0.44
2:F:378:ARG:CB	2:F:389:GLU:HB3	2.46	0.44
1:4:173:GLU:O	1:4:174:ASN:HB2	2.16	0.44
1:8:140:ARG:HH11	1:8:154:VAL:HG13	1.82	0.44
2:B:585:ARG:HD2	2:E:575:GLY:O	2.17	0.44
2:E:502:ASN:HD21	2:E:577:LYS:HB3	1.81	0.44
2:F:139:GLN:HB2	2:F:153:GLY:O	2.17	0.44
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	2.00	0.44
4:U:359:TYR:CE1	4:U:383:LEU:HB2	2.52	0.44
1:0:69:ASN:N	1:0:69:ASN:HD22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:16:ARG:HB3	1:8:117:PRO:HG3	2.00	0.44
2:A:377:PHE:CE1	2:A:396:LEU:HG	2.53	0.44
2:C:288:GLY:HA3	2:C:431:LEU:HA	1.99	0.44
2:C:360:ALA:HB1	2:C:408:ASN:HB2	2.00	0.44
2:D:292:TYR:HE1	2:D:434:LYS:HB2	1.82	0.44
2:D:448:ILE:HA	2:D:451:LYS:HD2	1.99	0.44
2:E:177:VAL:HG22	2:E:183:GLU:HG3	1.99	0.44
4:H:329:ARG:NH2	4:J:476:ASP:O	2.48	0.44
1:8:11:GLN:HG2	2:F:501:ALA:HA	1.99	0.44
2:C:235:LYS:HB3	2:C:238:VAL:HG22	1.98	0.44
2:C:266:ASP:HA	2:C:270:LEU:HD13	1.99	0.44
2:C:500:TYR:HB2	2:C:502:ASN:OD1	2.18	0.44
2:C:543:ARG:HB2	2:C:546:HIS:CD2	2.53	0.44
2:D:105:LEU:HD12	2:D:114:ASP:HB3	1.99	0.44
2:D:502:ASN:HD21	2:D:504:ASP:HB2	1.83	0.44
1:K:74:LEU:HD23	1:K:122:LEU:HD11	1.99	0.44
4:R:488:ARG:HB2	4:R:490:ILE:HG13	1.99	0.44
4:R:509:ARG:HA	4:R:509:ARG:HD2	1.83	0.44
1:Z:56:LEU:HG	1:Z:62:PHE:HB2	2.00	0.44
2:A:418:GLU:OE1	2:A:419:ASP:N	2.51	0.44
2:B:525:ARG:NH2	2:B:557:GLU:OE2	2.51	0.44
2:E:337:LEU:HD13	2:E:349:ILE:HG12	2.00	0.44
4:J:308:TYR:CE2	4:J:460:GLY:HA2	2.53	0.44
1:K:25:ALA:O	1:K:158:GLY:HA2	2.18	0.44
1:K:203:LEU:HB3	1:K:204:GLY:H	1.50	0.44
1:O:74:LEU:HD23	1:O:122:LEU:HD11	1.99	0.44
1:0:69:ASN:HD22	1:0:69:ASN:H	1.65	0.43
1:0:110:ILE:HG21	1:0:118:TYR:CD1	2.53	0.43
2:C:530:ALA:HB2	2:C:542:LEU:HD13	2.00	0.43
2:D:439:ARG:NH2	2:D:513:PHE:HA	2.33	0.43
2:E:527:LYS:NZ	2:F:282:SER:O	2.45	0.43
4:M:318:ARG:HD3	4:M:493:THR:HG23	2.00	0.43
4:V:344:GLY:C	4:V:345:ILE:HG12	2.38	0.43
1:0:203:LEU:HD12	1:0:208:LEU:HD21	2.00	0.43
1:4:140:ARG:HH11	1:4:154:VAL:HG13	1.80	0.43
1:8:173:GLU:O	1:8:174:ASN:HB2	2.18	0.43
2:C:388:VAL:HG22	2:C:391:THR:HG22	1.99	0.43
2:F:486:MET:HG3	2:F:555:PHE:HZ	1.83	0.43
4:S:450:MET:O	4:S:454:TYR:HB2	2.18	0.43
4:Y:359:TYR:CE1	4:Y:383:LEU:HB2	2.54	0.43
4:Y:382:ARG:HD3	1:Z:89:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:605:LEU:HG	1:4:111:PHE:CD2	2.53	0.43
2:A:447:ASP:O	2:A:451:LYS:HG2	2.17	0.43
2:C:183:GLU:HB2	2:F:161:ILE:HB	1.99	0.43
2:C:278:TYR:O	2:C:282:SER:N	2.51	0.43
2:F:427:ARG:HD2	2:F:428:PRO:O	2.19	0.43
1:I:69:ASN:HD22	1:I:69:ASN:N	2.17	0.43
4:N:366:TYR:CZ	4:N:370:GLU:HG3	2.53	0.43
1:2:118:TYR:HB3	1:2:120:VAL:HG22	2.00	0.43
2:B:385:SER:HB2	2:E:387:ASP:N	2.32	0.43
2:B:534:VAL:HG22	2:B:540:PRO:HA	2.01	0.43
2:E:142:ARG:NH2	2:E:151:GLU:OE1	2.52	0.43
2:E:574:SER:CB	2:E:580:ARG:HA	2.48	0.43
2:F:587:LEU:HD23	2:F:587:LEU:HA	1.88	0.43
1:K:56:LEU:HG	1:K:62:PHE:HB2	2.00	0.43
4:V:335:TYR:OH	4:V:353:VAL:HG22	2.19	0.43
1:0:173:GLU:O	1:0:174:ASN:HB2	2.17	0.43
1:2:203:LEU:HD12	1:2:208:LEU:HD21	2.01	0.43
2:C:341:PHE:HB3	2:F:340:LYS:HG3	2.00	0.43
2:E:570:TRP:HB3	2:E:581:ILE:CG2	2.49	0.43
2:F:321:ASP:OD1	2:F:321:ASP:N	2.51	0.43
1:X:79:ILE:HD13	4:Y:368:LYS:HB3	1.99	0.43
2:A:425:ILE:HG12	2:A:431:LEU:HD23	2.01	0.43
2:B:168:LEU:HD12	2:B:173:ARG:HB2	2.00	0.43
2:D:244:GLU:HB3	2:D:328:TYR:CD2	2.54	0.43
2:E:393:VAL:HG12	2:E:397:LEU:HD23	2.01	0.43
2:F:340:LYS:HE2	2:F:340:LYS:HB3	1.88	0.43
2:F:377:PHE:HB3	2:F:392:VAL:CG2	2.48	0.43
4:N:318:ARG:HD3	4:N:493:THR:HG23	2.00	0.43
2:A:378:ARG:HG3	2:A:379:THR:H	1.83	0.43
2:A:585:ARG:HD2	2:B:575:GLY:HA2	2.00	0.43
2:C:570:TRP:CD1	2:C:584:ILE:HD11	2.54	0.43
2:E:161:ILE:HD11	2:F:185:VAL:HG13	2.01	0.43
1:O:56:LEU:HG	1:O:62:PHE:HB2	2.01	0.43
1:Z:41:PHE:HB3	1:Z:53:ILE:HD13	1.99	0.43
2:A:99:SER:OG	2:B:123:ARG:HB3	2.18	0.43
2:A:270:LEU:HG	2:A:278:TYR:HE1	1.83	0.43
2:D:294:PRO:HD2	2:D:437:ILE:HB	1.99	0.43
2:E:235:LYS:HB2	2:E:235:LYS:HE2	1.82	0.43
1:O:118:TYR:HB3	1:O:120:VAL:HG22	2.01	0.43
1:Q:25:ALA:O	1:Q:158:GLY:HA2	2.19	0.43
1:0:32:ALA:HA	1:0:40:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:56:LEU:HD23	1:0:56:LEU:HA	1.77	0.43
1:4:30:VAL:HG13	1:4:43:ALA:HB2	2.00	0.43
1:4:69:ASN:HD22	1:4:69:ASN:H	1.66	0.43
2:A:166:GLU:HG2	2:A:175:LEU:HB3	2.00	0.43
2:A:455:GLU:O	2:A:471:ARG:NH2	2.37	0.43
2:E:164:LEU:HB2	2:E:220:LEU:HD23	2.00	0.43
1:I:25:ALA:O	1:I:158:GLY:HA2	2.18	0.43
1:O:33:LEU:HD12	1:O:40:LEU:HB3	2.00	0.43
1:Q:182:ARG:NH1	1:Q:234:LEU:O	2.51	0.43
4:S:366:TYR:CZ	4:S:370:GLU:HG3	2.54	0.43
4:U:314:MET:HE2	4:U:403:LEU:HG	2.00	0.43
4:W:344:GLY:C	4:W:345:ILE:HG12	2.37	0.43
4:W:366:TYR:CZ	4:W:370:GLU:HG3	2.54	0.43
4:Y:351:VAL:HG21	4:Y:398:LEU:HB3	2.00	0.43
2:A:235:LYS:HD2	2:B:175:LEU:HD22	2.01	0.43
2:D:493:ASN:HB2	2:D:509:TYR:HD1	1.84	0.43
2:E:291:LEU:HD23	2:E:435:ILE:HB	2.00	0.43
2:E:566:ASN:O	2:E:568:ASP:N	2.48	0.43
4:J:369:LEU:HD23	4:J:369:LEU:HA	1.83	0.43
4:N:429:TRP:HZ3	4:N:431:ILE:HG13	1.84	0.43
4:P:382:ARG:HD2	1:Q:89:TYR:CE1	2.54	0.43
1:Q:55:GLU:HB2	1:Q:222:PHE:CG	2.54	0.43
4:S:344:GLY:C	4:S:345:ILE:HG12	2.38	0.43
1:X:90:ASP:OD1	1:X:91:ARG:N	2.52	0.43
1:0:119:GLU:H	1:0:119:GLU:HG3	1.66	0.42
2:B:300:THR:HG21	2:E:402:GLY:HA2	2.01	0.42
2:C:332:ILE:HG21	2:C:352:ILE:HD13	2.01	0.42
4:H:433:GLU:HA	4:U:530:ASP:OD2	2.18	0.42
4:P:488:ARG:HB2	4:P:490:ILE:HG13	2.01	0.42
4:Y:369:LEU:HD23	4:Y:369:LEU:HA	1.84	0.42
2:A:187:TRP:HB2	2:A:228:TYR:CE2	2.54	0.42
2:B:222:VAL:HG12	2:B:229:ALA:HA	2.00	0.42
2:B:426:LEU:HD23	2:B:431:LEU:HD12	2.00	0.42
2:D:174:ALA:HB2	2:D:188:LEU:HD21	2.01	0.42
4:J:473:ASP:OD1	4:J:521:ARG:NH1	2.39	0.42
4:M:450:MET:O	4:M:454:TYR:HB2	2.19	0.42
1:T:74:LEU:HD23	1:T:122:LEU:HD11	2.01	0.42
1:4:68:PHE:HB3	2:B:607:GLN:HE21	1.84	0.42
2:B:301:LEU:N	5:B:701:ATP:O1A	2.45	0.42
2:B:376:ILE:HG13	2:B:377:PHE:HD1	1.84	0.42
2:B:477:ALA:O	2:B:481:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:344:GLY:C	4:M:345:ILE:HG12	2.37	0.42
1:T:56:LEU:HG	1:T:62:PHE:HB2	2.00	0.42
4:V:303:ILE:O	4:V:438:ALA:HA	2.19	0.42
1:4:8:SER:HB2	2:B:503:GLY:O	2.18	0.42
2:E:565:THR:HG21	2:E:582:VAL:HA	2.00	0.42
2:F:521:ASN:HD21	2:F:525:ARG:HH21	1.67	0.42
4:J:308:TYR:CD2	4:J:460:GLY:HA2	2.54	0.42
1:Q:69:ASN:HD22	1:Q:69:ASN:N	2.17	0.42
1:X:108:GLY:HA2	1:X:144:ASP:O	2.19	0.42
4:Y:486:LEU:HD12	4:Y:486:LEU:HA	1.86	0.42
2:A:255:GLY:H	5:A:701:ATP:HN61	1.68	0.42
2:B:397:LEU:HD22	2:B:430:ARG:NH1	2.34	0.42
2:C:453:LEU:HD12	2:C:479:ILE:HG12	2.02	0.42
2:F:245:GLU:OE2	2:F:326:LYS:NZ	2.51	0.42
2:F:373:MET:SD	2:F:413:GLY:HA3	2.60	0.42
2:F:496:LEU:HD21	2:F:562:PRO:HG3	2.02	0.42
1:I:33:LEU:HD12	1:I:40:LEU:HB3	2.02	0.42
1:I:118:TYR:HB3	1:I:120:VAL:HG22	2.01	0.42
1:K:118:TYR:HB3	1:K:120:VAL:HG22	2.02	0.42
4:Y:488:ARG:HB2	4:Y:490:ILE:HG13	2.02	0.42
1:8:23:GLY:HA2	1:8:26:ARG:NH2	2.34	0.42
2:E:530:ALA:O	2:E:534:VAL:HG23	2.20	0.42
1:K:181:LEU:HD23	1:K:233:LEU:HB3	2.01	0.42
1:X:56:LEU:HG	1:X:62:PHE:HB2	2.00	0.42
1:2:134:LYS:HB3	1:2:134:LYS:HE2	1.87	0.42
2:A:583:TYR:CE2	2:A:585:ARG:HB2	2.54	0.42
2:C:115:VAL:HG11	2:C:143:LEU:HD11	2.01	0.42
2:C:495:PHE:HZ	2:C:562:PRO:HD3	1.85	0.42
4:P:369:LEU:HD23	4:P:369:LEU:HA	1.81	0.42
4:P:475:ALA:HA	4:P:481:THR:HB	2.01	0.42
1:T:92:ARG:HH22	1:T:129:HIS:HB3	1.85	0.42
4:V:432:GLU:HG3	4:V:437:GLN:HB2	2.02	0.42
1:8:20:ALA:HA	1:8:119:GLU:HG2	2.02	0.42
2:A:259:ARG:O	2:A:263:GLN:HG2	2.20	0.42
2:E:383:GLY:HA3	2:E:387:ASP:OD1	2.20	0.42
2:F:235:LYS:HE3	2:F:351:LEU:HD22	2.02	0.42
4:H:432:GLU:CD	4:H:437:GLN:HE21	2.22	0.42
1:I:61:GLY:N	1:I:213:LEU:HD11	2.35	0.42
1:6:30:VAL:HG13	1:6:43:ALA:HB2	2.01	0.42
1:6:32:ALA:HA	1:6:40:LEU:O	2.20	0.42
1:8:30:VAL:HG13	1:8:43:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:105:LEU:HB2	2:A:114:ASP:HB2	2.01	0.42
2:A:500:TYR:CE2	2:A:506:GLU:HB2	2.55	0.42
2:C:418:GLU:N	2:C:418:GLU:OE1	2.53	0.42
2:E:373:MET:HB3	2:E:377:PHE:CE2	2.55	0.42
4:H:435:GLY:HA2	4:U:530:ASP:OD1	2.19	0.42
4:J:351:VAL:HG21	4:J:398:LEU:HB3	2.01	0.42
4:L:488:ARG:HB2	4:L:490:ILE:HG13	2.02	0.42
4:S:318:ARG:HD3	4:S:493:THR:HG23	2.00	0.42
4:U:369:LEU:HD23	4:U:369:LEU:HA	1.83	0.42
1:Z:69:ASN:HD22	1:Z:69:ASN:N	2.18	0.42
2:C:609:LEU:HA	2:C:609:LEU:HD23	1.79	0.42
2:E:300:THR:O	2:E:304:LYS:HG2	2.20	0.42
2:E:426:LEU:HD23	2:E:431:LEU:HD12	2.02	0.42
4:L:369:LEU:HD23	4:L:369:LEU:HA	1.85	0.42
1:0:134:LYS:HB3	1:0:134:LYS:HE2	1.89	0.41
1:4:89:TYR:CE1	4:M:382:ARG:HD3	2.55	0.41
2:A:184:ARG:NH2	2:A:224:THR:O	2.53	0.41
2:D:297:CYS:SG	2:D:439:ARG:NH1	2.93	0.41
2:F:333:LYS:O	2:F:336:GLU:HG2	2.19	0.41
1:8:32:ALA:HA	1:8:40:LEU:O	2.21	0.41
2:B:567:PRO:HA	2:B:570:TRP:CD1	2.47	0.41
2:E:362:GLU:HA	2:E:408:ASN:HD22	1.85	0.41
4:V:338:ASP:OD1	4:V:341:THR:N	2.53	0.41
2:B:528:LYS:HB3	2:B:528:LYS:HE3	1.87	0.41
1:Z:74:LEU:HD23	1:Z:122:LEU:HD11	2.02	0.41
2:1:605:LEU:CD2	1:4:111:PHE:CE2	3.03	0.41
2:B:108:HIS:CE1	2:B:123:ARG:HH12	2.39	0.41
2:B:256:GLY:N	2:B:447:ASP:OD2	2.48	0.41
2:C:154:THR:OG1	2:C:155:PHE:N	2.53	0.41
2:D:460:HIS:CD2	2:D:543:ARG:HE	2.37	0.41
2:D:495:PHE:HB2	2:D:510:PHE:CE1	2.55	0.41
2:D:570:TRP:HD1	2:D:584:ILE:HD12	1.85	0.41
2:E:237:GLU:HB2	2:E:355:ARG:HG2	2.02	0.41
2:E:499:THR:HA	2:E:504:ASP:O	2.21	0.41
4:J:475:ALA:HA	4:J:481:THR:HB	2.01	0.41
1:K:78:GLY:HA3	1:K:103:TYR:OH	2.20	0.41
4:S:471:LEU:HD23	4:S:471:LEU:HA	1.89	0.41
4:U:488:ARG:HB2	4:U:490:ILE:HG13	2.01	0.41
1:0:98:GLN:O	1:0:102:VAL:HG23	2.21	0.41
1:T:41:PHE:HB3	1:T:53:ILE:HD13	2.01	0.41
1:4:69:ASN:HD22	1:4:69:ASN:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:GLY:HA3	2:D:437:ILE:HB	2.01	0.41
2:D:441:ASP:N	2:D:444:ALA:HB3	2.36	0.41
2:D:525:ARG:HD2	2:D:554:GLU:HB2	2.02	0.41
1:2:32:ALA:HA	1:2:40:LEU:O	2.20	0.41
2:C:355:ARG:O	2:C:359:LYS:HG2	2.20	0.41
4:H:303:ILE:O	4:H:438:ALA:HA	2.20	0.41
1:K:164:ALA:O	1:K:168:LYS:HG3	2.20	0.41
1:Q:181:LEU:HD23	1:Q:233:LEU:HB3	2.03	0.41
4:W:380:ILE:HD11	4:W:421:VAL:HG21	2.01	0.41
4:W:471:LEU:HD23	4:W:471:LEU:HA	1.89	0.41
1:Z:24:ILE:HG22	1:Z:157:GLY:HA2	2.01	0.41
1:2:89:TYR:CE1	4:S:382:ARG:HD3	2.56	0.41
2:C:161:ILE:HG23	2:D:183:GLU:HG2	2.02	0.41
2:C:477:ALA:O	2:C:481:LYS:HG2	2.21	0.41
2:F:379:THR:OG1	2:F:420:MET:O	2.28	0.41
2:F:427:ARG:HH21	2:F:430:ARG:CZ	2.33	0.41
1:K:163:ILE:HG23	1:K:187:ALA:C	2.41	0.41
4:N:409:ILE:H	4:N:409:ILE:HG12	1.61	0.41
1:T:33:LEU:HD12	1:T:40:LEU:HB3	2.03	0.41
4:V:432:GLU:CD	4:V:437:GLN:HE21	2.24	0.41
1:4:182:ARG:NH1	1:4:234:LEU:O	2.54	0.41
1:6:140:ARG:HH11	1:6:154:VAL:HG13	1.83	0.41
2:A:285:PRO:HA	2:A:286:PRO:HD3	1.99	0.41
2:A:310:LEU:HD13	2:A:310:LEU:HA	1.79	0.41
2:A:419:ASP:OD1	2:A:420:MET:N	2.54	0.41
2:A:514:ASN:OD1	2:A:515:SER:N	2.54	0.41
2:B:360:ALA:HB1	2:B:408:ASN:HB2	2.02	0.41
2:C:344:GLU:HA	2:C:347:ARG:HG2	2.03	0.41
2:D:357:ARG:HH12	2:D:361:SER:HB2	1.86	0.41
2:D:370:PHE:HB3	2:D:373:MET:SD	2.61	0.41
2:D:437:ILE:N	2:D:437:ILE:HD12	2.36	0.41
2:D:485:ARG:HA	2:D:485:ARG:HH11	1.85	0.41
2:D:485:ARG:HA	2:D:485:ARG:NH1	2.36	0.41
2:E:531:ILE:HD11	2:F:277:LEU:HB3	2.02	0.41
4:M:303:ILE:O	4:M:438:ALA:HA	2.20	0.41
4:P:509:ARG:HA	4:P:512:GLU:CD	2.41	0.41
1:T:96:GLY:H	1:T:126:GLU:CD	2.25	0.41
4:W:450:MET:O	4:W:454:TYR:HB2	2.21	0.41
1:Z:174:ASN:HD22	1:Z:174:ASN:HA	1.60	0.41
1:4:32:ALA:HA	1:4:40:LEU:O	2.21	0.41
2:A:141:VAL:HA	2:A:152:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:429:GLY:H	2:C:432:ASP:HB3	1.86	0.41
2:D:269:GLU:OE2	2:D:313:LYS:HE2	2.21	0.41
1:T:118:TYR:HB3	1:T:120:VAL:HG22	2.02	0.41
4:W:303:ILE:O	4:W:438:ALA:HA	2.21	0.41
1:2:56:LEU:HA	1:2:56:LEU:HD23	1.77	0.40
2:D:609:LEU:HD23	2:D:609:LEU:HA	1.91	0.40
1:I:78:GLY:HA3	1:I:103:TYR:OH	2.22	0.40
1:I:208:LEU:HD23	1:I:208:LEU:HA	1.89	0.40
4:M:320:SER:HB3	4:M:331:VAL:HG21	2.03	0.40
1:2:214:ASP:OD2	1:2:217:ARG:HG2	2.22	0.40
2:C:397:LEU:HD21	2:C:425:ILE:HG12	2.03	0.40
2:C:499:THR:HB	2:C:583:TYR:HB2	2.02	0.40
2:E:497:GLU:HB2	2:E:587:LEU:HD11	2.03	0.40
2:E:500:TYR:CD1	2:E:504:ASP:HB3	2.56	0.40
2:E:544:ILE:HG22	2:E:548:LEU:HD13	2.02	0.40
2:F:326:LYS:HE3	2:F:326:LYS:HB3	1.82	0.40
2:F:561:LEU:N	2:F:562:PRO:HD2	2.37	0.40
4:M:456:GLN:HE21	4:M:465:ARG:HH21	1.68	0.40
4:M:471:LEU:HA	4:M:471:LEU:HD23	1.89	0.40
4:N:320:SER:HB3	4:N:331:VAL:HG21	2.03	0.40
1:0:11:GLN:CG	2:A:504:ASP:H	2.35	0.40
2:1:609:LEU:HD23	2:1:609:LEU:HA	1.75	0.40
1:K:108:GLY:HA2	1:K:144:ASP:O	2.21	0.40
1:O:78:GLY:HA3	1:O:103:TYR:OH	2.22	0.40
4:R:351:VAL:HG21	4:R:398:LEU:HB3	2.02	0.40
4:S:444:LEU:HA	4:S:444:LEU:HD12	1.83	0.40
1:T:108:GLY:HA2	1:T:144:ASP:O	2.22	0.40
1:X:118:TYR:HB3	1:X:120:VAL:HG22	2.03	0.40
1:4:96:GLY:H	1:4:126:GLU:CD	2.25	0.40
2:A:287:LYS:HD3	2:A:404:GLU:HA	2.02	0.40
2:C:575:GLY:HA2	2:C:580:ARG:HH22	1.87	0.40
2:D:499:THR:O	2:D:581:ILE:HG23	2.22	0.40
2:D:528:LYS:HB3	2:D:528:LYS:HE3	1.82	0.40
2:F:136:LYS:O	2:F:139:GLN:HG2	2.22	0.40
2:F:499:THR:HB	2:F:583:TYR:HB3	2.02	0.40
4:J:314:MET:HE2	4:J:403:LEU:HG	2.02	0.40
4:L:473:ASP:OD1	4:L:521:ARG:NH1	2.32	0.40
4:M:366:TYR:CZ	4:M:370:GLU:HG3	2.56	0.40
1:O:178:THR:HG22	1:O:182:ARG:HE	1.87	0.40
4:R:450:MET:HG3	4:R:470:ALA:HB2	2.04	0.40
4:S:338:ASP:OD1	4:S:341:THR:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:78:GLY:HA3	1:X:103:TYR:OH	2.22	0.40
1:Z:108:GLY:HA2	1:Z:144:ASP:O	2.21	0.40
1:6:144:ASP:OD2	2:B:606:GLY:HA3	2.22	0.40
2:A:144:ASN:HD21	2:A:146:ALA:HB3	1.86	0.40
2:A:255:GLY:O	5:A:701:ATP:N6	2.54	0.40
1:K:107:LEU:HD23	1:K:107:LEU:HA	1.93	0.40
4:L:450:MET:HG3	4:L:470:ALA:HB2	2.03	0.40
1:Z:16:ARG:NH2	1:Z:114:GLN:O	2.43	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	0	211/248 (85%)	202 (96%)	9 (4%)	0	100	100
1	2	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	4	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
1	6	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	8	211/248 (85%)	201 (95%)	10 (5%)	0	100	100
1	I	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
1	K	213/248 (86%)	205 (96%)	8 (4%)	0	100	100
1	O	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	Q	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	T	210/248 (85%)	202 (96%)	8 (4%)	0	100	100
1	X	210/248 (85%)	204 (97%)	6 (3%)	0	100	100
1	Z	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	d	211/248 (85%)	203 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	211/248 (85%)	202 (96%)	9 (4%)	0	100	100
2	1	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	A	458/609 (75%)	442 (96%)	15 (3%)	1 (0%)	47	78
2	B	465/609 (76%)	452 (97%)	13 (3%)	0	100	100
2	C	463/609 (76%)	451 (97%)	12 (3%)	0	100	100
2	D	447/609 (73%)	426 (95%)	17 (4%)	4 (1%)	17	53
2	E	477/609 (78%)	457 (96%)	20 (4%)	0	100	100
2	F	477/609 (78%)	460 (96%)	16 (3%)	1 (0%)	47	78
3	G	15/66 (23%)	15 (100%)	0	0	100	100
4	H	220/291 (76%)	211 (96%)	9 (4%)	0	100	100
4	J	221/291 (76%)	211 (96%)	10 (4%)	0	100	100
4	L	220/291 (76%)	209 (95%)	11 (5%)	0	100	100
4	M	220/291 (76%)	211 (96%)	8 (4%)	1 (0%)	29	66
4	N	220/291 (76%)	212 (96%)	7 (3%)	1 (0%)	29	66
4	P	221/291 (76%)	210 (95%)	11 (5%)	0	100	100
4	R	220/291 (76%)	210 (96%)	10 (4%)	0	100	100
4	S	220/291 (76%)	213 (97%)	6 (3%)	1 (0%)	29	66
4	U	232/291 (80%)	221 (95%)	11 (5%)	0	100	100
4	V	221/291 (76%)	214 (97%)	6 (3%)	1 (0%)	29	66
4	W	232/291 (80%)	225 (97%)	6 (3%)	1 (0%)	34	70
4	Y	221/291 (76%)	210 (95%)	11 (5%)	0	100	100
4	a	221/291 (76%)	210 (95%)	11 (5%)	0	100	100
4	b	221/291 (76%)	214 (97%)	6 (3%)	1 (0%)	29	66
All	All	8868/11875 (75%)	8531 (96%)	325 (4%)	12 (0%)	54	83

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	505	LYS
2	D	342	VAL
2	F	378	ARG
2	D	295	PRO
2	D	297	CYS
4	W	309	PRO

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Mol	Chain	Res	Type
4	b	309	PRO
4	M	309	PRO
4	N	309	PRO
4	S	309	PRO
4	V	309	PRO
2	D	296	GLY

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	0	165/192 (86%)	157 (95%)	8 (5%)	25	55
1	2	165/192 (86%)	159 (96%)	6 (4%)	35	62
1	4	165/192 (86%)	157 (95%)	8 (5%)	25	55
1	6	165/192 (86%)	156 (94%)	9 (6%)	21	53
1	8	165/192 (86%)	156 (94%)	9 (6%)	21	53
1	I	164/192 (85%)	154 (94%)	10 (6%)	18	50
1	K	166/192 (86%)	158 (95%)	8 (5%)	25	55
1	O	165/192 (86%)	155 (94%)	10 (6%)	18	50
1	Q	165/192 (86%)	154 (93%)	11 (7%)	16	47
1	T	164/192 (85%)	156 (95%)	8 (5%)	25	55
1	X	164/192 (85%)	159 (97%)	5 (3%)	41	66
1	Z	165/192 (86%)	156 (94%)	9 (6%)	21	53
1	d	165/192 (86%)	154 (93%)	11 (7%)	16	47
1	f	165/192 (86%)	153 (93%)	12 (7%)	14	44
2	1	4/511 (1%)	4 (100%)	0	100	100
2	A	397/511 (78%)	389 (98%)	8 (2%)	55	74
2	B	402/511 (79%)	394 (98%)	8 (2%)	55	74
2	C	400/511 (78%)	388 (97%)	12 (3%)	41	66
2	D	388/511 (76%)	377 (97%)	11 (3%)	43	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	409/511 (80%)	398 (97%)	11 (3%)	44	68
2	F	408/511 (80%)	403 (99%)	5 (1%)	71	84
3	G	10/50 (20%)	10 (100%)	0	100	100
4	H	164/217 (76%)	161 (98%)	3 (2%)	59	77
4	J	164/217 (76%)	158 (96%)	6 (4%)	34	61
4	L	164/217 (76%)	161 (98%)	3 (2%)	59	77
4	M	164/217 (76%)	160 (98%)	4 (2%)	49	71
4	N	164/217 (76%)	160 (98%)	4 (2%)	49	71
4	P	164/217 (76%)	159 (97%)	5 (3%)	41	66
4	R	164/217 (76%)	160 (98%)	4 (2%)	49	71
4	S	164/217 (76%)	159 (97%)	5 (3%)	41	66
4	U	171/217 (79%)	166 (97%)	5 (3%)	42	66
4	V	164/217 (76%)	161 (98%)	3 (2%)	59	77
4	W	171/217 (79%)	167 (98%)	4 (2%)	50	71
4	Y	164/217 (76%)	161 (98%)	3 (2%)	59	77
4	a	164/217 (76%)	161 (98%)	3 (2%)	59	77
4	b	164/217 (76%)	158 (96%)	6 (4%)	34	61
All	All	7036/9353 (75%)	6799 (97%)	237 (3%)	40	64

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	33	LEU
1	0	69	ASN
1	0	73	ASN
1	0	74	LEU
1	0	119	GLU
1	0	182	ARG
1	0	203	LEU
1	0	234	LEU
1	2	33	LEU
1	2	73	ASN
1	2	74	LEU
1	2	182	ARG
1	2	203	LEU
1	2	234	LEU

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Mol	Chain	Res	Type
1	4	33	LEU
1	4	69	ASN
1	4	73	ASN
1	4	74	LEU
1	4	119	GLU
1	4	182	ARG
1	4	203	LEU
1	4	234	LEU
1	6	11	GLN
1	6	33	LEU
1	6	73	ASN
1	6	74	LEU
1	6	119	GLU
1	6	123	CYS
1	6	182	ARG
1	6	203	LEU
1	6	234	LEU
1	8	26	ARG
1	8	33	LEU
1	8	69	ASN
1	8	73	ASN
1	8	74	LEU
1	8	147	ILE
1	8	182	ARG
1	8	203	LEU
1	8	234	LEU
2	A	215	ARG
2	A	310	LEU
2	A	337	LEU
2	A	393	VAL
2	A	418	GLU
2	A	430	ARG
2	A	492	ASP
2	A	506	GLU
2	B	276	GLU
2	B	345	THR
2	B	368	VAL
2	B	498	VAL
2	B	505	LYS
2	B	507	VAL
2	B	564	THR
2	B	605	LEU

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Mol	Chain	Res	Type
2	C	161	ILE
2	C	212	ARG
2	C	232	ARG
2	C	281	TYR
2	C	345	THR
2	C	382	THR
2	C	418	GLU
2	C	524	ASP
2	C	536	GLU
2	C	565	THR
2	C	570	TRP
2	C	582	VAL
2	D	177	VAL
2	D	237	GLU
2	D	244	GLU
2	D	262	GLU
2	D	283	LEU
2	D	300	THR
2	D	342	VAL
2	D	345	THR
2	D	418	GLU
2	D	439	ARG
2	D	502	ASN
2	E	145	GLU
2	E	235	LYS
2	E	345	THR
2	E	379	THR
2	E	408	ASN
2	E	511	LYS
2	E	566	ASN
2	E	573	ILE
2	E	574	SER
2	E	581	ILE
2	E	584	ILE
2	F	332	ILE
2	F	341	PHE
2	F	378	ARG
2	F	422	ASP
2	F	609	LEU
4	H	330	ASP
4	H	345	ILE
4	H	444	LEU

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Mol	Chain	Res	Type
1	I	33	LEU
1	I	69	ASN
1	I	73	ASN
1	I	74	LEU
1	I	123	CYS
1	I	147	ILE
1	I	174	ASN
1	I	182	ARG
1	I	205	VAL
1	I	217	ARG
4	J	330	ASP
4	J	345	ILE
4	J	354	GLU
4	J	434	GLU
4	J	444	LEU
4	J	486	LEU
1	K	10	GLU
1	K	26	ARG
1	K	33	LEU
1	K	69	ASN
1	K	73	ASN
1	K	74	LEU
1	K	123	CYS
1	K	182	ARG
4	L	345	ILE
4	L	444	LEU
4	L	486	LEU
4	M	330	ASP
4	M	345	ILE
4	M	412	SER
4	M	444	LEU
4	N	345	ILE
4	N	412	SER
4	N	444	LEU
4	N	509	ARG
1	O	11	GLN
1	O	26	ARG
1	O	33	LEU
1	O	69	ASN
1	O	73	ASN
1	O	74	LEU
1	O	123	CYS

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Mol	Chain	Res	Type
1	O	147	ILE
1	O	182	ARG
1	O	189	ARG
4	P	330	ASP
4	P	345	ILE
4	P	432	GLU
4	P	444	LEU
4	P	486	LEU
1	Q	10	GLU
1	Q	26	ARG
1	Q	33	LEU
1	Q	69	ASN
1	Q	73	ASN
1	Q	74	LEU
1	Q	123	CYS
1	Q	147	ILE
1	Q	182	ARG
1	Q	203	LEU
1	Q	234	LEU
4	R	345	ILE
4	R	357	ARG
4	R	444	LEU
4	R	486	LEU
4	S	330	ASP
4	S	338	ASP
4	S	345	ILE
4	S	412	SER
4	S	444	LEU
1	T	26	ARG
1	T	33	LEU
1	T	69	ASN
1	T	73	ASN
1	T	74	LEU
1	T	114	GLN
1	T	123	CYS
1	T	182	ARG
4	U	330	ASP
4	U	363	LEU
4	U	433	GLU
4	U	444	LEU
4	U	486	LEU
4	V	345	ILE

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Mol	Chain	Res	Type
4	V	444	LEU
4	V	509	ARG
4	W	330	ASP
4	W	345	ILE
4	W	354	GLU
4	W	444	LEU
1	X	33	LEU
1	X	69	ASN
1	X	92	ARG
1	X	123	CYS
1	X	182	ARG
4	Y	444	LEU
4	Y	486	LEU
4	Y	519	GLU
1	Z	26	ARG
1	Z	33	LEU
1	Z	69	ASN
1	Z	73	ASN
1	Z	74	LEU
1	Z	123	CYS
1	Z	147	ILE
1	Z	173	GLU
1	Z	182	ARG
4	a	444	LEU
4	a	486	LEU
4	a	519	GLU
4	b	345	ILE
4	b	412	SER
4	b	433	GLU
4	b	444	LEU
4	b	465	ARG
4	b	512	GLU
1	d	10	GLU
1	d	14	ARG
1	d	18	GLU
1	d	26	ARG
1	d	33	LEU
1	d	73	ASN
1	d	74	LEU
1	d	144	ASP
1	d	182	ARG
1	d	203	LEU

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Mol	Chain	Res	Type
1	d	234	LEU
1	f	10	GLU
1	f	19	LEU
1	f	22	LYS
1	f	33	LEU
1	f	69	ASN
1	f	73	ASN
1	f	74	LEU
1	f	144	ASP
1	f	147	ILE
1	f	182	ARG
1	f	203	LEU
1	f	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	69	ASN
1	0	80	GLN
1	0	98	GLN
1	0	114	GLN
1	2	11	GLN
1	2	80	GLN
1	2	98	GLN
1	2	114	GLN
1	4	11	GLN
1	4	69	ASN
1	4	80	GLN
1	4	98	GLN
1	4	114	GLN
1	6	80	GLN
1	6	114	GLN
1	8	11	GLN
1	8	69	ASN
1	8	80	GLN
1	8	114	GLN
2	A	408	ASN
2	A	416	ASN
2	B	566	ASN
2	C	514	ASN
2	C	520	GLN
2	C	545	GLN

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Mol	Chain	Res	Type
2	C	607	GLN
2	D	308	ASN
2	D	546	HIS
2	E	446	GLN
2	E	566	ASN
2	F	460	HIS
2	F	521	ASN
2	F	607	GLN
3	G	3	GLN
4	H	456	GLN
1	I	69	ASN
1	I	80	GLN
1	I	98	GLN
1	I	114	GLN
1	I	152	HIS
1	I	174	ASN
4	J	456	GLN
1	K	69	ASN
1	K	80	GLN
1	K	114	GLN
4	L	456	GLN
4	M	456	GLN
4	N	456	GLN
1	O	69	ASN
1	O	80	GLN
1	O	114	GLN
4	P	430	ASN
4	P	456	GLN
1	Q	11	GLN
1	Q	69	ASN
1	Q	80	GLN
1	Q	114	GLN
4	R	430	ASN
4	R	456	GLN
4	S	456	GLN
1	T	69	ASN
1	T	80	GLN
4	U	456	GLN
4	V	456	GLN
4	W	456	GLN
1	X	11	GLN
1	X	69	ASN

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Mol	Chain	Res	Type
1	X	80	GLN
1	X	114	GLN
1	X	129	HIS
4	Y	430	ASN
4	Y	456	GLN
1	Z	69	ASN
1	Z	80	GLN
1	Z	114	GLN
1	Z	174	ASN
4	a	430	ASN
4	a	456	GLN
4	b	456	GLN
1	d	11	GLN
1	d	69	ASN
1	d	80	GLN
1	d	114	GLN
1	f	11	GLN
1	f	69	ASN
1	f	80	GLN
1	f	114	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	F	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.60	5 (16%)
7	ADP	D	701	-	24,29,29	0.66	0	29,45,45	0.83	1 (3%)
5	ATP	C	701	6	26,33,33	0.91	1 (3%)	31,52,52	1.48	5 (16%)
5	ATP	B	701	6	26,33,33	0.93	1 (3%)	31,52,52	1.58	5 (16%)
5	ATP	A	701	6	26,33,33	0.93	1 (3%)	31,52,52	1.54	5 (16%)
5	ATP	E	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.62	5 (16%)

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
5	ATP	F	701	6	-	0/18/38/38	0/3/3/3
7	ADP	D	701	-	-	2/12/32/32	0/3/3/3
5	ATP	C	701	6	-	0/18/38/38	0/3/3/3
5	ATP	B	701	6	-	0/18/38/38	0/3/3/3
5	ATP	A	701	6	-	0/18/38/38	0/3/3/3
5	ATP	E	701	6	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	ATP	C5-C4	2.49	1.47	1.40
5	F	701	ATP	C5-C4	2.47	1.47	1.40
5	B	701	ATP	C5-C4	2.46	1.47	1.40
5	E	701	ATP	C5-C4	2.44	1.47	1.40
5	C	701	ATP	C5-C4	2.44	1.47	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	701	ATP	PA-O3A-PB	-4.42	117.65	132.83
5	E	701	ATP	PB-O3B-PG	-4.28	118.14	132.83
5	F	701	ATP	PA-O3A-PB	-4.17	118.50	132.83
5	B	701	ATP	PA-O3A-PB	-4.16	118.55	132.83
5	B	701	ATP	PB-O3B-PG	-4.14	118.61	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	701	ATP	PB-O3B-PG	-4.09	118.78	132.83
5	A	701	ATP	PB-O3B-PG	-3.93	119.34	132.83
5	A	701	ATP	PA-O3A-PB	-3.64	120.34	132.83
5	C	701	ATP	PB-O3B-PG	-3.64	120.35	132.83
5	C	701	ATP	N3-C2-N1	-3.09	123.84	128.68
5	F	701	ATP	N3-C2-N1	-3.09	123.85	128.68
5	B	701	ATP	N3-C2-N1	-3.03	123.94	128.68
5	C	701	ATP	PA-O3A-PB	-3.01	122.50	132.83
5	E	701	ATP	N3-C2-N1	-3.00	123.98	128.68
5	A	701	ATP	N3-C2-N1	-2.92	124.12	128.68
5	C	701	ATP	C3'-C2'-C1'	2.86	105.28	100.98
5	A	701	ATP	C3'-C2'-C1'	2.78	105.17	100.98
5	E	701	ATP	C3'-C2'-C1'	2.78	105.16	100.98
5	B	701	ATP	C3'-C2'-C1'	2.71	105.05	100.98
5	F	701	ATP	C3'-C2'-C1'	2.70	105.04	100.98
5	C	701	ATP	C4-C5-N7	-2.61	106.68	109.40
5	F	701	ATP	C4-C5-N7	-2.51	106.78	109.40
5	A	701	ATP	C4-C5-N7	-2.50	106.79	109.40
5	B	701	ATP	C4-C5-N7	-2.50	106.80	109.40
5	E	701	ATP	C4-C5-N7	-2.44	106.86	109.40
7	D	701	ADP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	701	ADP	C3'-C4'-C5'-O5'
7	D	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

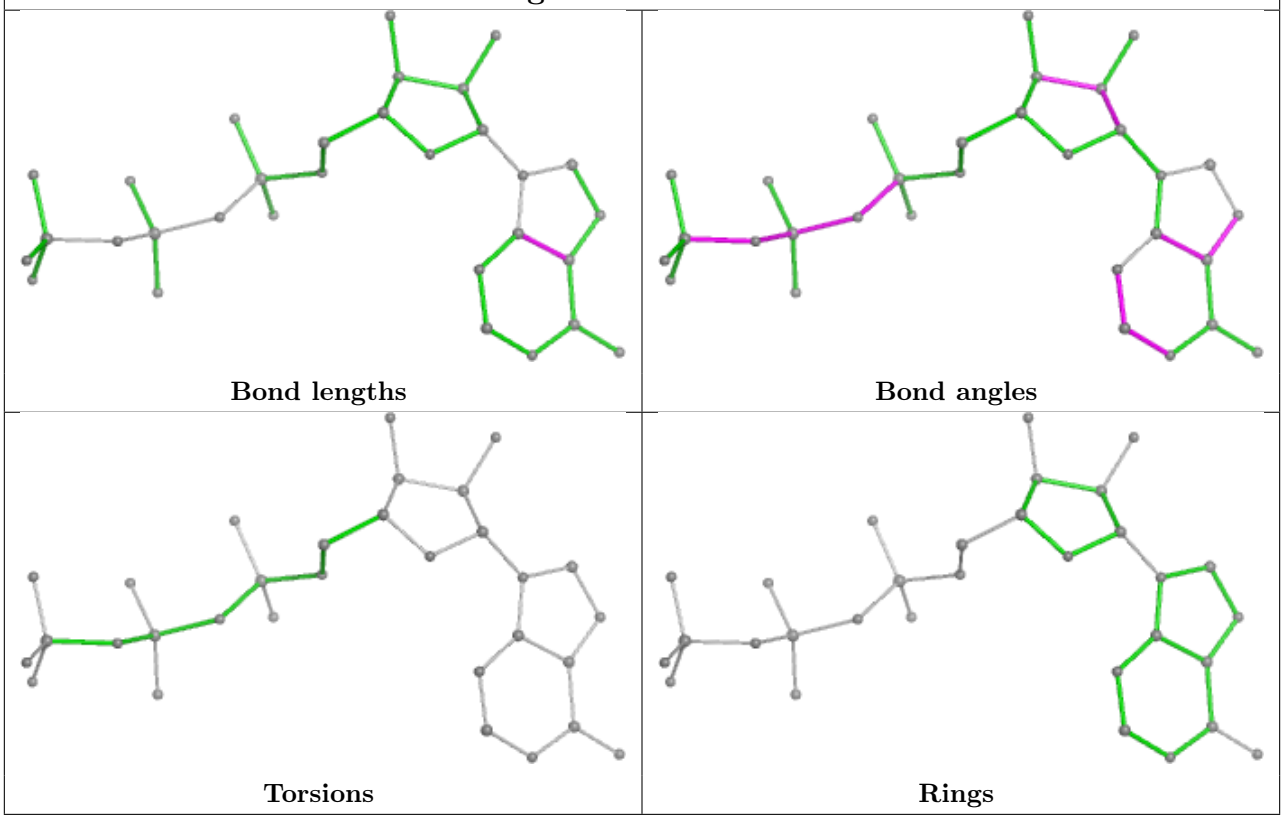
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	701	ATP	2	0
7	D	701	ADP	1	0
5	C	701	ATP	4	0
5	B	701	ATP	4	0
5	A	701	ATP	3	0
5	E	701	ATP	5	0

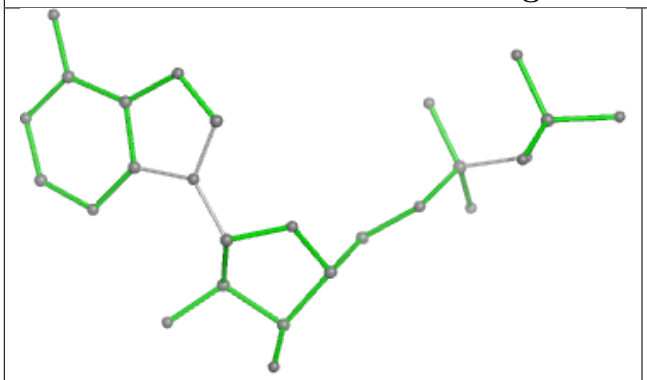
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

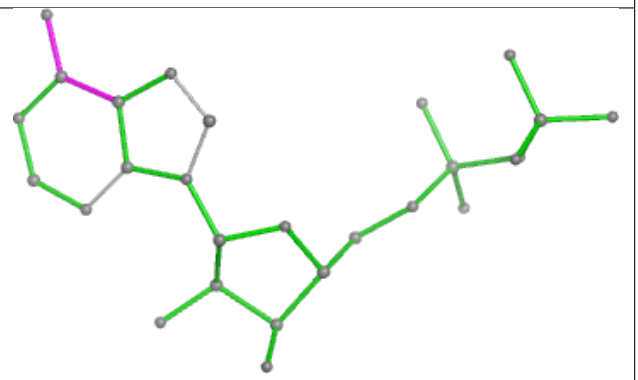
Ligand ATP F 701



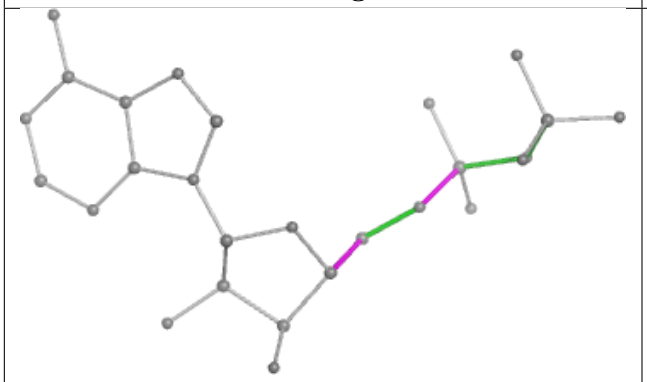
Ligand ADP D 701



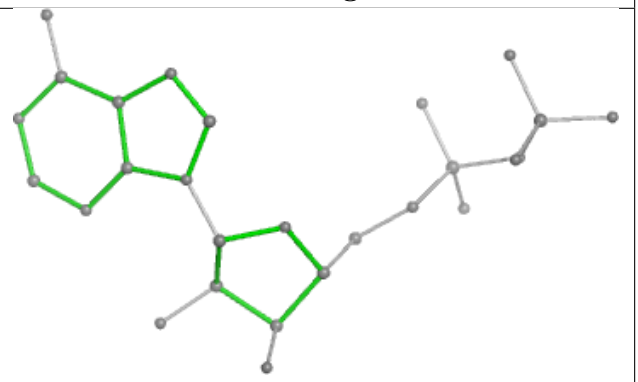
Bond lengths



Bond angles

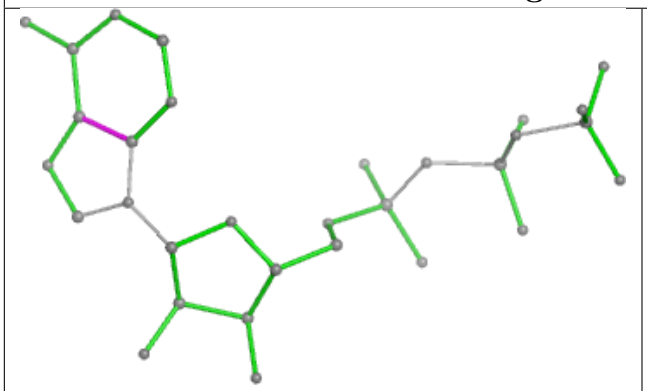


Torsions

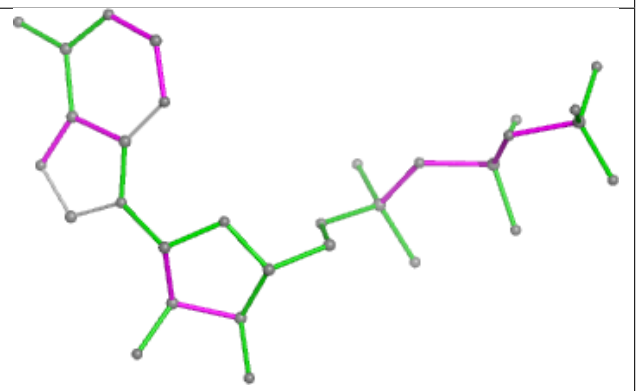


Rings

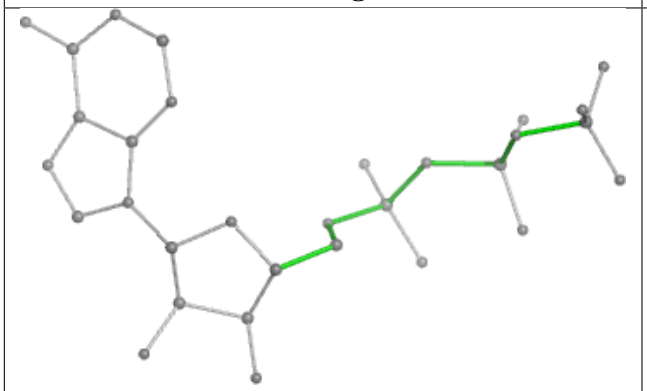
Ligand ATP C 701



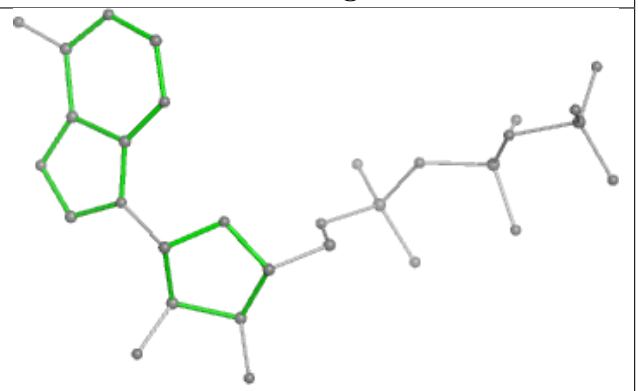
Bond lengths



Bond angles

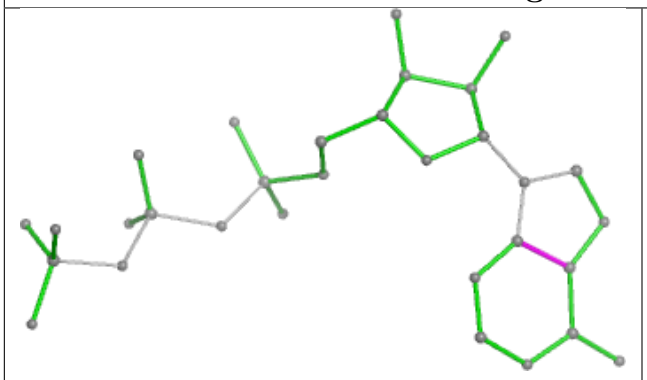


Torsions

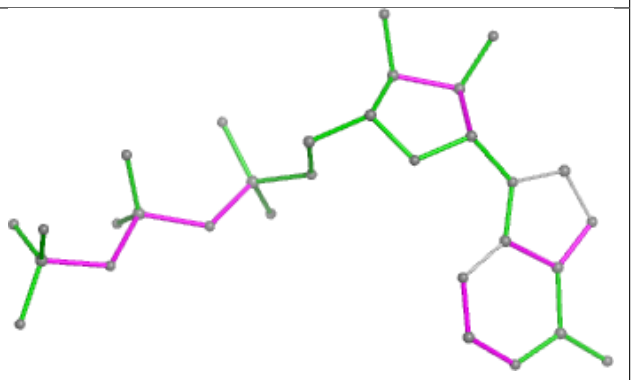


Rings

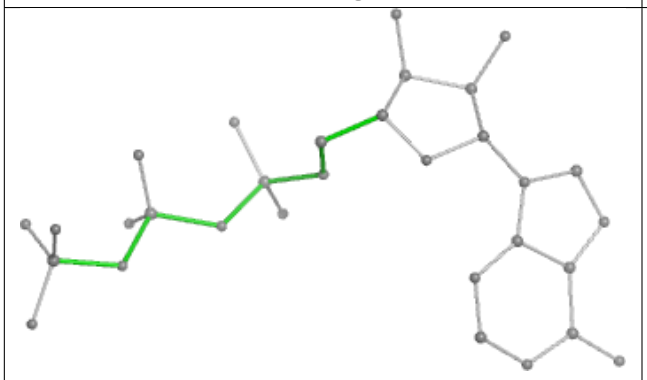
Ligand ATP B 701



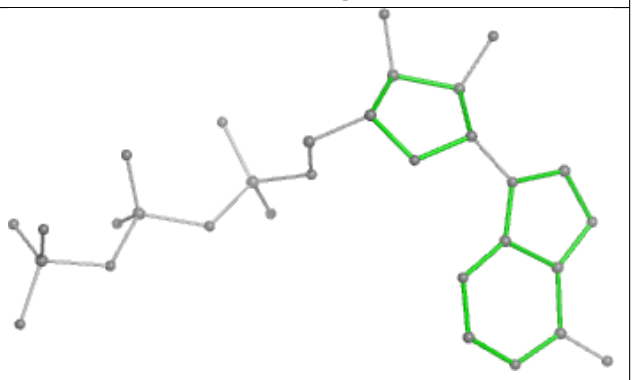
Bond lengths



Bond angles

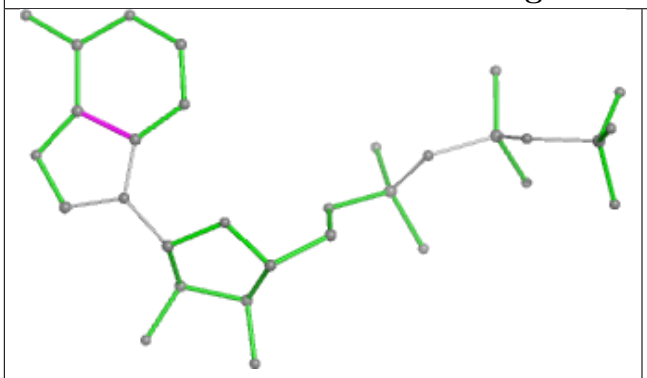


Torsions

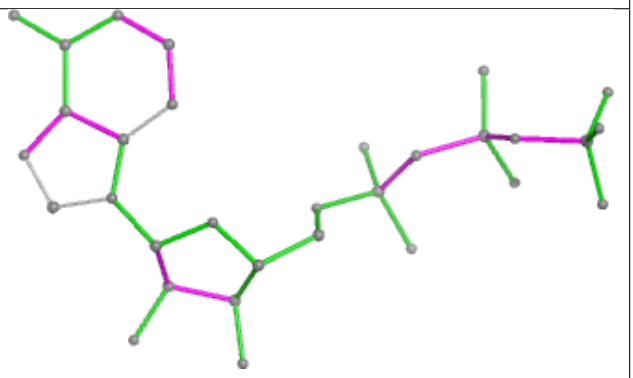


Rings

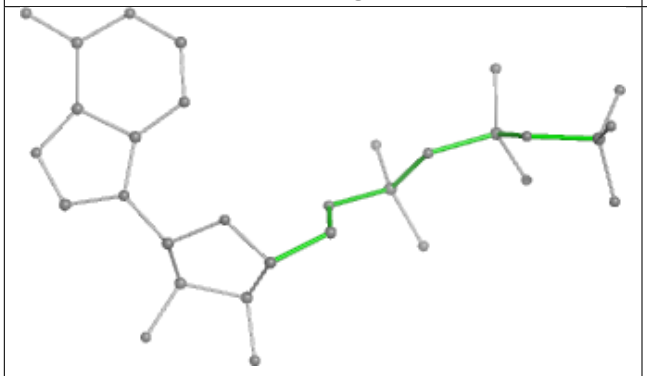
Ligand ATP A 701



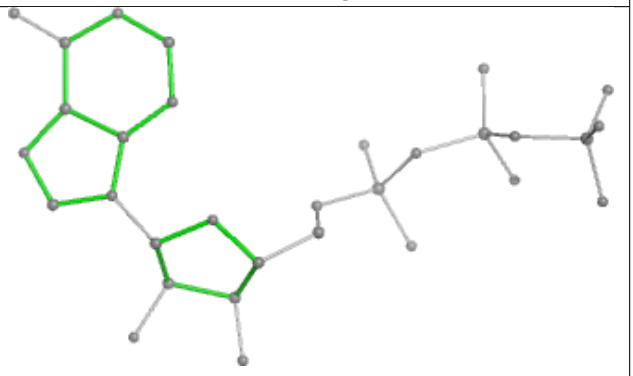
Bond lengths



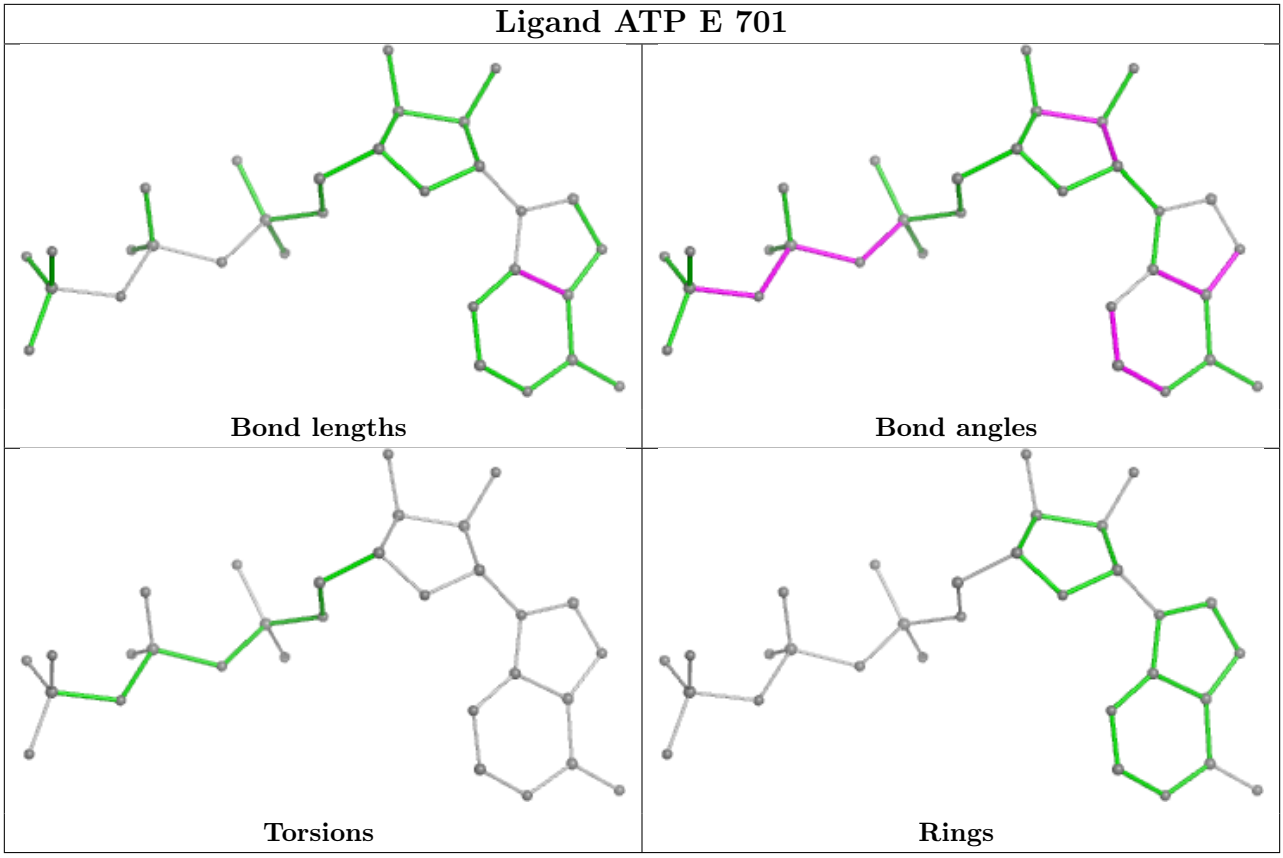
Bond angles



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.

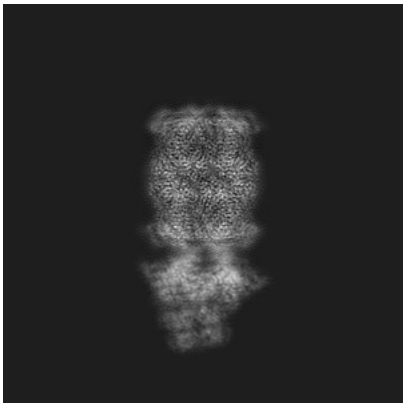
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13697. These allow visual inspection of the internal detail of the map and identification of artifacts.

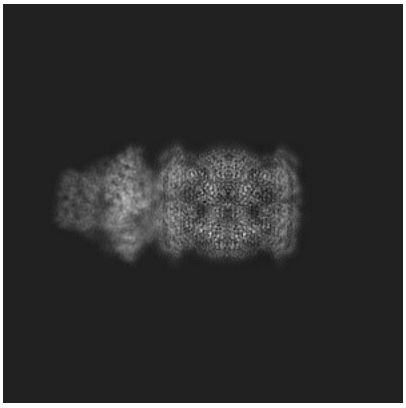
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

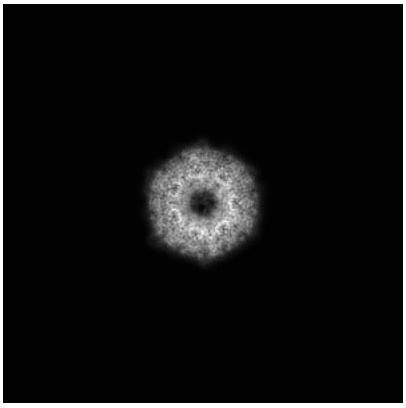
6.1.1 Primary map



X



Y

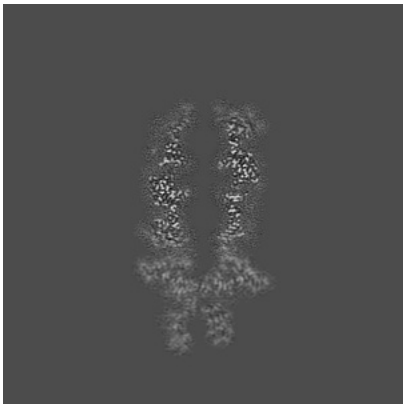


Z

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

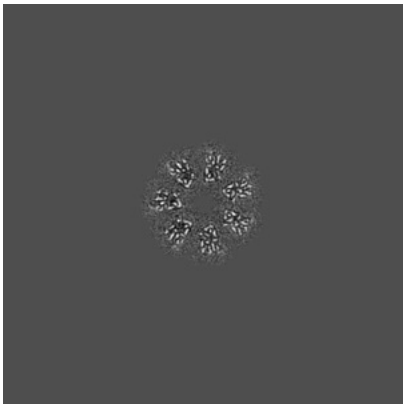
6.2 Central slices (i)

6.2.1 Primary map



X Index: 176

Y Index: 176

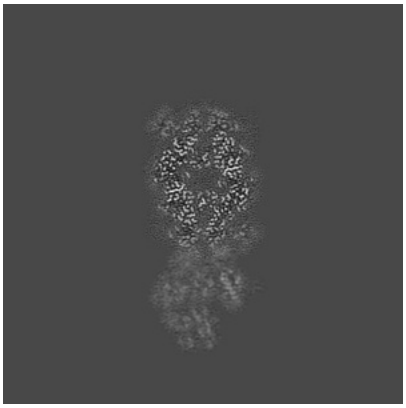


Z Index: 176

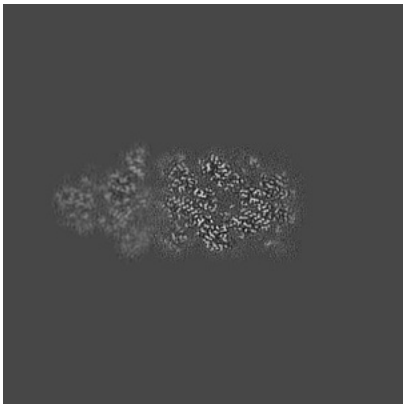
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

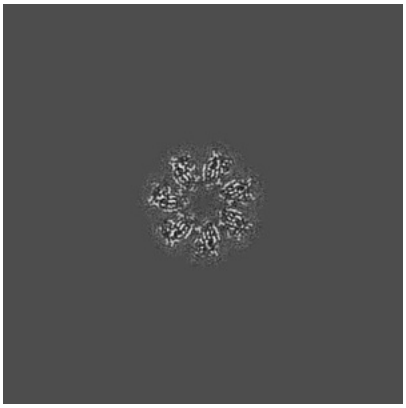
6.3.1 Primary map



X Index: 155



Y Index: 152

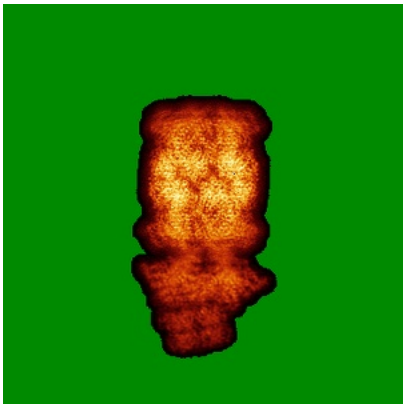


Z Index: 182

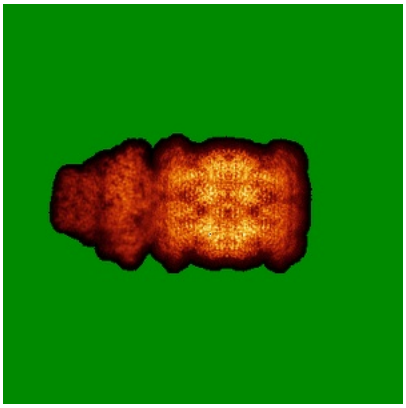
The images above show the largest variance slices of the map in three orthogonal directions.

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

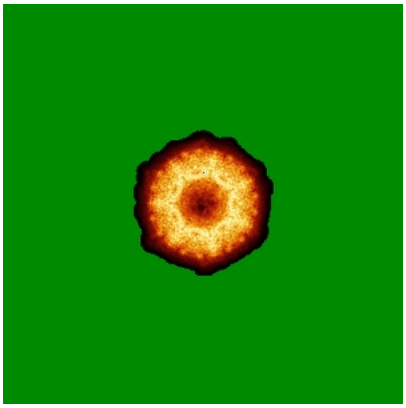
6.4.1 Primary map



X



Y

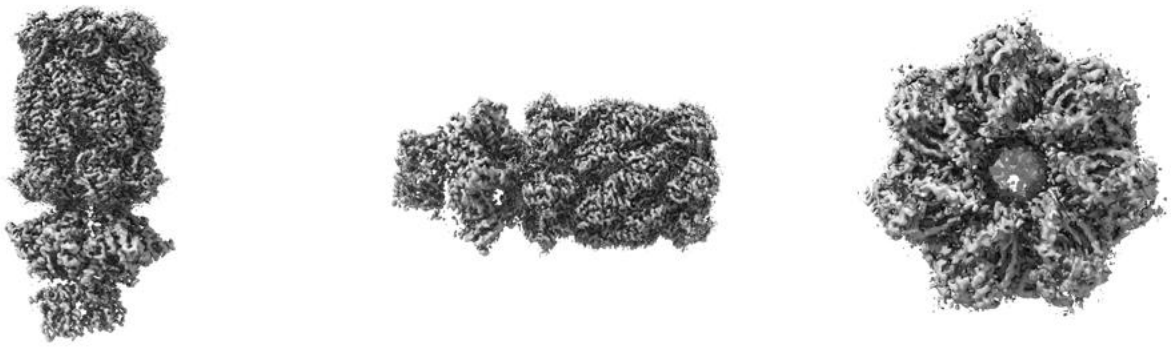


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

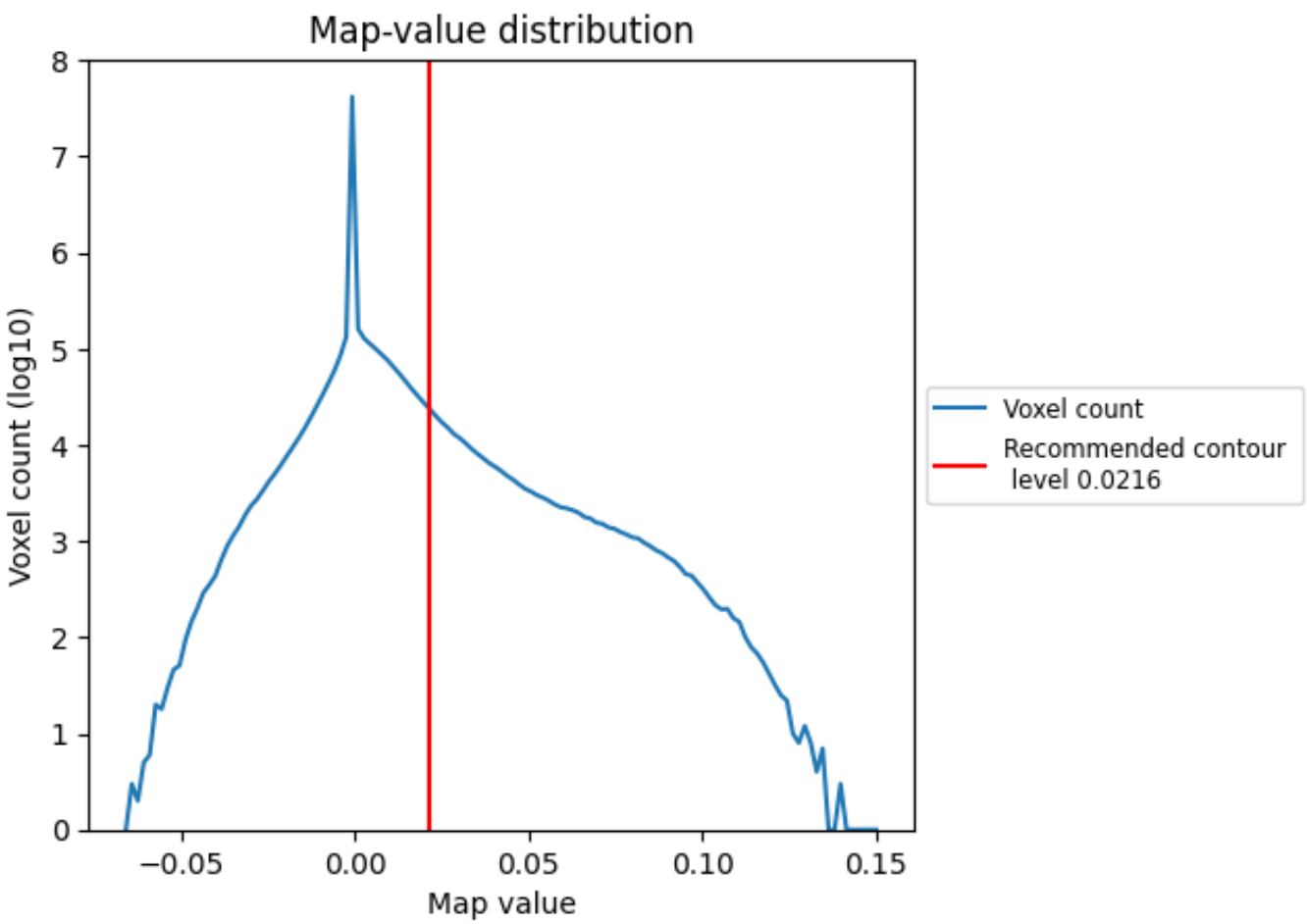
6.6 Mask visualisation (i)

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

7 Map analysis (i)

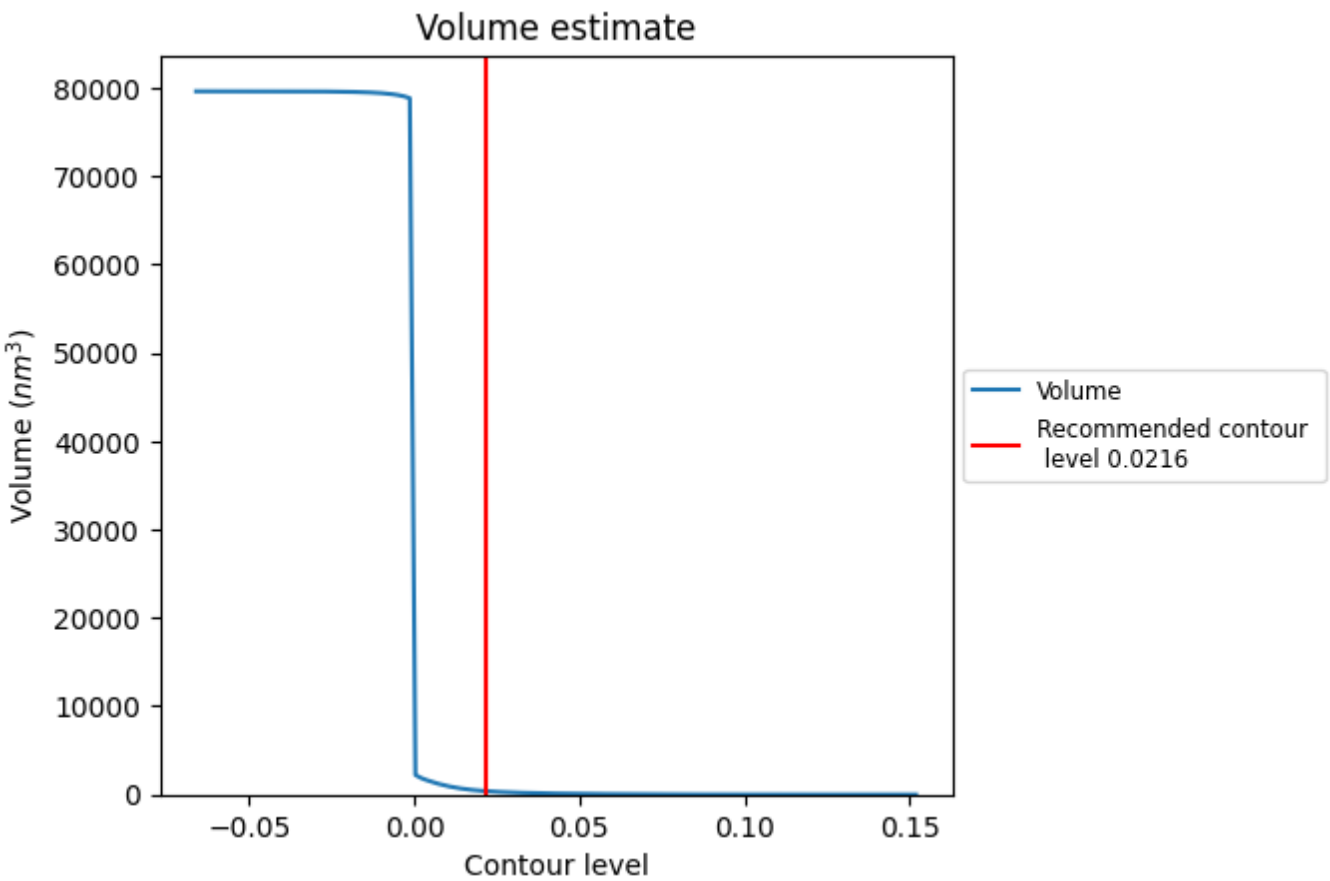
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

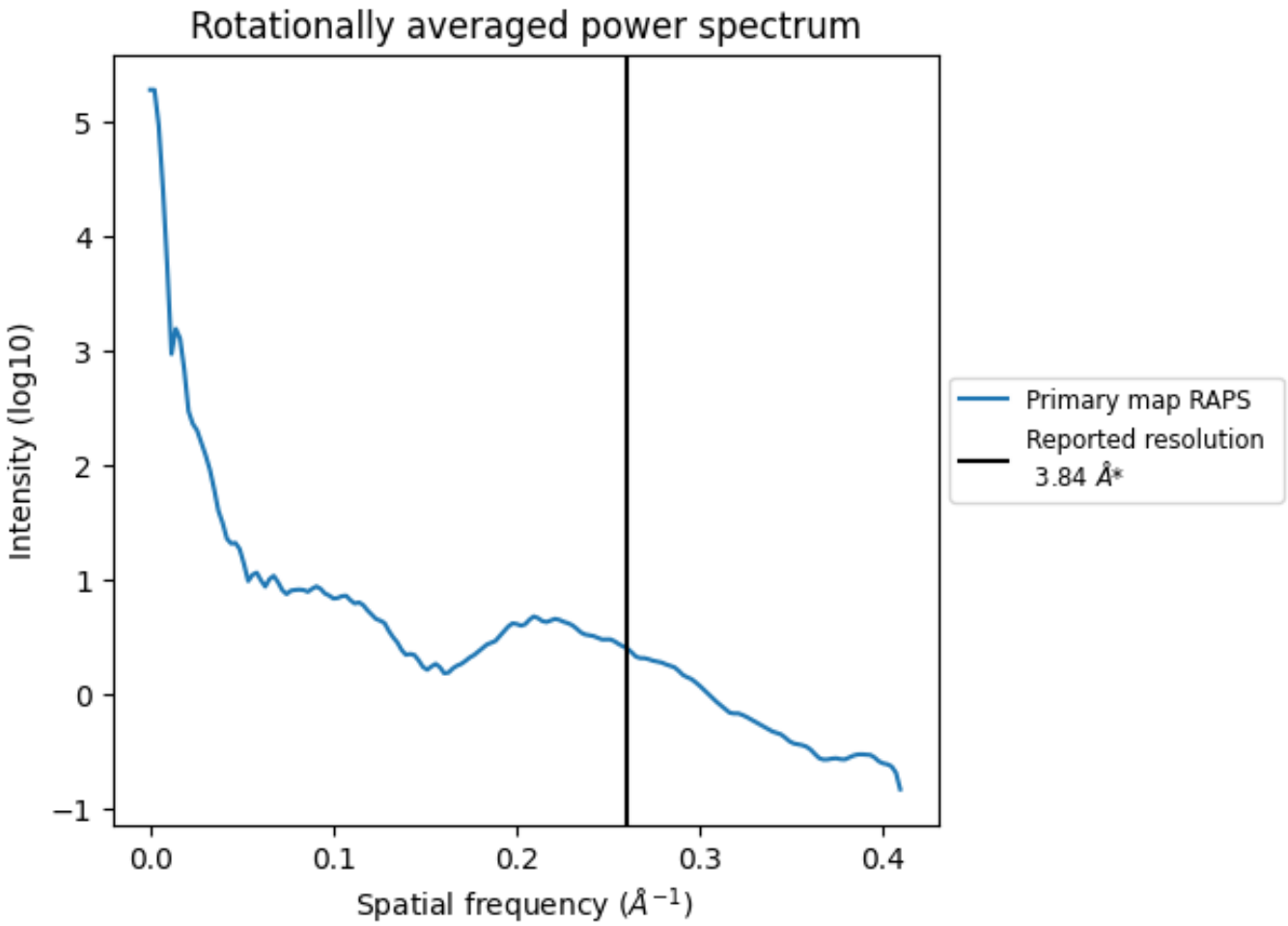
7.2 Volume estimate (i)



The volume at the recommended contour level is 393 nm^3; this corresponds to an approximate mass of 355 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 0.260 Å^{-1}

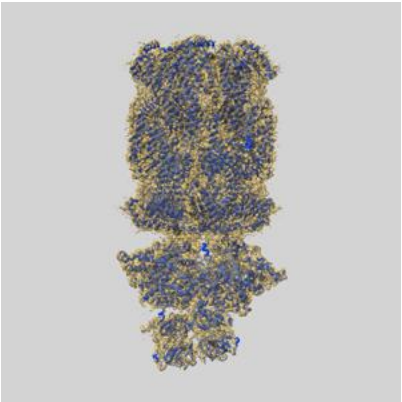
8 Fourier-Shell correlation (i)

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

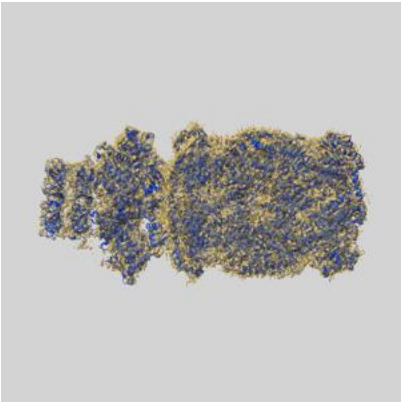
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13697 and PDB model 7PXC. Per-residue inclusion information can be found in section 3 on page 9.

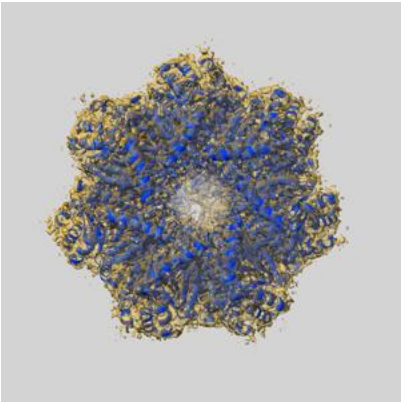
9.1 Map-model overlay (i)



X



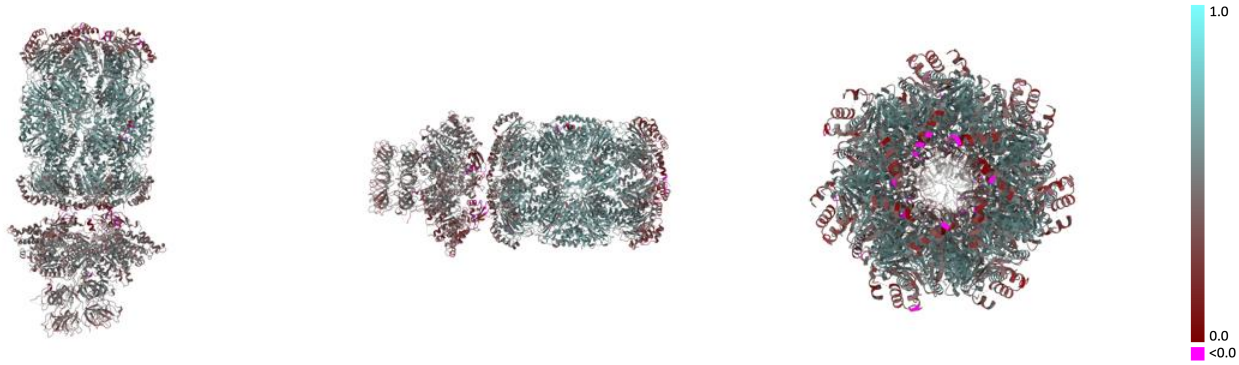
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

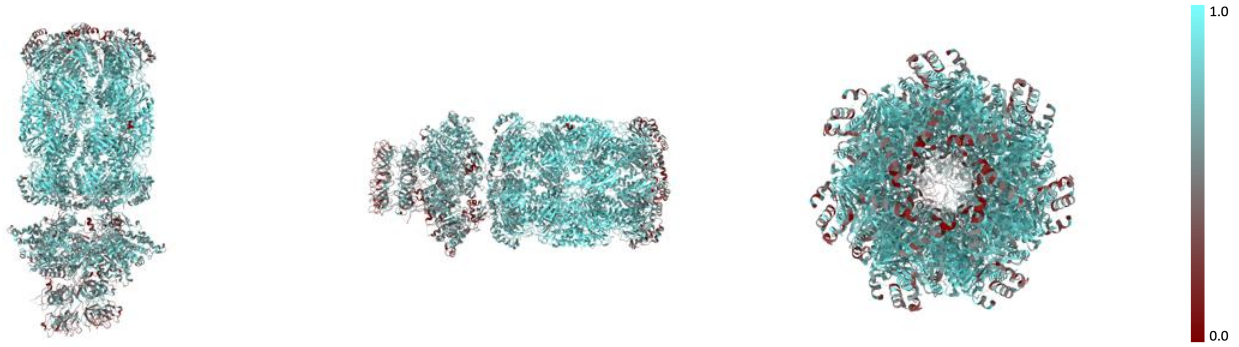
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

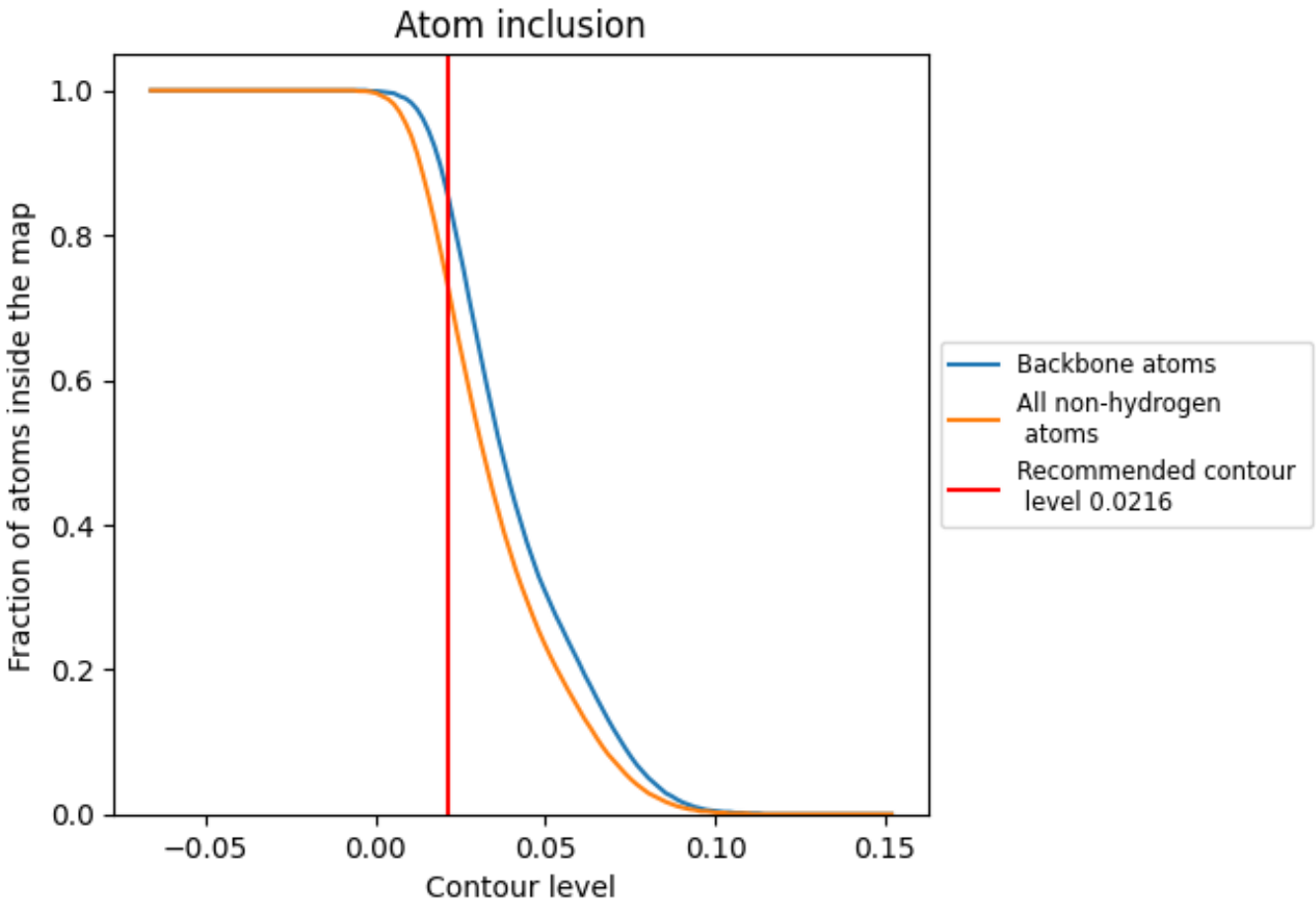
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0216).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.4740
0	0.7930	0.4880
1	0.5610	0.4540
2	0.7960	0.4980
4	0.7920	0.4940
6	0.8000	0.4850
8	0.7940	0.4930
A	0.5360	0.3790
B	0.6240	0.4190
C	0.5380	0.3730
D	0.3700	0.3090
E	0.6330	0.4250
F	0.6110	0.4180
G	0.3730	0.3670
H	0.9100	0.5780
I	0.6410	0.4170
J	0.8950	0.5810
K	0.6460	0.4150
L	0.9060	0.5830
M	0.9070	0.5810
N	0.9010	0.5810
O	0.6510	0.4210
P	0.9010	0.5890
Q	0.6510	0.4210
R	0.8940	0.5840
S	0.9040	0.5850
T	0.6510	0.4200
U	0.8540	0.5560
V	0.8950	0.5770
W	0.8590	0.5570
X	0.6510	0.4180
Y	0.9070	0.5840
Z	0.6480	0.4170
a	0.8910	0.5860
b	0.9010	0.5790

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Chain	Atom inclusion	Q-score
d	0.7890	0.4850
f	0.7930	0.4950