Full wwPDB EM Validation Report ⓘ

Jan 15, 2022 – 08:25 am GMT

PDB ID	:	7PXD
EMDB ID	:	EMD-13698
Title	:	Substrate-engaged mycobacterial Proteasome-associated ATPase in complex with open-gate 20S CP - composite map (state B)
Authors	:	Jomaa, A.; Kavalchuk, M.; Weber-Ban, E.
Deposited on	:	2021-10-08
Resolution	:	4.00 Å(reported)
Based on initial models	:	5KWA, 5LZP

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

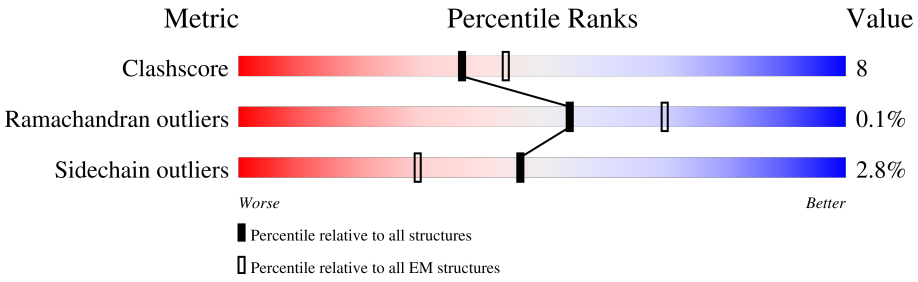
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	248	67% 17% • 13%
1	2	248	71% 14% • 13%
1	4	248	69% 15% • 13%
1	6	248	68% 17% • 13%
1	8	248	70% 14% • 13%
1	I	248	10% 63% 20% • 14%
1	K	248	7% 67% 19% • 12%
1	O	248	6% 69% 16% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	248	7% 67% 16% 13%
1	T	248	7% 66% 18% 14%
1	X	248	10% 69% 16% 14%
1	Z	248	12% 65% 20% 13%
1	d	248	83% 13%
1	f	248	82% 13%
2	1	609	99%
2	A	609	10% 58% 19% 23%
2	B	609	8% 53% 25% 21%
2	C	609	20% 53% 24% 23%
2	D	609	23% 52% 23% 25%
2	E	609	10% 60% 19% 21%
2	F	609	13% 58% 21% 21%
3	G	66	14% 23% 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%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Y	291	
4	a	291	
4	b	291	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 68900 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
1	0	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	2	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	4	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	6	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	8	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	I	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	K	217	Total	C	N	O	S	0	0
			1668	1044	305	316	3		
1	O	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	Q	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	T	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	X	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	Z	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	d	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	f	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

- Molecule 2 is a protein called AAA ATPase forming ring-shaped complexes.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	471	Total	C	N	O	S	0	0
			3692	2334	636	711	11		
2	B	481	Total	C	N	O	S	0	0
			3761	2371	648	731	11		
2	C	471	Total	C	N	O	S	0	0
			3685	2326	634	714	11		
2	D	457	Total	C	N	O	S	0	0
			3584	2270	613	690	11		
2	E	483	Total	C	N	O	S	0	0
			3775	2378	651	735	11		
2	F	483	Total	C	N	O	S	0	0
			3773	2377	651	734	11		

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP A0A045GWT8
G	0	SER	-	expression tag	UNP A0A045GWT8

- Molecule 4 is a protein called Proteasome subunit beta.

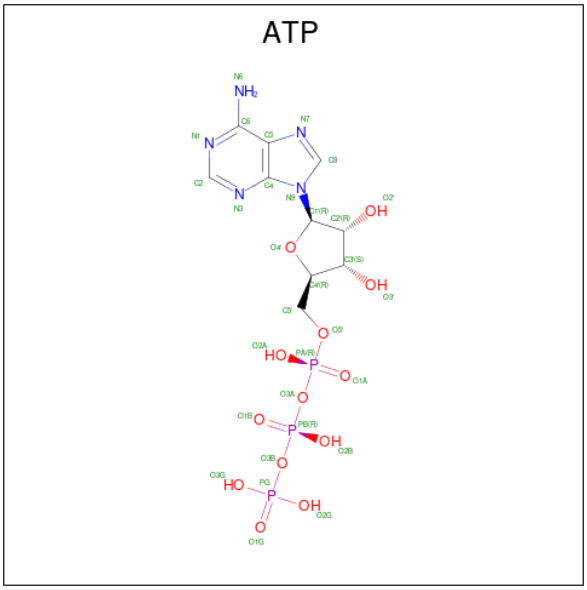
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
4	J	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
4	L	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
4	M	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
4	N	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
4	P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

Continued on next page...

Continued from previous page...

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

- 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
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

Continued from previous page...

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

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

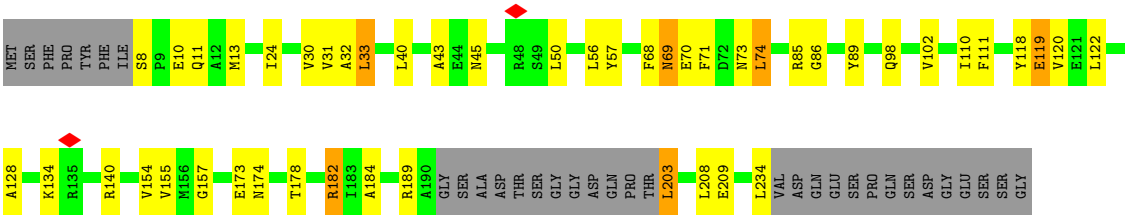
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

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.

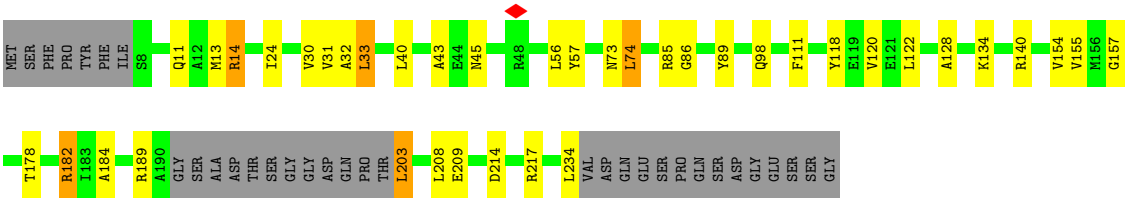
• Molecule 1: Proteasome subunit alpha

Chain 0:



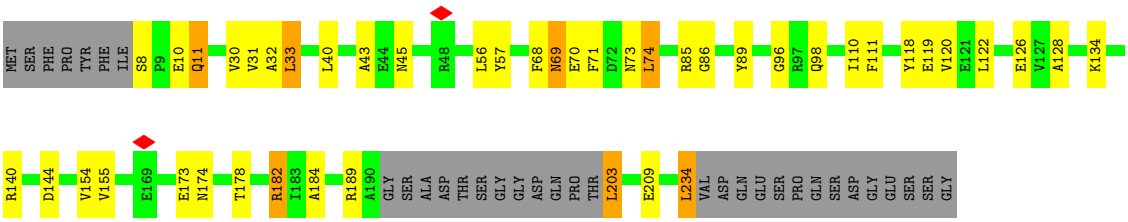
• Molecule 1: Proteasome subunit alpha

Chain 2:



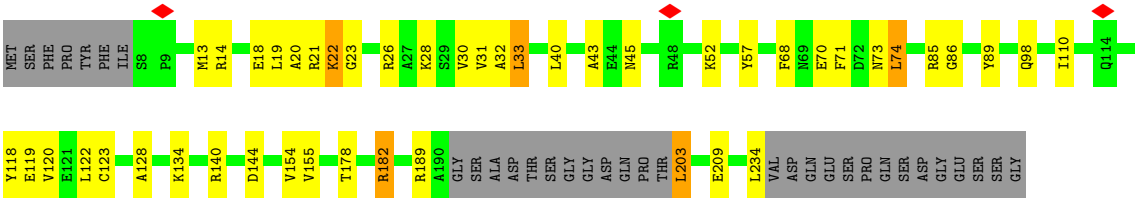
• Molecule 1: Proteasome subunit alpha

Chain 4:



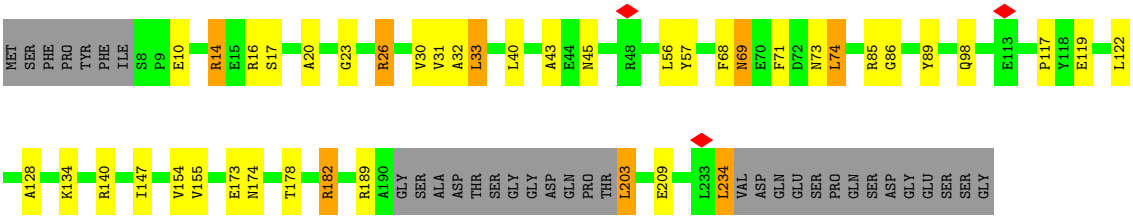
• Molecule 1: Proteasome subunit alpha

Chain 6:



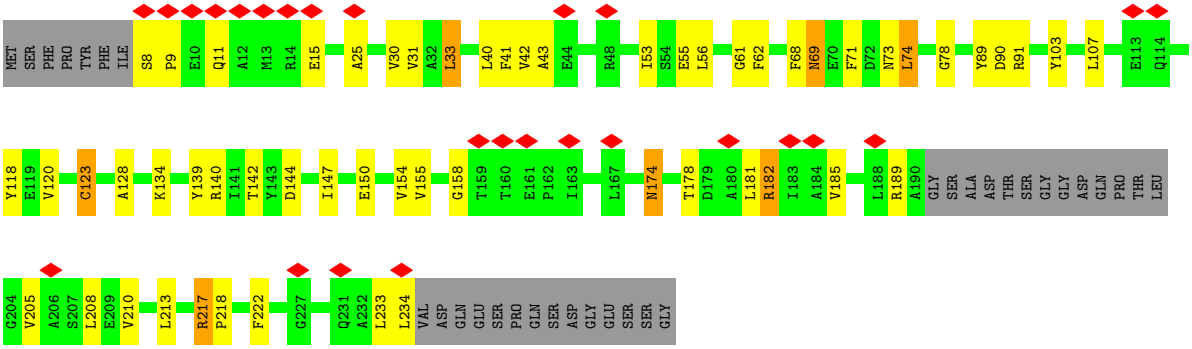
• Molecule 1: Proteasome subunit alpha

Chain 8:



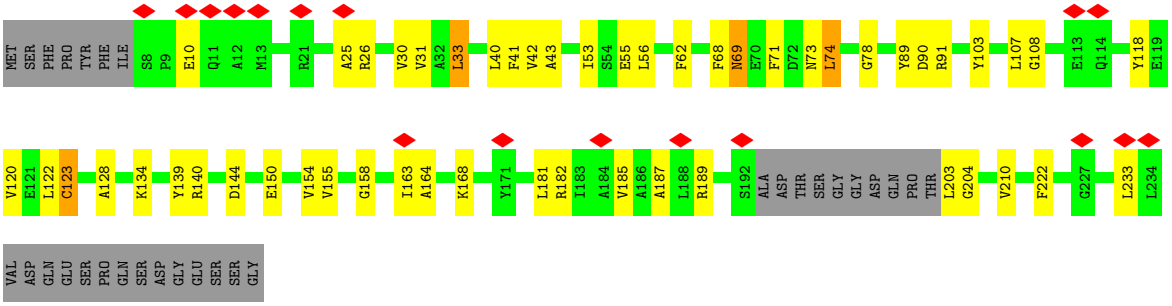
• Molecule 1: Proteasome subunit alpha

Chain I:



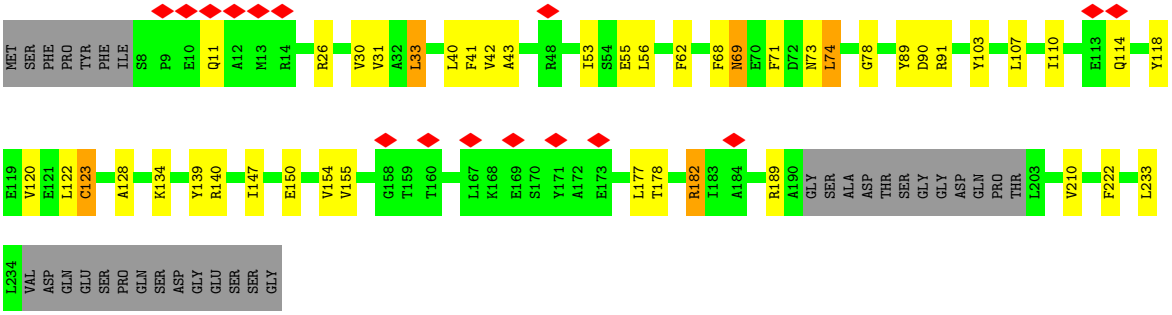
• Molecule 1: Proteasome subunit alpha

Chain K:



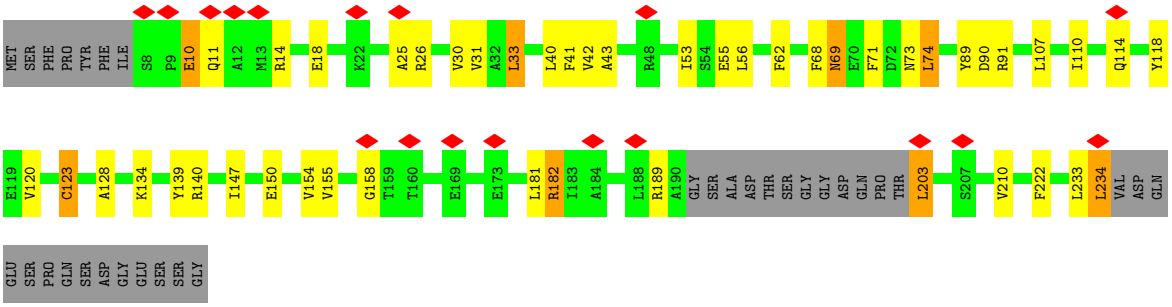
• Molecule 1: Proteasome subunit alpha

Chain O:



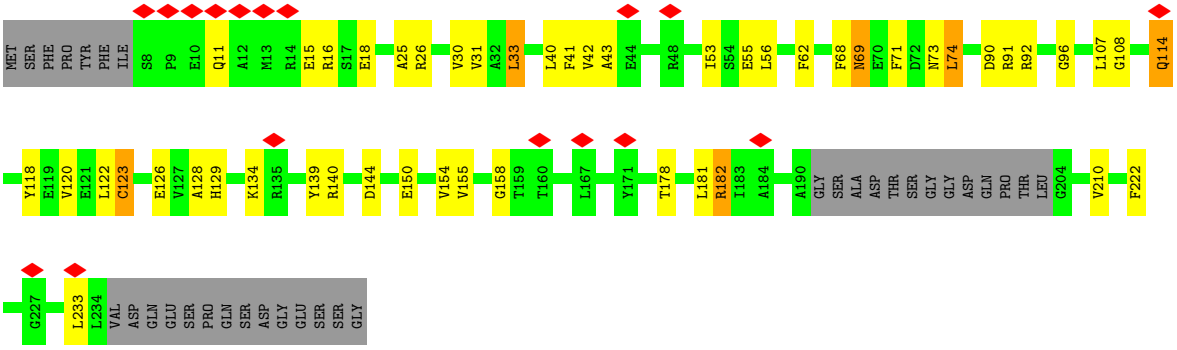
• Molecule 1: Proteasome subunit alpha

Chain Q:



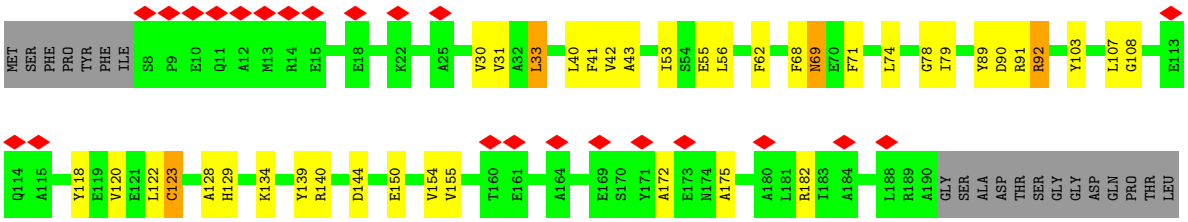
• Molecule 1: Proteasome subunit alpha

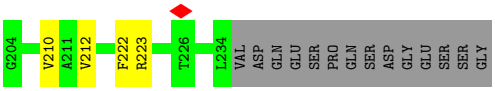
Chain T:



• Molecule 1: Proteasome subunit alpha

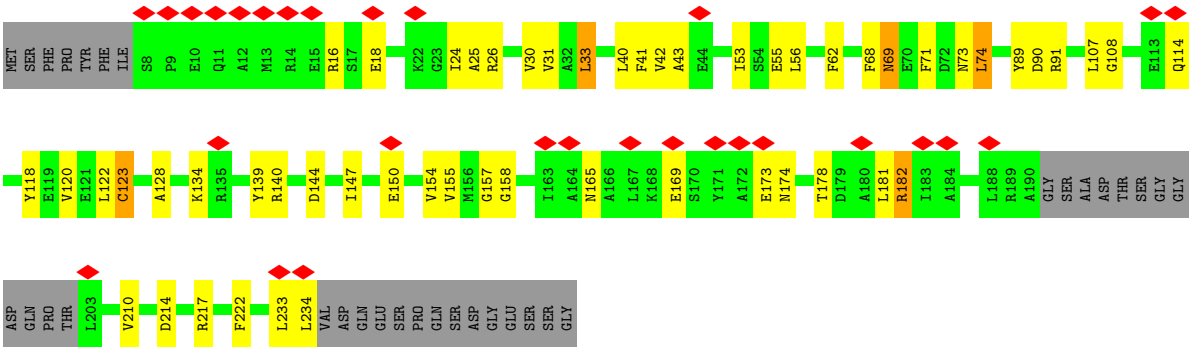
Chain X:





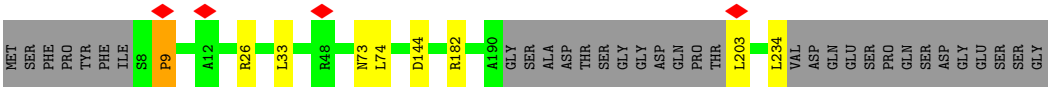
• Molecule 1: Proteasome subunit alpha

Chain Z:



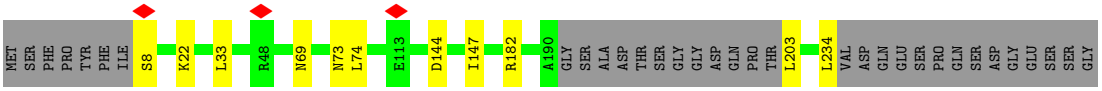
• Molecule 1: Proteasome subunit alpha

Chain d:



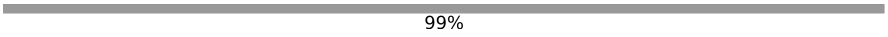
• Molecule 1: Proteasome subunit alpha

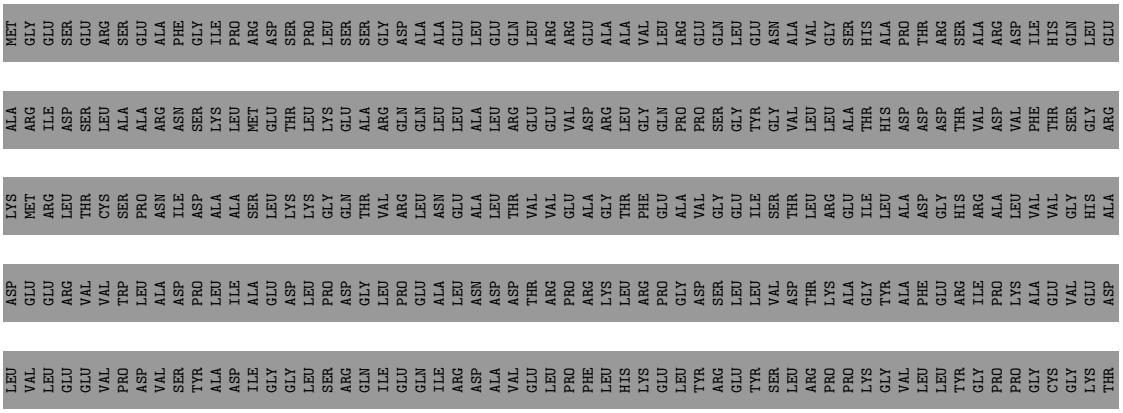
Chain f:



• Molecule 2: AAA ATPase forming ring-shaped complexes

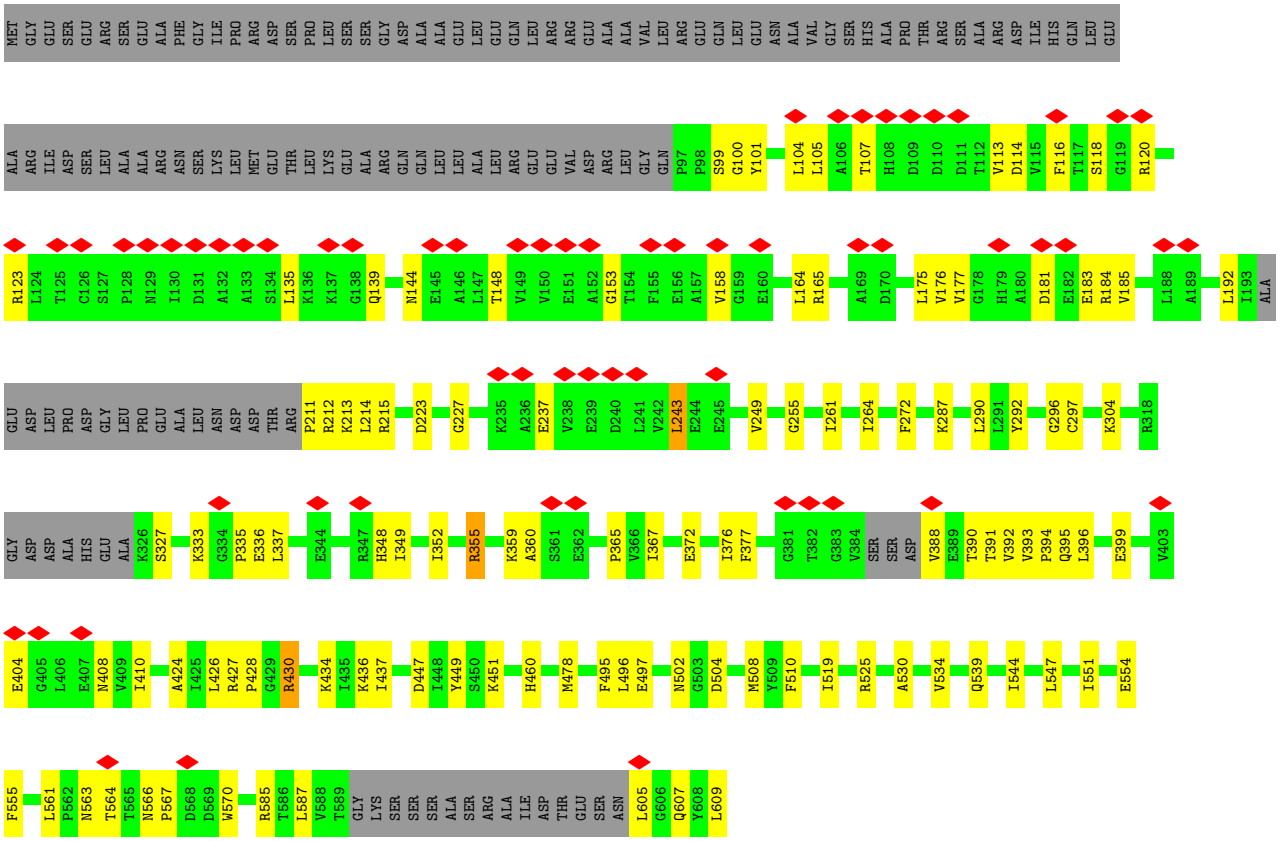
Chain 1:





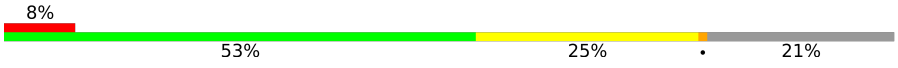
• Molecule 2: AAA ATPase forming ring-shaped complexes

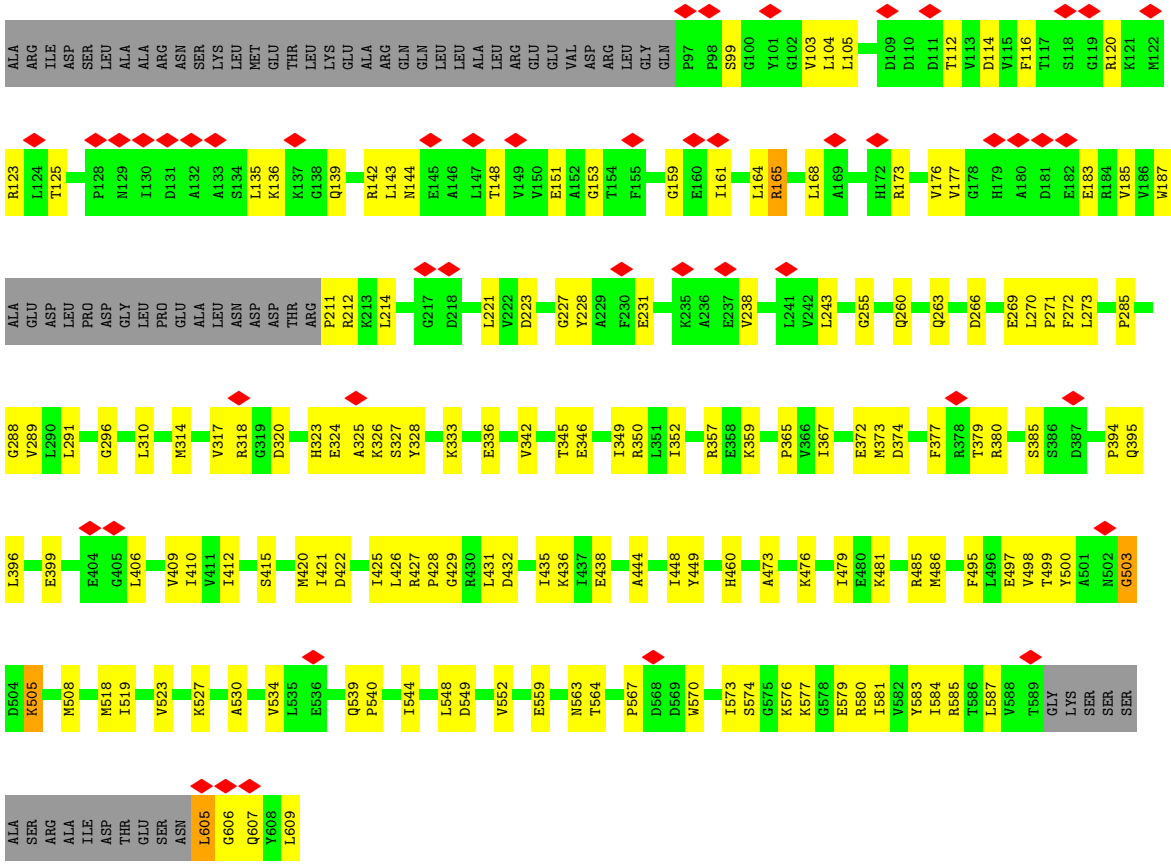
Chain A:



• Molecule 2: AAA ATPase forming ring-shaped complexes

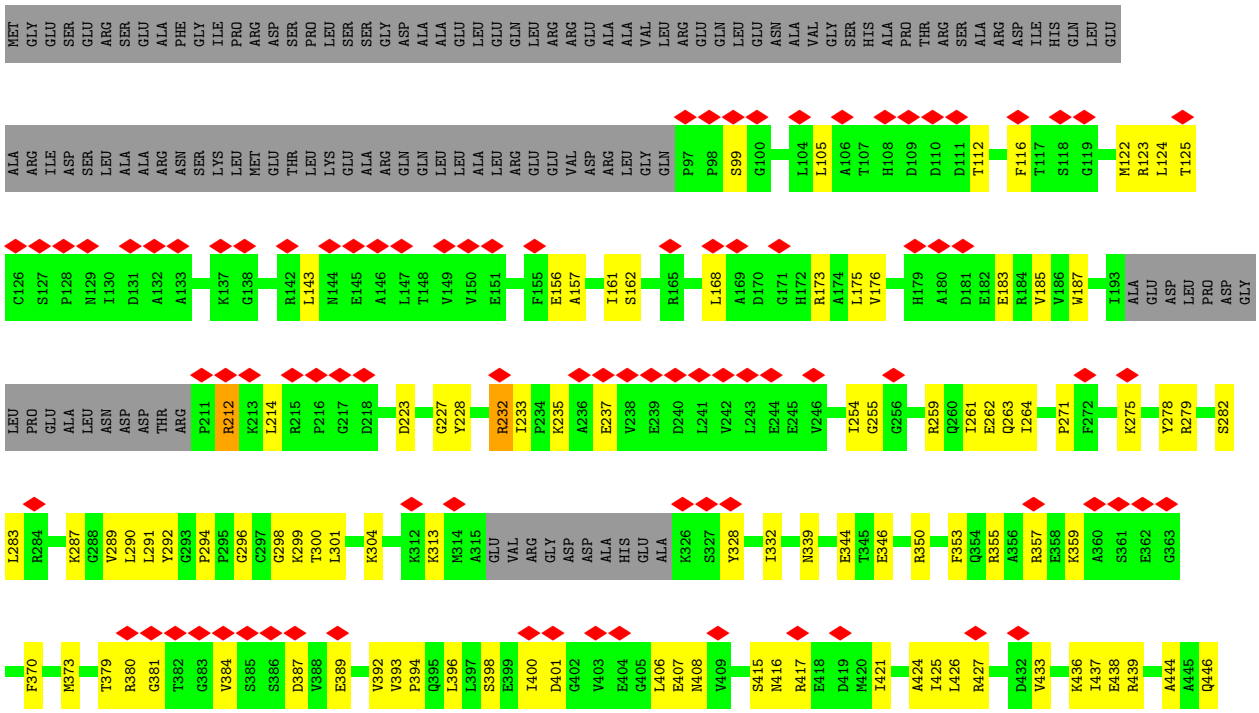
Chain B:

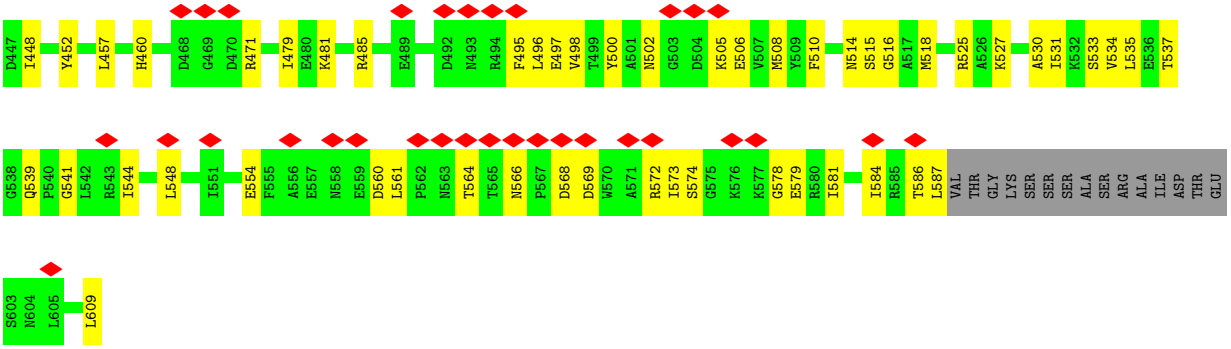




• Molecule 2: AAA ATPase forming ring-shaped complexes

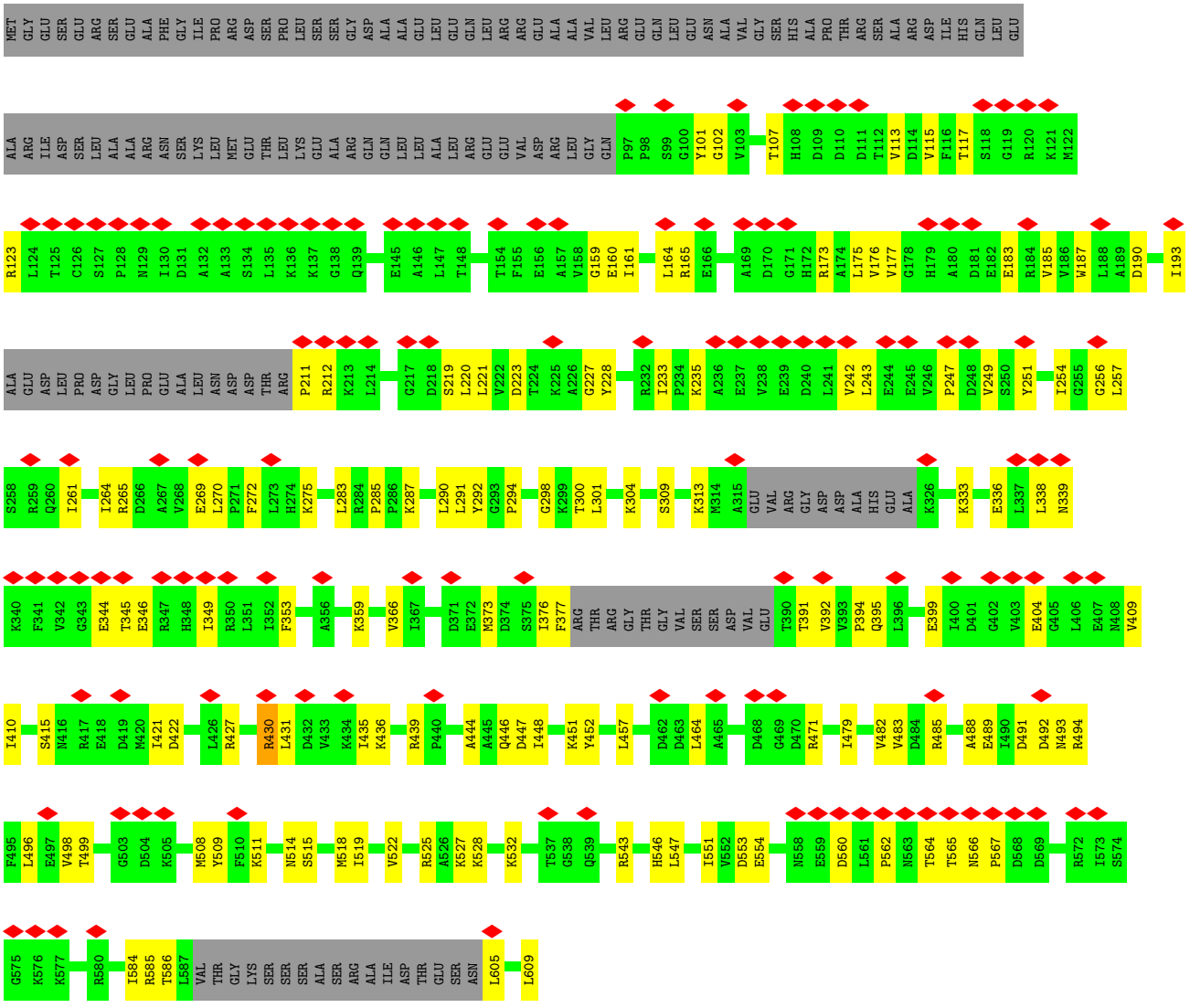
Chain C:





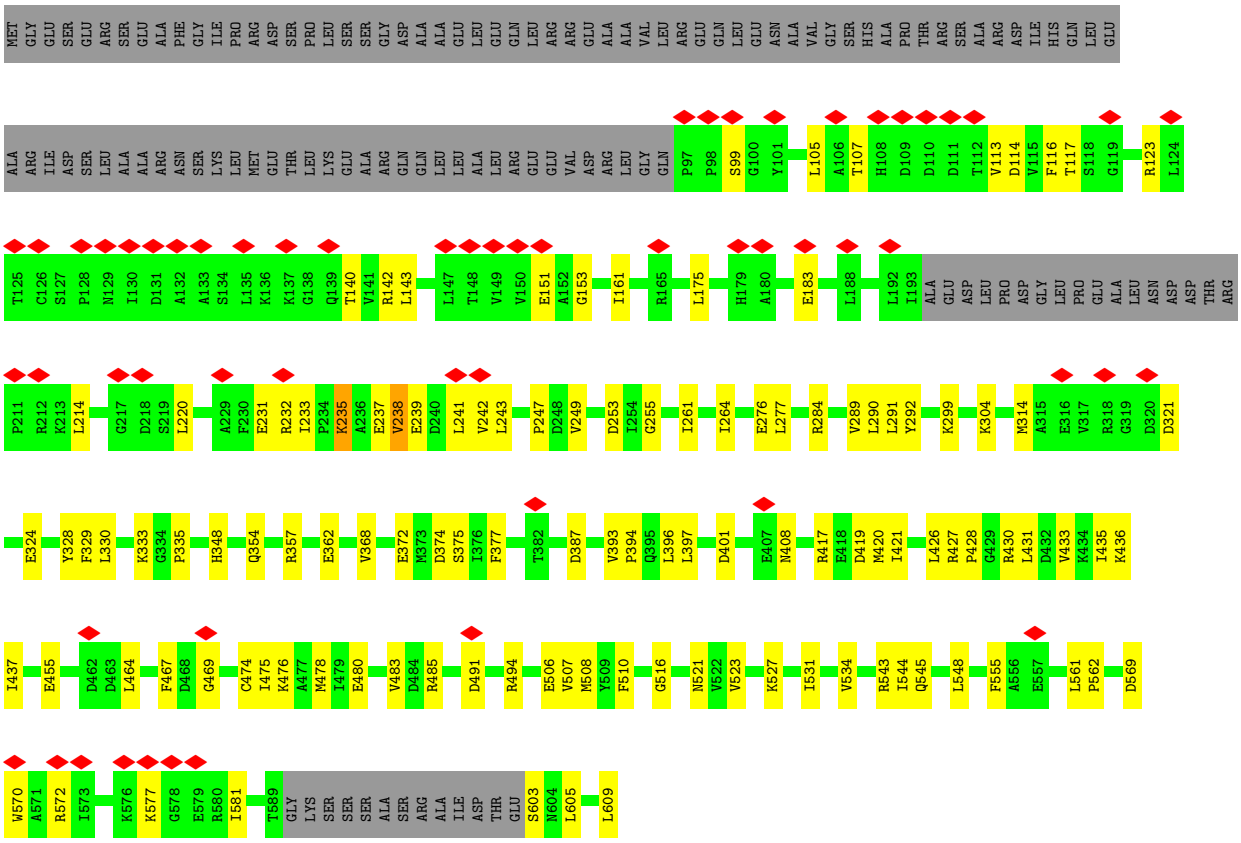
• Molecule 2: AAA ATPase forming ring-shaped complexes

Chain D:



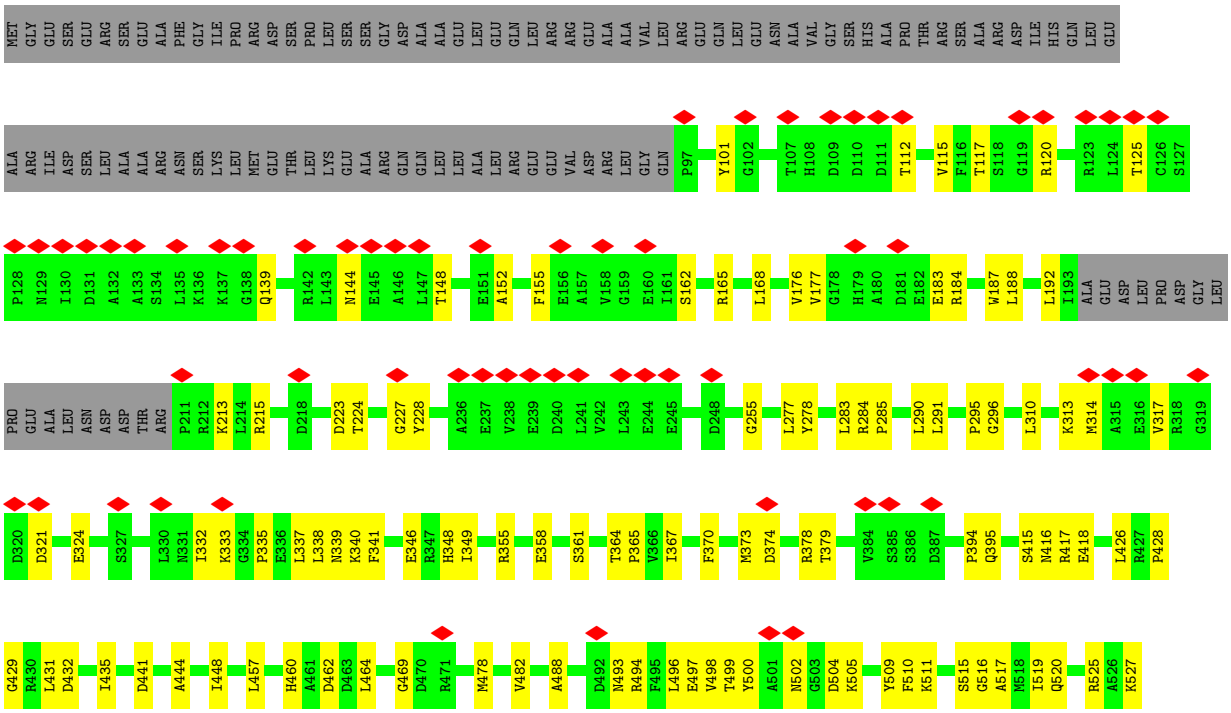
• Molecule 2: AAA ATPase forming ring-shaped complexes

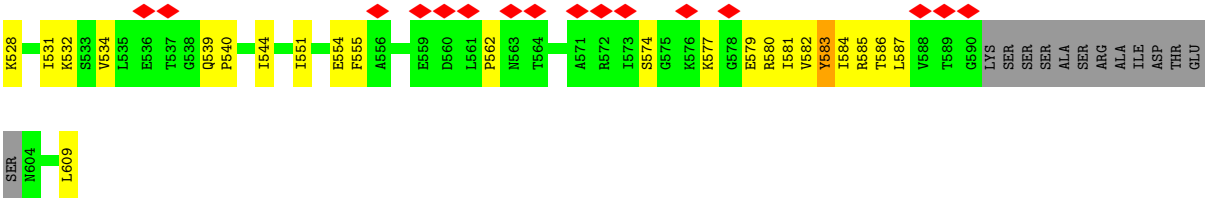
Chain E:



• Molecule 2: AAA ATPase forming ring-shaped complexes

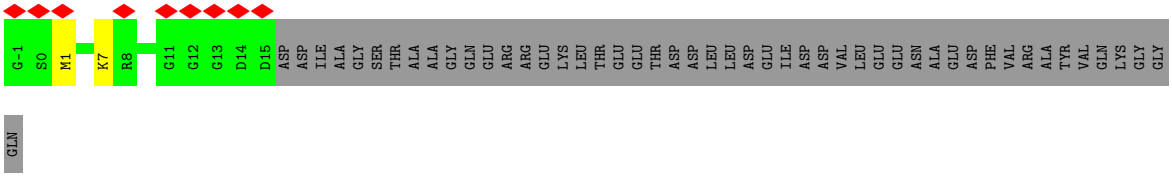
Chain F:





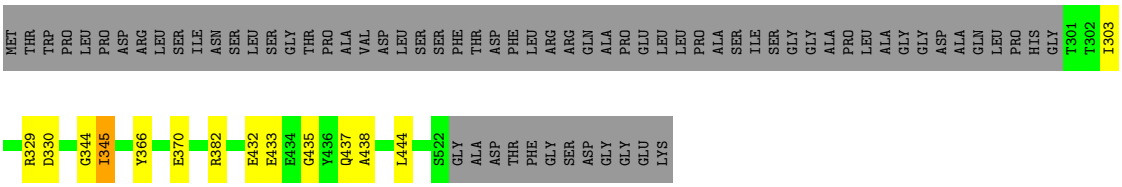
• Molecule 3: Prokaryotic ubiquitin-like protein Pup

Chain G:



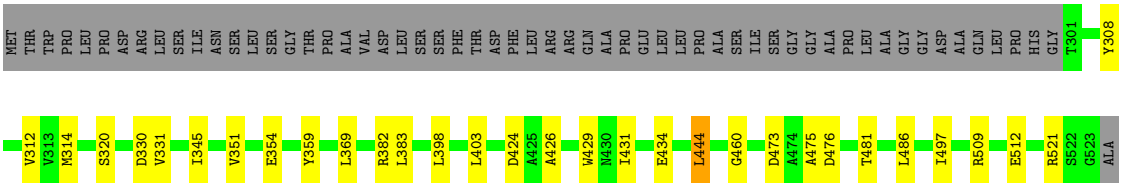
• Molecule 4: Proteasome subunit beta

Chain H:



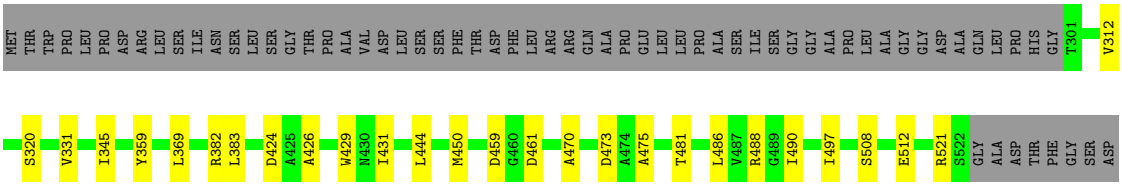
• Molecule 4: Proteasome subunit beta

Chain J:



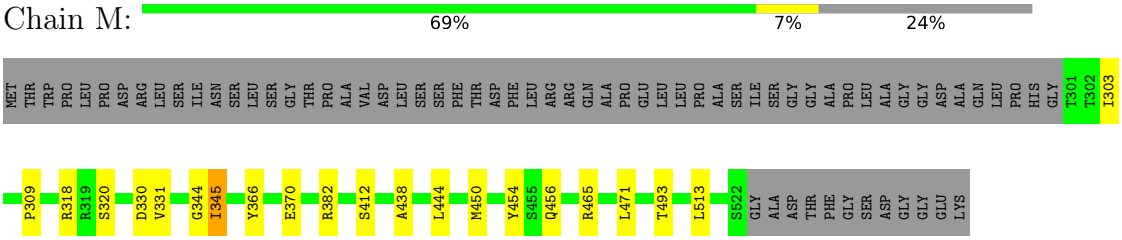
• Molecule 4: Proteasome subunit beta

Chain L:



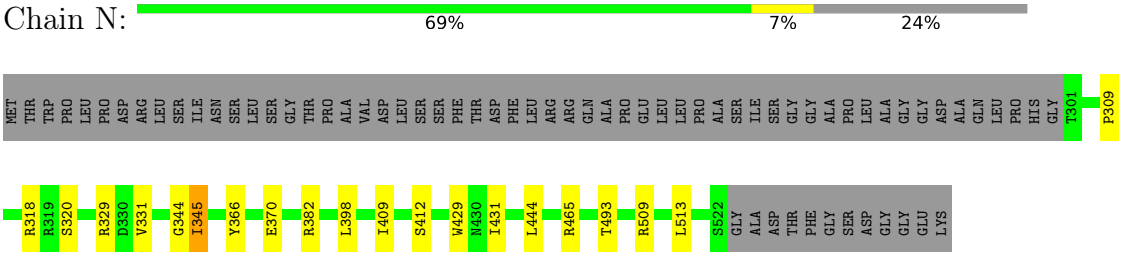
• Molecule 4: Proteasome subunit beta

Chain M:



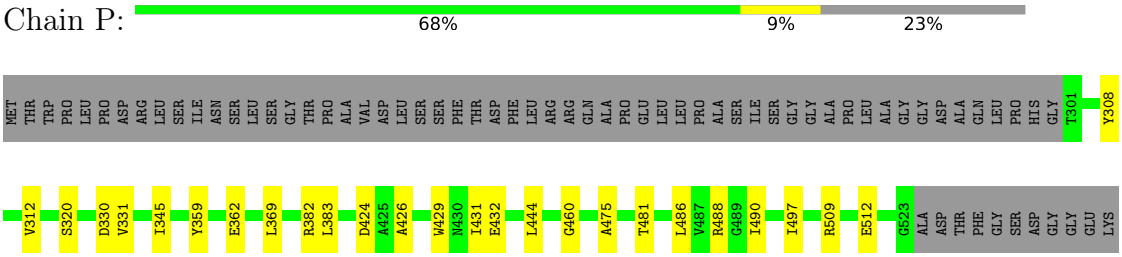
• Molecule 4: Proteasome subunit beta

Chain N:



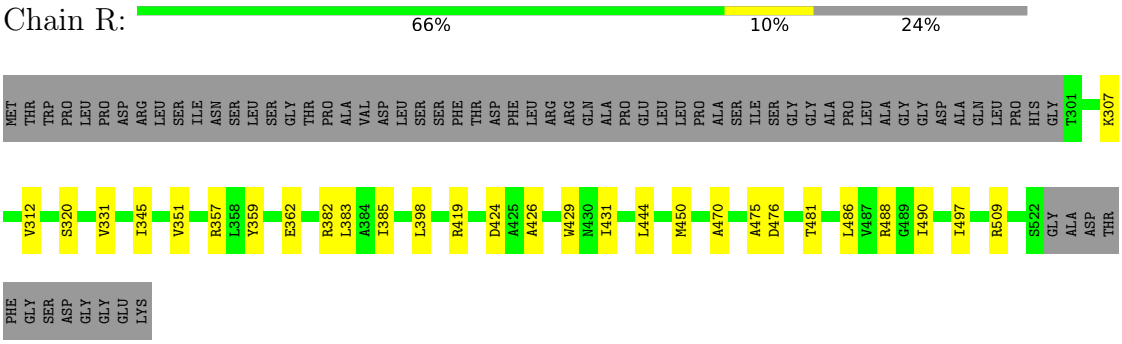
• Molecule 4: Proteasome subunit beta

Chain P:



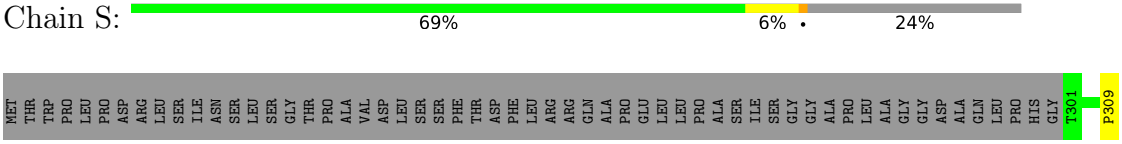
• Molecule 4: Proteasome subunit beta

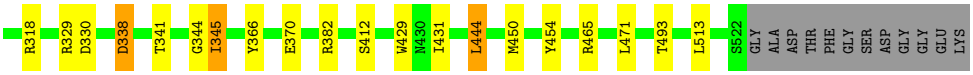
Chain R:



• Molecule 4: Proteasome subunit beta

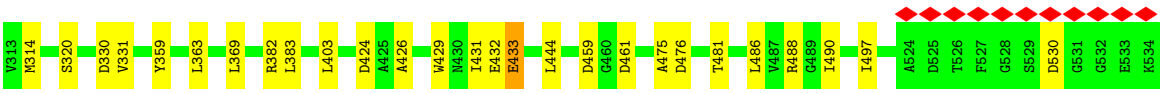
Chain S:





• Molecule 4: Proteasome subunit beta

Chain U:

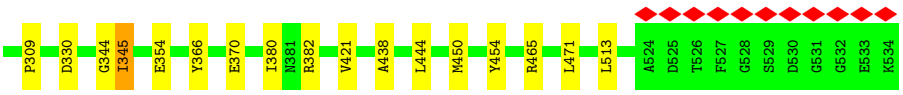


• Molecule 4: Proteasome subunit beta

Chain V:

• Molecule 4: Proteasome subunit beta

Chain W:

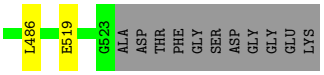


• Molecule 4: Proteasome subunit beta

Chain Y:

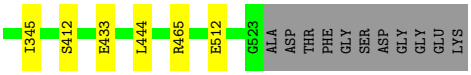
• Molecule 4: Proteasome subunit beta

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	50814	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	0.003	Depositor
Recommended contour level	0.0177	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: ATP, MG

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	0.43	0/1683	0.59	0/2274
1	f	0.47	0/1683	0.59	0/2274
2	1	0.57	0/42	0.55	0/54
2	A	0.30	0/3751	0.47	0/5069
2	B	0.29	0/3823	0.46	0/5170
2	C	0.31	0/3745	0.47	0/5062
2	D	0.27	0/3643	0.46	0/4923
2	E	0.29	0/3837	0.45	0/5189
2	F	0.32	0/3835	0.47	0/5186
3	G	0.23	0/111	0.43	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	0/69759	0.53	0/94368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	39	0
1	2	1658	0	1659	29	0
1	4	1658	0	1659	53	0
1	6	1658	0	1659	35	0
1	8	1658	0	1659	31	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
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	3692	0	3718	95	0
2	B	3761	0	3768	124	0
2	C	3685	0	3700	109	0
2	D	3584	0	3604	103	0
2	E	3775	0	3779	83	0
2	F	3773	0	3777	108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	112	0	102	1	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	2	0
5	B	31	0	12	2	0
5	C	31	0	12	6	0
5	D	31	0	12	1	0
5	E	31	0	12	2	0
5	F	31	0	12	7	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	68900	0	68660	1058	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 8.

All (1058) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:373:MET:HB3	2:B:415:SER:HB3	1.46	0.95
1:0:111:PHE:CE2	2:D:605:LEU:HD23	2.00	0.95
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
1:6:26:ARG:HH12	2:F:502:ASN:HB2	1.38	0.85
1:X:42:VAL:HG22	1:X:210:VAL:HG22	1.62	0.82
2:B:429:GLY:H	2:B:432:ASP:HB3	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
1:2:111:PHE:HE2	2:A:605:LEU:CD2	1.94	0.80
2:E:220:LEU:HD23	2:E:232:ARG:HB3	1.61	0.80
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.64	0.80
4:J:509:ARG:NH1	4:J:512:GLU:OE1	2.14	0.79
2:A:426:LEU:HD12	2:A:434:LYS:HE3	1.64	0.79
1:K:140:ARG:NH1	1:K:154:VAL:HG13	1.99	0.78
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.66	0.77
1:Z:31:VAL:HG12	1:Z:155:VAL:HG22	1.66	0.77
2:A:118:SER:HB3	2:A:120:ARG:HH12	1.49	0.77
1:I:140:ARG:NH1	1:I:154:VAL:HG13	2.00	0.77
2:C:161:ILE:HD11	2:D:185:VAL:HG23	1.67	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
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
2:F:482:VAL:HG23	2:F:551:ILE:HD11	1.68	0.75
1:8:10:GLU:HB2	2:F:582:VAL:HG11	1.68	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
2:F:502:ASN:HB3	2:F:579:GLU:HG2	1.69	0.74
1:O:42:VAL:HG22	1:O:210:VAL:HG22	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:VAL:HG22	1:K:210:VAL:HG22	1.69	0.74
2:1:605:LEU:HD21	1:4:111:PHE:CG	2.22	0.74
2:B:142:ARG:HH21	2:B:151:GLU:HG2	1.51	0.74
1:T:42:VAL:HG22	1:T:210:VAL:HG22	1.68	0.74
2:A:237:GLU:HB2	2:B:165:ARG:HH12	1.53	0.73
2:B:563:ASN:OD1	2:B:564:THR:N	2.22	0.72
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:449:TYR:OH	2:B:486:MET:SD	2.46	0.71
2:C:393:VAL:HG23	2:C:425:ILE:HD11	1.71	0.71
2:A:372:GLU:OE2	2:B:380:ARG:NH2	2.23	0.71
2:E:603:SER:O	2:F:504:ASP:HA	1.91	0.70
1:0:111:PHE:CE2	2:D:605:LEU:CD2	2.73	0.70
2:C:569:ASP:O	2:C:572:ARG:HG2	1.92	0.70
2:F:494:ARG:HB3	2:F:587:LEU:HD13	1.71	0.70
2:F:574:SER:HB2	2:F:581:ILE:HG13	1.74	0.70
2:A:243:LEU:HD21	2:A:327:SER:HA	1.73	0.70
1:0:111:PHE:HE2	2:D:605:LEU:CD2	1.99	0.70
2:A:563:ASN:HD22	2:B:426:LEU:HB3	1.57	0.70
2:F:577:LYS:HE3	2:F:579:GLU:HB2	1.74	0.69
2:C:339:ASN:HD22	2:C:344:GLU:HG2	1.57	0.69
2:E:508:MET:HE1	2:E:570:TRP:HE1	1.56	0.69
1:X:74:LEU:HD23	1:X:122:LEU:HD11	1.75	0.69
2:1:605:LEU:HD22	1:4:144:ASP:C	2.14	0.67
2:F:517:ALA:HB2	5:F:701:ATP:H4'	1.76	0.67
2:1:605:LEU:HD23	1:4:144:ASP:HB3	1.70	0.67
2:B:266:ASP:HA	2:B:270:LEU:HD13	1.77	0.67
2:B:449:TYR:HB3	2:B:479:ILE:HG12	1.77	0.67
2:C:485:ARG:HD3	2:C:548:LEU:HD22	1.77	0.67
2:F:295:PRO:HG3	2:F:416:ASN:HD21	1.59	0.67
2:B:255:GLY:O	5:B:701:ATP:N6	2.28	0.66
2:D:333:LYS:HE2	2:D:336:GLU:HG2	1.75	0.66
2:A:365:PRO:HA	2:A:408:ASN:HB2	1.78	0.66
2:A:349:ILE:HD13	2:A:396:LEU:HD21	1.76	0.66
2:F:516:GLY:HA3	5:F:701:ATP:N3	2.11	0.66
2:B:374:ASP:HA	2:B:421:ILE:HD11	1.78	0.65
2:C:379:THR:HG22	2:C:381:GLY:H	1.61	0.65
2:B:485:ARG:HD3	2:B:548:LEU:HD22	1.77	0.65
2:E:570:TRP:HB3	2:E:581:ILE:HD12	1.78	0.65
2:B:243:LEU:HD11	2:B:327:SER:HA	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:242:VAL:HG13	2:D:243:LEU:H	1.60	0.65
2:E:255:GLY:O	5:E:701:ATP:N6	2.27	0.65
1:I:8:SER:HB3	1:I:9:PRO:HD3	1.79	0.65
2:D:446:GLN:HG3	2:D:483:VAL:HG11	1.77	0.65
2:E:175:LEU:HD11	2:E:183:GLU:HB2	1.79	0.65
2:B:164:LEU:HA	2:B:176:VAL:HG12	1.79	0.64
2:A:337:LEU:HD13	2:A:349:ILE:HD11	1.79	0.64
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
2:A:184:ARG:NH2	2:D:160:GLU:OE1	2.31	0.64
1:Z:181:LEU:HD22	1:Z:233:LEU:HD23	1.79	0.64
1:6:19:LEU:O	1:6:22:LYS:HG3	1.96	0.64
2:A:213:LYS:O	2:A:215:ARG:NH1	2.31	0.64
2:E:362:GLU:HA	2:E:408:ASN:HD22	1.62	0.64
4:R:362:GLU:OE2	4:R:382:ARG:HD3	1.98	0.64
1:6:74:LEU:HD23	1:6:122:LEU:HD11	1.79	0.64
2:B:192:LEU:HB3	2:B:214:LEU:HD11	1.80	0.64
2:E:220:LEU:CD2	2:E:232:ARG:HB3	2.27	0.64
1:0:85:ARG:HH12	1:0:98:GLN:NE2	1.96	0.63
2:A:290:LEU:HD22	2:A:426:LEU:HD11	1.80	0.63
2:C:437:ILE:H	2:C:437:ILE:HD12	1.63	0.63
2:D:290:LEU:HD12	2:D:431:LEU:HD23	1.80	0.63
2:C:123:ARG:NH2	2:F:101:TYR:OH	2.31	0.63
1:8:140:ARG:NH1	1:8:154:VAL:HG13	2.13	0.63
2:A:255:GLY:O	5:A:701:ATP:N6	2.32	0.63
2:B:142:ARG:HH12	2:B:153:GLY:HA3	1.64	0.63
2:B:260:GLN:HA	2:B:263:GLN:HE21	1.63	0.63
2:C:287:LYS:NZ	2:C:401:ASP:OD1	2.31	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:349:ILE:HD12	2:B:396:LEU:HD21	1.79	0.62
2:B:377:PHE:CE1	2:B:396:LEU:HD13	2.34	0.62
2:F:184:ARG:NH2	2:F:224:THR:O	2.33	0.62
2:A:424:ALA:O	2:A:430:ARG:NH2	2.32	0.62
2:B:574:SER:HB2	2:B:581:ILE:HG12	1.82	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
2:F:361:SER:H	2:F:364:THR:HB	1.65	0.62
2:B:503:GLY:HA2	2:B:577:LYS:NZ	2.14	0.62
2:E:237:GLU:HG2	2:E:241:LEU:HG	1.82	0.62
4:U:429:TRP:HZ3	4:U:431:ILE:HG13	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:605:LEU:CD2	1:4:144:ASP:HA	2.30	0.62
2:E:247:PRO:HG2	2:E:304:LYS:HB2	1.82	0.62
2:F:534:VAL:HG22	2:F:540:PRO:HA	1.82	0.62
1:8:14:ARG:HG2	2:F:582:VAL:HG23	1.82	0.61
2:C:373:MET:HB2	2:C:415:SER:HB2	1.82	0.61
2:F:464:LEU:HB3	2:F:469:GLY:HA2	1.83	0.61
4:R:382:ARG:HH21	4:R:385:ILE:HD13	1.64	0.61
2:A:105:LEU:HD12	2:A:114:ASP:HB3	1.83	0.61
2:C:389:GLU:HA	2:C:392:VAL:HG12	1.80	0.61
4:P:362:GLU:OE2	4:P:382:ARG:HD3	2.00	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
2:B:243:LEU:HD12	2:B:326:LYS:HG3	1.83	0.61
2:D:173:ARG:HG2	2:D:187:TRP:CD1	2.36	0.61
1:4:74:LEU:HD23	1:4:122:LEU:HD11	1.83	0.60
2:E:485:ARG:HG3	2:E:548:LEU:HD22	1.83	0.60
1:Z:182:ARG:NH1	1:Z:234:LEU:O	2.34	0.60
2:B:139:GLN:NE2	2:B:153:GLY:O	2.34	0.60
2:B:518:MET:HB3	2:E:428:PRO:HG2	1.83	0.60
2:C:421:ILE:HB	2:C:426:LEU:HD11	1.83	0.60
2:C:416:ASN:HD22	2:C:566:ASN:HD22	1.49	0.60
2:D:233:ILE:O	2:D:235:LYS:NZ	2.34	0.60
2:F:498:VAL:HG13	2:F:581:ILE:HG23	1.84	0.60
1:0:140:ARG:NH1	1:0:154:VAL:HG13	2.17	0.60
1:X:128:ALA:HB2	1:X:134:LYS:HB3	1.83	0.60
2:C:350:ARG:NH2	2:F:335:PRO:O	2.34	0.60
1:8:74:LEU:HD23	1:8:122:LEU:HD11	1.83	0.59
2:D:247:PRO:HB2	2:D:304:LYS:HB3	1.83	0.59
1:2:140:ARG:NH1	1:2:154:VAL:HG13	2.17	0.59
2:D:272:PHE:HA	2:D:275:LYS:HE3	1.84	0.59
1:2:85:ARG:HH12	1:2:98:GLN:NE2	1.99	0.59
2:D:261:ILE:O	2:D:265:ARG:HG3	2.01	0.59
2:C:173:ARG:HG2	2:C:187:TRP:HD1	1.67	0.59
2:F:373:MET:HB3	2:F:415:SER:HB2	1.83	0.59
1:2:31:VAL:HG12	1:2:155:VAL:HG22	1.84	0.59
1:6:20:ALA:HA	1:6:119:GLU:HG2	1.84	0.59
2:F:177:VAL:HG12	2:F:183:GLU:HG3	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:A:296:GLY:HA3	2:B:427:ARG:HD3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:249:VAL:HG21	2:D:301:LEU:HD22	1.85	0.58
1:0:10:GLU:HA	1:0:13:MET:HE2	1.86	0.58
2:C:527:LYS:HD3	2:D:283:LEU:HB2	1.85	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:F:502:ASN:CB	2:F:579:GLU:HG2	2.33	0.58
1:6:26:ARG:NH1	2:F:502:ASN:HB2	2.16	0.58
2:D:562:PRO:O	2:D:565:THR:OG1	2.22	0.58
2:E:531:ILE:HD11	2:F:277:LEU:HB3	1.86	0.58
1:2:45:ASN:ND2	1:2:209:GLU:OE1	2.35	0.58
2:E:330:LEU:HD12	2:E:368:VAL:HG22	1.85	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
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
2:C:357:ARG:HH12	2:C:406:LEU:HA	1.68	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
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
1:4:31:VAL:HG12	1:4:155:VAL:HG22	1.85	0.57
2:C:168:LEU:HD13	2:C:173:ARG:HB3	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:B:255:GLY:H	5:B:701:ATP:HN61	1.52	0.57
1:T:128:ALA:HB2	1:T:134:LYS:HB3	1.86	0.57
2:B:105:LEU:HD12	2:B:114:ASP:HB3	1.87	0.57
2:B:497:GLU:HB2	2:B:587:LEU:HD11	1.86	0.57
2:C:417:ARG:HD2	2:C:568:ASP:HB2	1.85	0.57
1:Z:30:VAL:HG13	1:Z:43:ALA:HB2	1.86	0.57
2:C:384:VAL:HB	2:C:387:ASP:HB2	1.87	0.57
2:D:164:LEU:HD22	2:D:220:LEU:HD11	1.87	0.57
1:O:74:LEU:HD21	1:O:107:LEU:HD21	1.86	0.57
1:Q:74:LEU:HD21	1:Q:107:LEU:HD21	1.86	0.57
2:C:259:ARG:O	2:C:262:GLU:HG2	2.05	0.57
2:D:377:PHE:HB2	2:D:422:ASP:HB2	1.86	0.57
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.85	0.57
1:6:118:TYR:HB3	1:6:120:VAL:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:HB2	2:B:324:GLU:HB3	1.86	0.57
2:B:323:HIS:HA	2:B:326:LYS:NZ	2.19	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:427:ARG:HD3	2:A:428:PRO:HD2	1.87	0.57
2:B:323:HIS:O	2:B:326:LYS:HG2	2.05	0.57
2:F:497:GLU:OE1	2:F:505:LYS:HE3	2.04	0.57
2:D:290:LEU:HD11	2:D:421:ILE:HD13	1.87	0.56
2:A:211:PRO:N	2:A:212:ARG:HA	2.20	0.56
2:A:349:ILE:HG21	2:A:396:LEU:HD21	1.86	0.56
2:B:425:ILE:HG23	2:B:426:LEU:HD12	1.86	0.56
2:C:212:ARG:HH12	2:C:214:LEU:HD23	1.70	0.56
2:C:292:TYR:O	2:C:436:LYS:HA	2.05	0.56
2:C:457:LEU:O	2:C:471:ARG:NH2	2.38	0.56
1:8:31:VAL:HG12	1:8:155:VAL:HG22	1.87	0.56
2:F:509:TYR:HB2	2:F:511:LYS:HG2	1.87	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:F:374:ASP:HB2	2:F:417:ARG:HB2	1.88	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:561:LEU:HD13	2:B:426:LEU:HD23	1.87	0.56
2:C:161:ILE:HB	2:D:183:GLU:HG3	1.86	0.56
2:C:502:ASN:HB3	2:C:579:GLU:HG3	1.87	0.56
2:D:285:PRO:HG2	2:D:287:LYS:HE3	1.86	0.56
1:8:189:ARG:NH1	1:8:203:LEU:N	2.53	0.56
2:C:173:ARG:HE	2:C:185:VAL:HG12	1.71	0.56
1:K:74:LEU:HD21	1:K:107:LEU:HD21	1.88	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
1:6:22:LYS:HD3	2:F:502:ASN:CB	2.35	0.56
1:8:128:ALA:HB2	1:8:134:LYS:HB3	1.87	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
2:F:187:TRP:HB2	2:F:228:TYR:CE1	2.41	0.56
2:F:488:ALA:O	2:F:493:ASN:ND2	2.38	0.56
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
1:Q:189:ARG:NH1	1:Q:203:LEU:N	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:291:LEU:HD23	2:E:435:ILE:HB	1.87	0.55
2:F:500:TYR:CD1	2:F:577:LYS:HG2	2.42	0.55
2:B:333:LYS:HB2	2:B:336:GLU:HB2	1.87	0.55
2:E:142:ARG:NH1	2:E:151:GLU:OE1	2.27	0.55
4:J:320:SER:HB3	4:J:331:VAL:HG21	1.87	0.55
4:L:320:SER:HB3	4:L:331:VAL:HG21	1.88	0.55
4:U:432:GLU:OE2	4:U:433:GLU:N	2.39	0.55
2:A:460:HIS:HE2	2:A:539:GLN:HB3	1.72	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:E:335:PRO:HG3	2:E:375:SER:HB2	1.89	0.55
2:F:498:VAL:HG22	2:F:584:ILE:HG12	1.88	0.55
4:Y:429:TRP:HZ3	4:Y:431:ILE:HG13	1.72	0.55
2:E:543:ARG:HH12	2:E:545:GLN:HB3	1.72	0.55
2:F:314:MET:HE2	2:F:365:PRO:HD2	1.89	0.55
2:F:496:LEU:HD23	2:F:586:THR:HA	1.88	0.55
2:A:211:PRO:HG2	2:A:213:LYS:HG2	1.88	0.55
2:C:291:LEU:HB3	2:C:437:ILE:HD11	1.89	0.55
2:C:328:TYR:HD2	2:C:359:LYS:HB3	1.70	0.55
2:F:144:ASN:HD21	2:F:148:THR:HB	1.71	0.55
1:I:174:ASN:N	1:I:174:ASN:HD22	2.05	0.55
2:A:376:ILE:HG23	2:A:377:PHE:CD2	2.42	0.55
1:O:68:PHE:HA	1:O:71:PHE:CE2	2.42	0.55
1:8:14:ARG:HA	1:8:14:ARG:HH11	1.73	0.54
2:B:367:ILE:HD13	2:B:410:ILE:HB	1.90	0.54
2:C:498:VAL:HG13	2:C:581:ILE:HG23	1.89	0.54
1:T:140:ARG:HH11	1:T:154:VAL:HG13	1.73	0.54
2:E:292:TYR:CZ	2:E:436:LYS:HB2	2.42	0.54
2:C:294:PRO:HD2	2:C:438:GLU:HA	1.88	0.54
2:B:449:TYR:CE1	2:B:519:ILE:HG23	2.42	0.54
2:D:338:LEU:HD21	2:D:376:ILE:HG12	1.89	0.54
1:0:45:ASN:ND2	1:0:209:GLU:OE1	2.40	0.54
1:2:128:ALA:HB2	1:2:134:LYS:HB3	1.89	0.54
2:C:500:TYR:HE2	2:C:506:GLU:HB2	1.72	0.54
2:E:464:LEU:HD22	2:E:469:GLY:HA2	1.89	0.54
4:P:320:SER:HB3	4:P:331:VAL:HG21	1.89	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
2:D:525:ARG:HD3	2:D:553:ASP:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:45:ASN:ND2	1:8:209:GLU:OE1	2.41	0.54
2:B:99:SER:HB2	2:B:143:LEU:O	2.08	0.54
2:B:574:SER:OG	2:B:580:ARG:HA	2.08	0.54
1:T:181:LEU:HD23	1:T:233:LEU:HB3	1.88	0.54
1:0:128:ALA:HB2	1:0:134:LYS:HB3	1.88	0.54
2:A:164:LEU:HA	2:A:176:VAL:HG12	1.90	0.54
2:A:376:ILE:HD11	2:A:392:VAL:HG11	1.89	0.54
1:O:177:LEU:HG	1:O:233:LEU:HD21	1.90	0.54
1:T:68:PHE:HA	1:T:71:PHE:CE2	2.43	0.53
1:K:89:TYR:CE1	4:R:382:ARG:HD2	2.43	0.53
2:A:335:PRO:O	2:B:350:ARG:NH2	2.41	0.53
2:B:317:VAL:HG12	2:B:318:ARG:HG3	1.91	0.53
1:Z:140:ARG:HH11	1:Z:154:VAL:HG13	1.70	0.53
2:F:374:ASP:N	2:F:374:ASP:OD1	2.42	0.53
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.89	0.53
2:B:563:ASN:HB2	2:E:419:ASP:HB2	1.91	0.53
4:J:424:ASP:OD1	4:J:426:ALA:N	2.41	0.53
1:O:69:ASN:HD22	1:O:69:ASN:H	1.56	0.53
2:B:498:VAL:HG22	2:B:584:ILE:HG22	1.90	0.53
1:T:92:ARG:NH1	1:T:129:HIS:CG	2.77	0.53
1:0:11:GLN:HB3	2:A:504:ASP:H	1.72	0.53
2:B:238:VAL:HG22	2:B:352:ILE:HD13	1.91	0.53
2:F:339:ASN:HD21	2:F:348:HIS:CE1	2.27	0.53
2:A:372:GLU:HG2	2:B:394:PRO:HB3	1.89	0.53
1:I:68:PHE:HA	1:I:71:PHE:CE2	2.44	0.53
2:A:377:PHE:CZ	2:A:396:LEU:HG	2.44	0.53
1:O:110:ILE:HA	1:O:114:GLN:HG3	1.91	0.53
1:8:89:TYR:CD1	4:N:382:ARG:HD3	2.44	0.53
2:F:496:LEU:HD22	2:F:584:ILE:HG22	1.91	0.53
1:T:30:VAL:HG13	1:T:43:ALA:HB2	1.89	0.53
1:X:140:ARG:HH11	1:X:154:VAL:HG13	1.74	0.53
2:B:99:SER:OG	2:E:123:ARG:NE	2.33	0.52
2:C:460:HIS:HA	2:C:541:GLY:HA3	1.91	0.52
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.44	0.52
1:4:68:PHE:HB3	2:B:607:GLN:HG3	1.91	0.52
2:B:187:TRP:HB2	2:B:228:TYR:CE1	2.45	0.52
2:B:460:HIS:HE1	2:B:539:GLN:HB3	1.75	0.52
2:F:335:PRO:HA	2:F:338:LEU:HD13	1.91	0.52
2:F:340:LYS:O	2:F:341:PHE:CD1	2.62	0.52
2:D:366:VAL:O	2:D:409:VAL:HA	2.09	0.52
1:I:8:SER:CB	1:I:9:PRO:HD3	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:421:ILE:HB	2:E:426:LEU:HD11	1.91	0.52
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.90	0.52
2:B:357:ARG:HB2	2:B:406:LEU:HD11	1.92	0.52
2:A:333:LYS:HB2	2:A:336:GLU:HG3	1.92	0.52
2:C:560:ASP:O	2:C:564:THR:OG1	2.21	0.52
1:I:140:ARG:HH11	1:I:154:VAL:HG13	1.71	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:A:185:VAL:HG13	2:D:161:ILE:HD11	1.91	0.52
2:B:168:LEU:HD12	2:B:173:ARG:HB2	1.90	0.52
2:C:255:GLY:H	5:C:701:ATP:N6	2.08	0.52
2:C:301:LEU:HD11	5:C:701:ATP:H2'	1.92	0.52
1:I:178:THR:HG22	1:I:182:ARG:HE	1.74	0.52
2:C:353:PHE:O	2:C:357:ARG:HG3	2.10	0.52
2:D:249:VAL:HB	2:D:304:LYS:HB2	1.92	0.52
1:T:11:GLN:O	1:T:15:GLU:HG2	2.10	0.52
2:A:497:GLU:HB2	2:A:587:LEU:HD11	1.91	0.52
1:K:150:GLU:HG3	1:K:154:VAL:HG22	1.92	0.52
2:C:355:ARG:HD2	2:C:359:LYS:HE2	1.91	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
1:4:10:GLU:HG3	2:B:505:LYS:HZ2	1.75	0.51
1:4:68:PHE:HA	1:4:71:PHE:CE2	2.45	0.51
2:C:122:MET:HG3	2:C:124:LEU:HD11	1.91	0.51
2:D:211:PRO:N	2:D:212:ARG:HA	2.26	0.51
2:B:177:VAL:HG12	2:B:183:GLU:HG3	1.92	0.51
2:B:310:LEU:HD21	2:B:328:TYR:HB2	1.93	0.51
2:D:448:ILE:HG22	2:D:452:TYR:CE2	2.45	0.51
2:D:525:ARG:HE	2:D:554:GLU:HB3	1.75	0.51
1:I:123:CYS:HA	1:I:139:TYR:O	2.11	0.51
2:B:345:THR:O	2:B:349:ILE:HG12	2.11	0.51
2:F:290:LEU:HB2	2:F:431:LEU:HD13	1.93	0.51
1:Z:90:ASP:OD1	1:Z:91:ARG:N	2.44	0.51
1:6:14:ARG:O	1:6:18:GLU:HG2	2.11	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: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:68:PHE:HA	1:Z:71:PHE:CE2	2.46	0.51
2:C:278:TYR:O	2:C:282:SER:N	2.43	0.51
2:E:235:LYS:HE3	2:E:348:HIS:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:26:ARG:HD2	2:F:504:ASP:OD2	2.10	0.51
2:D:499:THR:HG1	2:D:585:ARG:HH21	1.59	0.51
2:A:547:LEU:O	2:A:551:ILE:HG12	2.10	0.51
2:B:372:GLU:HB3	2:E:394:PRO:HB3	1.92	0.51
1:K:90:ASP:OD1	1:K:91:ARG:N	2.44	0.51
2:E:290:LEU:HB2	2:E:431:LEU:HD23	1.93	0.51
1:I:11:GLN:O	1:I:15:GLU:HB2	2.11	0.51
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:A:249:VAL:HG11	2:A:304:LYS:HG3	1.92	0.50
2:B:314:MET:HB2	2:B:325:ALA:HA	1.93	0.50
2:D:448:ILE:HA	2:D:451:LYS:HD2	1.92	0.50
2:F:291:LEU:HD23	2:F:435:ILE:HB	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:497:GLU:HB3	2:A:585:ARG:HB3	1.94	0.50
2:E:401:ASP:OD1	2:E:430:ARG:NE	2.43	0.50
4:R:320:SER:HB3	4:R:331:VAL:HG21	1.92	0.50
1:6:22:LYS:HD3	2:F:502:ASN:HB3	1.92	0.50
2:D:254:ILE:HA	5:D:701:ATP:N6	2.26	0.50
2:E:478:MET:HG3	2:E:544:ILE:HD13	1.93	0.50
1:Z:118:TYR:HB3	1:Z:120:VAL:HG22	1.93	0.50
2:A:100:GLY:HA2	2:B:120:ARG:HH22	1.77	0.50
1:I:181:LEU:HD23	1:I:233:LEU:HB3	1.92	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
1:2:11:GLN:HA	1:2:14:ARG:NH1	2.27	0.50
2:E:494:ARG:HE	2:E:507:VAL:HG21	1.75	0.50
1:T:150:GLU:HG3	1:T:154:VAL:HG22	1.94	0.50
1:Z:25:ALA:O	1:Z:158:GLY:HA2	2.11	0.50
1:6:19:LEU:HD12	1:6:22:LYS:HE2	1.94	0.50
2:B:269:GLU:O	2:B:273:LEU:N	2.38	0.50
2:E:299:LYS:HG2	2:E:437:ILE:HD12	1.93	0.50
2:E:491:ASP:HA	2:E:494:ARG:HH22	1.77	0.50
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.59	0.50
1:2:13:MET:SD	2:A:605:LEU:CG	2.78	0.50
2:F:255:GLY:H	5:F:701:ATP:HN61	1.59	0.50
2:F:332:ILE:HD12	2:F:337:LEU:HD11	1.94	0.50
1:Z:178:THR:HG22	1:Z:182:ARG:HE	1.77	0.50
1:4:89:TYR:CD1	4:M:382:ARG:HD3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:LEU:HD11	2:C:116:PHE:HB2	1.94	0.50
2:C:535:LEU:HD13	2:D:270:LEU:HD11	1.94	0.50
2:D:175:LEU:HD11	2:D:183:GLU:HB2	1.93	0.50
2:E:354:GLN:O	2:E:357:ARG:HG2	2.11	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
2:A:223:ASP:O	2:A:227:GLY:N	2.39	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:D:165:ARG:HG3	2:D:177:VAL:HG13	1.94	0.49
1:0:89:TYR:CD1	4:W:382:ARG:HD3	2.47	0.49
2:D:391:THR:O	2:D:394:PRO:HD2	2.12	0.49
2:D:488:ALA:O	2:D:493:ASN:ND2	2.44	0.49
1:I:142:THR:OG1	1:I:144:ASP:OD1	2.29	0.49
1:X:92:ARG:NH1	1:X:129:HIS:CD2	2.80	0.49
1:6:89:TYR:CD1	4:H:382:ARG:HD3	2.47	0.49
2:A:192:LEU:HB3	2:A:214:LEU:HD11	1.94	0.49
2:A:348:HIS:O	2:A:352:ILE:HG12	2.11	0.49
2:B:323:HIS:HA	2:B:326:LYS:HZ2	1.78	0.49
2:D:257:LEU:O	2:D:261:ILE:HG12	2.12	0.49
2:F:374:ASP:CB	2:F:417:ARG:HB2	2.42	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:360:ALA:HA	2:A:408:ASN:HD21	1.77	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:B:112:THR:HG22	2:B:125:THR:HA	1.95	0.49
2:C:439:ARG:HE	2:C:572:ARG:HH22	1.59	0.49
2:C:485:ARG:NH1	2:C:548:LEU:HB3	2.27	0.49
2:D:515:SER:O	2:D:519:ILE:HG13	2.12	0.49
2:F:162:SER:HB3	2:F:176:VAL:HB	1.93	0.49
2:F:478:MET:HB3	2:F:544:ILE:HD13	1.94	0.49
1:I:55:GLU:HB2	1:I:222:PHE:CG	2.47	0.49
2:D:251:TYR:HE1	2:D:309:SER:HB2	1.78	0.49
2:E:238:VAL:HG13	2:E:239:GLU:OE1	2.12	0.49
1:4:70:GLU:HB3	1:4:118:TYR:CD2	2.48	0.49
1:T:18:GLU:OE2	1:T:18:GLU:HA	2.12	0.49
2:F:139:GLN:HG3	2:F:155:PHE:HE1	1.76	0.49
1:K:41:PHE:HB3	1:K:53:ILE:HD13	1.95	0.49
4:M:465:ARG:HG3	4:M:513:LEU:HD22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:GLU:HG3	2:D:161:ILE:HB	1.94	0.49
2:E:233:ILE:HG13	2:F:168:LEU:HD21	1.94	0.49
2:E:372:GLU:HG2	2:F:394:PRO:HB3	1.95	0.49
1:T:55:GLU:HB2	1:T:222:PHE:CG	2.48	0.49
2:B:385:SER:HB2	2:E:387:ASP:H	1.78	0.48
2:F:580:ARG:NH2	2:F:581:ILE:HB	2.27	0.48
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.75	0.48
4:U:459:ASP:OD1	4:U:461:ASP:N	2.44	0.48
1:4:33:LEU:HD12	1:4:40:LEU:HB3	1.94	0.48
1:6:110:ILE:HG21	1:6:118:TYR:CD1	2.48	0.48
2:C:187:TRP:HB2	2:C:228:TYR:CE1	2.48	0.48
2:D:107:THR:HA	2:D:113:VAL:HG12	1.96	0.48
2:E:506:GLU:HG3	2:E:577:LYS:HE2	1.95	0.48
1:2:33:LEU:HD12	1:2:40:LEU:HB3	1.94	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:D:294:PRO:HB3	2:D:439:ARG:HH21	1.79	0.48
2:E:420:MET:HE3	2:E:420:MET:HA	1.96	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
2:C:439:ARG:NE	2:C:572:ARG:HH22	2.12	0.48
2:D:254:ILE:HD11	2:D:261:ILE:HD11	1.95	0.48
1:Z:214:ASP:OD2	1:Z:217:ARG:HG2	2.13	0.48
1:0:50:LEU:HB3	2:A:609:LEU:HD11	1.95	0.48
1:6:33:LEU:HD12	1:6:40:LEU:HB3	1.94	0.48
1:6:68:PHE:HB2	2:E:609:LEU:HG	1.95	0.48
4:L:382:ARG:HD3	1:X:89:TYR:CD1	2.48	0.48
1:0:68:PHE:CD1	2:A:609:LEU:HD12	2.49	0.48
2:A:165:ARG:HB2	2:A:175:LEU:HD23	1.96	0.48
2:D:313:LYS:HA	2:D:313:LYS:HD3	1.72	0.48
2:F:460:HIS:ND1	2:F:540:PRO:O	2.25	0.48
4:L:459:ASP:OD1	4:L:461:ASP:N	2.44	0.48
4:W:465:ARG:HG3	4:W:513:LEU:HD22	1.95	0.48
2:D:457:LEU:HD21	2:D:527:LYS:HE2	1.96	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:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.96	0.48
1:0:178:THR:HG22	1:0:182:ARG:HE	1.79	0.48
2:D:528:LYS:O	2:D:532:LYS:HG2	2.13	0.48
2:F:223:ASP:O	2:F:227:GLY:N	2.41	0.48
2:B:223:ASP:O	2:B:227:GLY:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:531:ILE:HG21	2:F:278:TYR:CE1	2.49	0.48
4:L:359:TYR:CE1	4:L:383:LEU:HB2	2.49	0.48
2:B:328:TYR:CZ	2:B:359:LYS:HE3	2.49	0.47
2:D:522:VAL:HG22	2:D:554:GLU:HG2	1.95	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
1:4:110:ILE:HG21	1:4:118:TYR:CD1	2.49	0.47
2:A:297:CYS:HB3	2:A:437:ILE:HG22	1.96	0.47
2:C:271:PRO:HA	2:C:278:TYR:CE2	2.49	0.47
2:F:313:LYS:O	2:F:317:VAL:HB	2.14	0.47
1:O:55:GLU:HB2	1:O:222:PHE:CG	2.49	0.47
1:Z:69:ASN:H	1:Z:69:ASN:HD22	1.61	0.47
1:0:24:ILE:HG22	1:0:157:GLY:HA2	1.95	0.47
2:A:336:GLU:HA	2:B:350:ARG:CZ	2.45	0.47
2:E:455:GLU:HA	2:E:475:ILE:HD12	1.95	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
2:E:243:LEU:HD13	2:E:329:PHE:HD2	1.80	0.47
2:F:500:TYR:CD2	2:F:577:LYS:HE2	2.48	0.47
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:A:101:TYR:H	2:B:120:ARG:HH12	1.62	0.47
2:F:429:GLY:N	2:F:432:ASP:OD1	2.36	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
1:6:22:LYS:HD2	1:6:22:LYS:C	2.34	0.47
2:C:275:LYS:O	2:C:279:ARG:HG2	2.14	0.47
2:D:187:TRP:HB2	2:D:228:TYR:CE1	2.49	0.47
4:L:312:VAL:HG12	4:L:497:ILE:HB	1.96	0.47
1:Z:123:CYS:HA	1:Z:139:TYR:O	2.15	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:144:ASN:HD21	2:B:148:THR:HB	1.80	0.47
2:B:288:GLY:HA3	2:B:431:LEU:HA	1.96	0.47
2:B:473:ALA:HA	2:B:476:LYS:HE2	1.96	0.47
2:B:503:GLY:HA2	2:B:577:LYS:HZ1	1.76	0.47
2:C:232:ARG:NH1	2:C:233:ILE:O	2.48	0.47
2:C:235:LYS:HG2	2:C:237:GLU:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:ILE:HG21	2:C:426:LEU:HD21	1.96	0.47
2:C:481:LYS:HB3	2:C:544:ILE:HD11	1.97	0.47
2:D:219:SER:HB2	2:D:235:LYS:HZ2	1.80	0.47
2:D:496:LEU:HD22	2:D:586:THR:HG22	1.97	0.47
2:D:543:ARG:HD3	2:D:546:HIS:CE1	2.50	0.47
2:E:105:LEU:HD12	2:E:114:ASP:HB3	1.96	0.47
2:F:165:ARG:HH21	2:F:177:VAL:HG21	1.80	0.47
2:F:188:LEU:HD12	2:F:192:LEU:HB3	1.97	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	2.49	0.47
1:Q:33:LEU:HD12	1:Q:40:LEU:HB3	1.96	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
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
2:A:525:ARG:NH1	2:A:554:GLU:OE2	2.46	0.47
2:C:99:SER:HB2	2:C:143:LEU:O	2.15	0.47
2:D:287:LYS:NZ	2:D:404:GLU:OE2	2.40	0.47
2:E:516:GLY:HA3	5:E:701:ATP:N3	2.30	0.47
2:F:582:VAL:O	2:F:583:TYR:HB2	2.14	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
1:6:70:GLU:HB3	1:6:118:TYR:CD2	2.50	0.47
2:B:485:ARG:HH11	2:B:548:LEU:HD22	1.79	0.47
2:C:516:GLY:HA3	5:C:701:ATP:N3	2.30	0.47
2:E:235:LYS:C	2:E:235:LYS:HD2	2.35	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:C:99:SER:OG	2:D:123:ARG:HB3	2.15	0.46
2:C:294:PRO:O	2:C:299:LYS:NZ	2.48	0.46
2:F:583:TYR:CE2	2:F:585:ARG:HB2	2.50	0.46
1:Q:110:ILE:HA	1:Q:114:GLN:HG3	1.96	0.46
2:A:478:MET:HG3	2:A:544:ILE:HD13	1.97	0.46
2:C:271:PRO:HA	2:C:278:TYR:HE2	1.80	0.46
2:D:242:VAL:HG13	2:D:243:LEU:N	2.30	0.46
2:D:292:TYR:CZ	2:D:436:LYS:HB2	2.50	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:B:104:LEU:HD22	2:B:135:LEU:HD12	1.97	0.46
2:C:254:ILE:HD11	2:C:301:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:TYR:CD2	2:C:359:LYS:HD2	2.50	0.46
4:Y:459:ASP:OD1	4:Y:461:ASP:N	2.48	0.46
2:D:547:LEU:O	2:D:551:ILE:HG13	2.15	0.46
2:F:444:ALA:O	2:F:448:ILE:HG13	2.15	0.46
4:L:475:ALA:HA	4:L:481:THR:HB	1.97	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
2:B:342:VAL:HA	3:G:7:LYS:HE3	1.97	0.46
2:B:609:LEU:HD23	2:B:609:LEU:HA	1.78	0.46
2:C:156:GLU:OE2	2:C:157:ALA:N	2.48	0.46
2:C:514:ASN:HA	2:C:518:MET:SD	2.55	0.46
2:D:509:TYR:HB2	2:D:511:LYS:HG2	1.98	0.46
2:E:523:VAL:HG12	2:E:527:LYS:HD2	1.98	0.46
2:F:498:VAL:HG11	2:F:581:ILE:HG12	1.97	0.46
1:K:185:VAL:O	1:K:189:ARG:HB2	2.15	0.46
1:2:33:LEU:HD21	1:2:184:ALA:HB2	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
1:Z:33:LEU:HD12	1:Z:40:LEU:HB3	1.97	0.46
2:A:272:PHE:CE1	2:A:408:ASN:HA	2.51	0.46
2:C:122:MET:HG3	2:C:124:LEU:CD1	2.46	0.46
2:D:291:LEU:HD23	2:D:435:ILE:HB	1.97	0.46
2:F:112:THR:HG22	2:F:125:THR:HA	1.97	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
1:6:68:PHE:CD1	2:E:609:LEU:HD12	2.51	0.46
2:C:298:GLY:HA2	5:C:701:ATP:O1A	2.16	0.46
2:F:115:VAL:HG12	2:F:117:THR:HG23	1.97	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:377:PHE:HE1	2:B:396:LEU:HD13	1.79	0.46
2:C:569:ASP:O	2:C:573:ILE:HG13	2.16	0.46
2:D:251:TYR:CE1	2:D:309:SER:HB2	2.51	0.46
2:D:444:ALA:O	2:D:448:ILE:HG13	2.16	0.46
2:E:243:LEU:H	2:E:243:LEU:HD23	1.81	0.46
4:H:366:TYR:CZ	4:H:370:GLU:HG3	2.51	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
2:A:144:ASN:OD1	2:A:148:THR:N	2.38	0.46
2:B:314:MET:CB	2:B:325:ALA:HA	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:439:ARG:HB3	2:D:514:ASN:O	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:E:531:ILE:HA	2:E:534:VAL:HG12	1.97	0.45
2:F:499:THR:CG2	2:F:583:TYR:HD2	2.30	0.45
4:J:359:TYR:CE1	4:J:383:LEU:HB2	2.52	0.45
4:J:429:TRP:CZ3	4:J:431:ILE:HG13	2.51	0.45
4:L:508:SER:O	4:L:512:GLU:HG3	2.16	0.45
2:B:161:ILE:HB	2:E:183:GLU:HG2	1.98	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
2:C:298:GLY:N	5:C:701:ATP:O2B	2.46	0.45
2:D:173:ARG:HG2	2:D:187:TRP:HD1	1.79	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:A:213:LYS:HE3	2:A:213:LYS:HB3	1.65	0.45
2:A:391:THR:O	2:A:394:PRO:HD2	2.16	0.45
1:T:25:ALA:O	1:T:158:GLY:HA2	2.16	0.45
1:0:8:SER:N	2:A:502:ASN:HB3	2.32	0.45
2:A:449:TYR:CE1	2:A:519:ILE:HG23	2.51	0.45
2:C:530:ALA:O	2:C:534:VAL:HG13	2.17	0.45
2:D:346:GLU:HG2	2:D:392:VAL:HG13	1.98	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
1:4:10:GLU:HB3	2:B:505:LYS:H	1.82	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:B:406:LEU:HD23	2:B:409:VAL:HG11	1.98	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:A:355:ARG:O	2:A:359:LYS:HG2	2.17	0.45
1:O:69:ASN:HD22	1:O:69:ASN:N	2.14	0.45
2:A:107:THR:HG22	2:A:113:VAL:HG12	1.99	0.45
2:B:291:LEU:HD23	2:B:435:ILE:HB	1.99	0.45
2:C:296:GLY:O	2:C:515:SER:HB2	2.17	0.45
4:N:398:LEU:N	4:N:398:LEU:HD12	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:VAL:HA	2:B:185:VAL:HG23	1.98	0.45
1:X:33:LEU:HD12	1:X:40:LEU:HB3	1.99	0.45
1:X:150:GLU:HG3	1:X:154:VAL:HG22	1.98	0.45
1:2:30:VAL:HG13	1:2:43:ALA:HB2	1.98	0.45
2:A:104:LEU:HD22	2:A:135:LEU:HD12	1.99	0.45
2:B:577:LYS:HG3	2:B:579:GLU:OE1	2.17	0.45
2:C:112:THR:HG22	2:C:125:THR:HG22	1.99	0.45
2:D:498:VAL:HG22	2:D:584:ILE:HG23	1.99	0.45
2:E:321:ASP:HB2	2:E:324:GLU:HG2	1.99	0.45
1:I:41:PHE:HB3	1:I:53:ILE:HD13	1.99	0.45
1:K:33:LEU:HD12	1:K:40:LEU:HB3	1.99	0.45
1:X:172:ALA:HB3	1:X:175:ALA:HB2	1.98	0.45
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
1:I:56:LEU:HG	1:I:62:PHE:HB2	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
2:B:395:GLN:HE21	2:B:399:GLU:HG2	1.83	0.44
2:D:427:ARG:HB2	2:D:430:ARG:HH22	1.82	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:A:255:GLY:H	5:A:701:ATP:HN61	1.64	0.44
2:C:533:SER:O	2:C:537:THR:HG22	2.17	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
2:A:530:ALA:O	2:A:534:VAL:HG13	2.18	0.44
2:B:500:TYR:CD2	2:B:577:LYS:HG2	2.52	0.44
2:C:407:GLU:HG2	2:C:408:ASN:N	2.32	0.44
2:F:528:LYS:HD3	2:F:532:LYS:HE3	1.98	0.44
1:K:69:ASN:HD22	1:K:69:ASN:N	2.16	0.44
2:A:177:VAL:HG13	2:A:181:ASP:HA	1.99	0.44
2:A:367:ILE:HG12	2:A:410:ILE:HB	1.99	0.44
2:A:510:PHE:CE2	2:A:555:PHE:HB3	2.53	0.44
2:B:500:TYR:CG	2:B:577:LYS:HG2	2.52	0.44
2:C:427:ARG:HH12	2:F:296:GLY:N	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:452:TYR:OH	5:C:701:ATP:O2'	2.30	0.44
2:E:289:VAL:HG13	2:E:433:VAL:HG23	2.00	0.44
2:E:480:GLU:HA	2:E:483:VAL:HG22	1.99	0.44
2:E:603:SER:HB2	2:F:505:LYS:HG2	1.99	0.44
2:F:510:PHE:CZ	2:F:555:PHE:HB3	2.52	0.44
1:0:69:ASN:N	1:0:69:ASN:HD22	2.15	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:C:424:ALA:O	2:C:427:ARG:HG2	2.17	0.44
2:F:213:LYS:O	2:F:215:ARG:NH1	2.51	0.44
2:F:520:GLN:NE2	5:F:701:ATP:O2'	2.51	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
1:8:16:ARG:HB3	1:8:117:PRO:HG3	2.00	0.44
2:B:500:TYR:HB3	2:B:579:GLU:O	2.18	0.44
2:C:259:ARG:HA	2:C:262:GLU:HG2	1.98	0.44
2:E:249:VAL:HG23	2:E:253:ASP:HB2	1.99	0.44
2:E:284:ARG:HA	2:E:284:ARG:HD2	1.76	0.44
4:H:329:ARG:NH2	4:J:476:ASP:O	2.48	0.44
2:B:142:ARG:NH2	2:B:151:GLU:HG2	2.25	0.44
2:B:296:GLY:HA3	2:E:427:ARG:HD2	2.00	0.44
2:C:380:ARG:HH11	2:C:394:PRO:HG3	1.82	0.44
2:C:497:GLU:HB2	2:C:587:LEU:HD11	1.99	0.44
2:D:395:GLN:HE21	2:D:399:GLU:HG2	1.83	0.44
2:E:393:VAL:O	2:E:397:LEU:HG	2.18	0.44
2:F:139:GLN:NE2	2:F:152:ALA:HB1	2.32	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
1:8:14:ARG:HG3	2:F:499:THR:CG2	2.48	0.44
2:B:211:PRO:HB2	2:B:212:ARG:H	1.64	0.44
2:E:510:PHE:CE2	2:E:555:PHE:HB3	2.53	0.44
2:F:310:LEU:HD22	2:F:367:ILE:HD13	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:74:LEU:HD23	1:K:122:LEU:HD11	1.99	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
1:4:8:SER:HB3	2:B:499:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:SER:OG	2:C:176:VAL:HB	2.17	0.43
2:F:457:LEU:HD11	2:F:527:LYS:HE2	2.00	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
2:A:261:ILE:HA	2:A:264:ILE:HG22	2.00	0.43
2:A:447:ASP:O	2:A:451:LYS:HG2	2.17	0.43
2:B:192:LEU:HD11	2:B:231:GLU:HA	2.00	0.43
2:C:537:THR:HG23	2:C:539:GLN:HG3	2.00	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
2:1:605:LEU:HG	1:4:111:PHE:CD2	2.53	0.43
1:8:173:GLU:O	1:8:174:ASN:HB2	2.18	0.43
2:B:444:ALA:O	2:B:448:ILE:HG13	2.19	0.43
2:D:223:ASP:O	2:D:227:GLY:N	2.49	0.43
1:I:69:ASN:HD22	1:I:69:ASN:N	2.17	0.43
1:K:56:LEU:HG	1:K:62:PHE:HB2	2.00	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:272:PHE:CD2	2:B:365:PRO:HG3	2.53	0.43
2:F:378:ARG:HB3	2:F:379:THR:H	1.70	0.43
2:F:441:ASP:H	2:F:444:ALA:HB3	1.83	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:A:388:VAL:HG12	2:A:390:THR:H	1.84	0.43
2:B:104:LEU:HD23	2:B:136:LYS:O	2.18	0.43
2:B:270:LEU:HA	2:B:273:LEU:HB2	2.00	0.43
2:D:256:GLY:HA3	2:D:444:ALA:HB2	2.01	0.43
1:X:79:ILE:HD13	4:Y:368:LYS:HB3	1.99	0.43
1:6:13:MET:HB3	2:B:605:LEU:HD23	2.00	0.43
2:A:99:SER:OG	2:B:123:ARG:HB3	2.19	0.43
2:C:283:LEU:HD22	2:F:531:ILE:HD12	2.00	0.43
2:D:272:PHE:CE2	2:D:410:ILE:HD11	2.54	0.43
2:D:479:ILE:HA	2:D:482:VAL:HG12	2.01	0.43
2:E:476:LYS:O	2:E:480:GLU:OE1	2.37	0.43
2:E:494:ARG:NH2	2:E:494:ARG:HB2	2.34	0.43
2:F:332:ILE:HD11	2:F:370:PHE:CE2	2.54	0.43
1:Z:41:PHE:HB3	1:Z:53:ILE:HD13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:14:ARG:NE	2:F:499:THR:OG1	2.51	0.43
2:C:289:VAL:HG22	2:C:433:VAL:HB	2.00	0.43
2:C:380:ARG:NH1	2:C:394:PRO:HG3	2.34	0.43
2:C:574:SER:O	2:C:578:GLY:N	2.39	0.43
2:D:565:THR:HG22	2:D:566:ASN:N	2.34	0.43
2:E:117:THR:HG23	2:F:120:ARG:HH21	1.84	0.43
2:F:337:LEU:HD13	2:F:349:ILE:HD11	1.99	0.43
4:N:318:ARG:HD3	4:N:493:THR:HG23	2.00	0.43
1:0:32:ALA:HA	1:0:40:LEU:O	2.19	0.43
2:E:527:LYS:HB2	2:F:283:LEU:HD13	2.00	0.43
2:E:569:ASP:HA	2:E:572:ARG:NH2	2.34	0.43
2:F:176:VAL:O	2:F:183:GLU:HA	2.18	0.43
1:O:56:LEU:HG	1:O:62:PHE:HB2	2.01	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
1:0:56: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:B:103:VAL:CG1	2:B:116:PHE:HB3	2.49	0.43
2:B:427:ARG:HD2	2:B:428:PRO:O	2.19	0.43
2:B:523:VAL:HG12	2:B:527:LYS:HE3	2.01	0.43
2:D:339:ASN:HB2	2:D:345:THR:N	2.32	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:D:247:PRO:HB3	2:D:304:LYS:HD2	2.01	0.43
2:F:346:GLU:HB3	2:F:395:GLN:HE21	1.83	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
2:A:292:TYR:CZ	2:A:436:LYS:HB2	2.54	0.42
2:A:430:ARG:H	2:A:430:ARG:HD3	1.84	0.42
2:B:495:PHE:HE1	2:B:559:GLU:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:PRO:HG2	2:B:570:TRP:CE3	2.53	0.42
2:D:164:LEU:HA	2:D:176:VAL:HG12	2.01	0.42
2:D:464:LEU:HD11	2:D:471:ARG:HG2	2.00	0.42
2:E:521:ASN:ND2	2:F:428:PRO:HB3	2.34	0.42
2:F:496:LEU:HD11	2:F:562:PRO:HB3	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
1:0:119:GLU:H	1:0:119:GLU:HG3	1.66	0.42
2:A:510:PHE:HB3	2:A:555:PHE:CE1	2.53	0.42
2:B:346:GLU:O	2:B:350:ARG:HG3	2.20	0.42
2:C:175:LEU:HD11	2:C:183:GLU:HB3	2.01	0.42
2:D:115:VAL:HG12	2:D:117:THR:HG23	2.00	0.42
2:F:284:ARG:HE	2:F:285:PRO:HD2	1.83	0.42
2:F:355:ARG:O	2:F:358:GLU:HG3	2.19	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:A:495:PHE:HB2	2:A:510:PHE:CD1	2.54	0.42
2:C:292:TYR:CZ	2:C:436:LYS:HB2	2.55	0.42
2:E:99:SER:HB2	2:E:143:LEU:O	2.20	0.42
2:E:107:THR:HG22	2:E:113:VAL:HG12	2.01	0.42
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
1:6:23:GLY:HA3	1:6:119:GLU:OE1	2.19	0.42
2:A:123:ARG:NH2	2:D:101:TYR:OH	2.52	0.42
2:B:549:ASP:HA	2:B:552:VAL:HG22	2.01	0.42
2:B:583:TYR:HE2	2:B:585:ARG:HD3	1.83	0.42
2:C:261:ILE:HA	2:C:264:ILE:HG22	2.02	0.42
2:C:300:THR:O	2:C:304:LYS:HG3	2.19	0.42
2:E:220:LEU:HA	2:E:231:GLU:O	2.20	0.42
2:F:321:ASP:OD1	2:F:324:GLU:HB2	2.18	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:B:508:MET:CE	2:B:573:ILE:HG21	2.50	0.42
2:C:498:VAL:O	2:C:505:LYS:HB3	2.18	0.42
2:D:219:SER:OG	2:D:235:LYS:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:161:ILE:HG22	2:F:183:GLU:O	2.19	0.42
2:F:255:GLY:O	5:F:701:ATP:N6	2.50	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:C:437:ILE:HD12	2:C:437:ILE:N	2.32	0.42
2:C:446:GLN:HG3	2:C:479:ILE:HG22	2.01	0.42
2:D:243:LEU:HD21	2:D:359:LYS:HD3	2.01	0.42
2:D:261:ILE:O	2:D:264:ILE:HG22	2.20	0.42
2:E:561:LEU:N	2:E:562:PRO:HD2	2.34	0.42
2:F:418:GLU:CD	2:F:418:GLU:H	2.23	0.42
1:I:33:LEU:HD12	1:I:40:LEU:HB3	2.02	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:B:272:PHE:CE2	2:B:365:PRO:HG3	2.55	0.42
2:B:534:VAL:HG22	2:B:540:PRO:HA	2.02	0.42
2:C:496:LEU:HD23	2:C:586:THR:HA	2.01	0.42
2:D:339:ASN:HB3	2:D:344:GLU:HB3	2.02	0.42
2:D:349:ILE:HG23	2:D:353:PHE:HE2	1.84	0.42
2:D:518:MET:O	2:D:522:VAL:HG23	2.20	0.42
2:F:290:LEU:HD22	2:F:426:LEU:HD22	2.01	0.42
4:H:432:GLU:CD	4:H:437:GLN:HE21	2.22	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:E:140:THR:O	2:E:153:GLY:N	2.53	0.42
2:E:237:GLU:O	2:E:241:LEU:N	2.53	0.42
2:F:187:TRP:CD1	2:F:228:TYR:HE1	2.38	0.42
2:F:460:HIS:CE1	2:F:539:GLN:HB3	2.54	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
2:B:379:THR:HG22	2:B:422:ASP:HA	2.02	0.42
2:D:159:GLY:N	2:D:221:LEU:HD11	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:488:ARG:HB2	4:L:490:ILE:HG13	2.02	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:A:566:ASN:OD1	2:A:567:PRO:HD2	2.20	0.42
2:B:544:ILE:O	2:B:548:LEU:HG	2.20	0.42
2:E:242:VAL:HG11	2:E:333:LYS:HG3	2.02	0.42
4:L:369:LEU:HD23	4:L:369:LEU:HA	1.85	0.42
4:S:318:ARG:HD3	4:S:493:THR:HG23	2.00	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:C:346:GLU:O	2:C:350:ARG:HG3	2.20	0.41
2:C:609:LEU:HA	2:C:609:LEU:HD23	1.79	0.41
2:F:255:GLY:H	5:F:701:ATP:N6	2.18	0.41
2:A:563:ASN:OD1	2:A:564:THR:N	2.53	0.41
2:B:289:VAL:HB	2:B:412:ILE:HG12	2.02	0.41
2:B:379:THR:HG23	2:B:420:MET:O	2.20	0.41
2:D:489:GLU:HG2	2:D:511:LYS:NZ	2.35	0.41
2:F:515:SER:O	2:F:519:ILE:HG12	2.20	0.41
4:V:338:ASP:OD1	4:V:341:THR:N	2.53	0.41
1:8:32:ALA:HA	1:8:40:LEU:O	2.21	0.41
2:B:271:PRO:HB3	2:B:285:PRO:HB3	2.02	0.41
2:C:223:ASP:O	2:C:227:GLY:N	2.45	0.41
2:C:525:ARG:CZ	2:C:554:GLU:HA	2.50	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
1:6:18:GLU:HA	1:6:21:ARG:HE	1.85	0.41
2:A:139:GLN:NE2	2:A:153:GLY:O	2.31	0.41
2:A:272:PHE:HE1	2:A:408:ASN:HA	1.84	0.41
2:A:395:GLN:O	2:A:399:GLU:HG2	2.20	0.41
2:B:500:TYR:CD1	2:B:581:ILE:HD13	2.55	0.41
2:C:173:ARG:HG2	2:C:187:TRP:CD1	2.51	0.41
2:C:531:ILE:O	2:C:535:LEU:HG	2.20	0.41
2:E:374:ASP:OD2	2:E:417:ARG:HB2	2.19	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
1:0:98:GLN:O	1:0:102:VAL:HG23	2.21	0.41
2:A:287:LYS:HD2	2:A:404:GLU:HG3	2.02	0.41
2:B:289:VAL:O	2:B:412:ILE:HA	2.21	0.41
2:C:444:ALA:O	2:C:448:ILE:HG13	2.21	0.41
2:D:261:ILE:HA	2:D:264:ILE:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:ARG:NH1	2:D:269:GLU:OE1	2.54	0.41
2:D:496:LEU:HB2	2:D:508:MET:HG3	2.03	0.41
1:T:41:PHE:HB3	1:T:53:ILE:HD13	2.01	0.41
4:U:488:ARG:HB2	4:U:490:ILE:HG13	2.02	0.41
1:2:32:ALA:HA	1:2:40:LEU:O	2.20	0.41
1:4:69:ASN:HD22	1:4:69:ASN:N	2.18	0.41
2:A:105:LEU:HD21	2:A:116:PHE:HB2	2.03	0.41
2:B:530:ALA:O	2:B:534:VAL:HG23	2.21	0.41
2:C:313:LYS:HD3	2:C:313:LYS:HA	1.93	0.41
2:C:396:LEU:O	2:C:400:ILE:HG12	2.20	0.41
2:E:377:PHE:HZ	2:E:396:LEU:HD13	1.85	0.41
2:A:496:LEU:HB2	2:A:508:MET:HB2	2.02	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:A:393:VAL:CG1	2:A:394:PRO:HD3	2.51	0.41
2:A:570:TRP:CE3	2:A:570:TRP:HA	2.55	0.41
2:B:436:LYS:HE2	2:B:438:GLU:HG2	2.02	0.41
2:F:497:GLU:HB3	2:F:587:LEU:HD21	2.03	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
1:4:11:GLN:HB2	2:B:505:LYS:HB2	2.03	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:D:339:ASN:H	2:D:345:THR:HB	1.85	0.41
2:E:105:LEU:HD21	2:E:116:PHE:HB2	2.02	0.41
2:E:261:ILE:HA	2:E:264:ILE:HG22	2.03	0.41
2:E:314:MET:HG3	2:E:328:TYR:CD2	2.55	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:V:432:GLU:CD	4:V:437:GLN:HE21	2.24	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
1:8:14:ARG:HG2	2:F:582:VAL:CG2	2.49	0.41
1:8:17:SER:HB2	2:E:605:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:337:LEU:O	2:A:337:LEU:HD12	2.21	0.41
2:B:159:GLY:N	2:B:221:LEU:HD11	2.36	0.41
2:C:287:LYS:HG3	2:C:406:LEU:HD11	2.02	0.41
2:C:495:PHE:HB2	2:C:510:PHE:CD1	2.56	0.41
2:D:102:GLY:HA3	2:D:117:THR:HG22	2.02	0.41
2:D:485:ARG:NH2	2:D:492:ASP:OD2	2.54	0.41
2:F:525:ARG:HH21	2:F:554:GLU:HG2	1.86	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
1:4:32:ALA:HA	1:4:40:LEU:O	2.21	0.40
1:8:14:ARG:HA	1:8:14:ARG:HD2	1.26	0.40
2:A:563:ASN:ND2	2:B:426:LEU:HB3	2.31	0.40
2:C:437:ILE:HG22	2:C:438:GLU:H	1.86	0.40
2:D:265:ARG:HG2	2:D:265:ARG:HH11	1.85	0.40
2:D:447:ASP:O	2:D:451:LYS:HG3	2.21	0.40
2:D:609:LEU:HD23	2:D:609:LEU:HA	1.91	0.40
2:E:377:PHE:CZ	2:E:396:LEU:HD13	2.56	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: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
1:2:214:ASP:OD2	1:2:217:ARG:HG2	2.22	0.40
2:A:355:ARG:HA	2:A:355:ARG:HD3	1.75	0.40
2:B:573:ILE:HA	2:B:576:LYS:HE3	2.03	0.40
2:C:259:ARG:O	2:C:263:GLN:OE1	2.39	0.40
2:C:495:PHE:HZ	2:C:561:LEU:HB2	1.85	0.40
2:C:508:MET:SD	2:C:508:MET:N	2.94	0.40
2:D:190:ASP:HA	2:D:193:ILE:HG22	2.02	0.40
2:D:298:GLY:C	2:D:300:THR:H	2.24	0.40
2:E:276:GLU:HG2	2:E:277:LEU:HD22	2.04	0.40
4:M:320:SER:HB3	4:M:331:VAL:HG21	2.03	0.40
2:1:609:LEU:HD23	2:1:609:LEU:HA	1.75	0.40
1:6:28:LYS:HB2	1:6:52:LYS:HZ2	1.86	0.40
2:B:481:LYS:HA	2:B:481:LYS:HD3	1.82	0.40
2:C:290:LEU:HD22	2:C:426:LEU:HD22	2.03	0.40
2:D:566:ASN:N	2:D:567:PRO:HD2	2.36	0.40
2:E:467:PHE:HD2	2:E:474:CYS:HA	1.86	0.40
2:F:296:GLY:O	5:F:701:ATP:H5'1	2.21	0.40
1:K:108:GLY:HA2	1:K:144:ASP:O	2.21	0.40
4:N:320:SER:HB3	4:N:331:VAL:HG21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:GLY:HA3	1:X:103:TYR:OH	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:C:332:ILE:HD13	2:C:370:PHE:HE1	1.86	0.40
2:E:214:LEU:HD13	2:E:232:ARG:HE	1.86	0.40
2:F:460:HIS:HD2	2:F:462:ASP:HB2	1.85	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
4:R:450:MET:HG3	4:R:470:ALA:HB2	2.04	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:C:398:SER:HB2	2:F:333:LYS:HG3	2.04	0.40
2:C:496:LEU:HD13	2:C:584:ILE:HG21	2.03	0.40
2:D:373:MET:HB2	2:D:415:SER:HB2	2.04	0.40
2:D:491:ASP:OD1	2:D:494:ARG:NH1	2.55	0.40
2:D:560:ASP:O	2:D:564:THR:OG1	2.26	0.40
2:F:165:ARG:CG	2:F:177:VAL:HG13	2.52	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:O:178:THR:HG22	1:O:182:ARG:HE	1.87	0.40
4:S:338:ASP:OD1	4:S:341:THR:N	2.55	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%)	201 (95%)	10 (5%)	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%)	202 (96%)	8 (4%)	1 (0%)	29	67
1	f	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
2	1	3/609 (0%)	2 (67%)	1 (33%)	0	100	100
2	A	461/609 (76%)	446 (97%)	15 (3%)	0	100	100
2	B	475/609 (78%)	454 (96%)	20 (4%)	1 (0%)	47	79
2	C	463/609 (76%)	448 (97%)	15 (3%)	0	100	100
2	D	447/609 (73%)	424 (95%)	23 (5%)	0	100	100
2	E	477/609 (78%)	450 (94%)	27 (6%)	0	100	100
2	F	477/609 (78%)	457 (96%)	19 (4%)	1 (0%)	47	79
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	67
4	N	220/291 (76%)	212 (96%)	7 (3%)	1 (0%)	29	67
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	67
4	U	232/291 (80%)	221 (95%)	11 (5%)	0	100	100
4	V	221/291 (76%)	214 (97%)	6 (3%)	1 (0%)	29	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	W	232/291 (80%)	225 (97%)	6 (3%)	1 (0%)	34 71
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 67
All	All	8881/11875 (75%)	8519 (96%)	353 (4%)	9 (0%)	54 84

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	d	9	PRO
2	F	583	TYR
4	W	309	PRO
4	b	309	PRO
4	M	309	PRO
4	N	309	PRO
4	S	309	PRO
4	V	309	PRO
2	B	503	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 53
1	2	165/192 (86%)	158 (96%)	7 (4%)	30 56
1	4	165/192 (86%)	156 (94%)	9 (6%)	21 50
1	6	165/192 (86%)	157 (95%)	8 (5%)	25 53
1	8	165/192 (86%)	155 (94%)	10 (6%)	18 47
1	I	164/192 (85%)	154 (94%)	10 (6%)	18 47
1	K	166/192 (86%)	158 (95%)	8 (5%)	25 53
1	O	165/192 (86%)	155 (94%)	10 (6%)	18 47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	165/192 (86%)	154 (93%)	11 (7%)	16 44
1	T	164/192 (85%)	156 (95%)	8 (5%)	25 52
1	X	164/192 (85%)	159 (97%)	5 (3%)	41 64
1	Z	165/192 (86%)	156 (94%)	9 (6%)	21 50
1	d	165/192 (86%)	156 (94%)	9 (6%)	21 50
1	f	165/192 (86%)	154 (93%)	11 (7%)	16 44
2	1	4/511 (1%)	4 (100%)	0	100 100
2	A	400/511 (78%)	397 (99%)	3 (1%)	81 89
2	B	407/511 (80%)	404 (99%)	3 (1%)	84 90
2	C	400/511 (78%)	398 (100%)	2 (0%)	88 93
2	D	388/511 (76%)	387 (100%)	1 (0%)	92 95
2	E	409/511 (80%)	407 (100%)	2 (0%)	88 93
2	F	408/511 (80%)	407 (100%)	1 (0%)	93 96
3	G	10/50 (20%)	9 (90%)	1 (10%)	7 29
4	H	164/217 (76%)	161 (98%)	3 (2%)	59 77
4	J	164/217 (76%)	158 (96%)	6 (4%)	34 60
4	L	164/217 (76%)	161 (98%)	3 (2%)	59 77
4	M	164/217 (76%)	160 (98%)	4 (2%)	49 69
4	N	164/217 (76%)	160 (98%)	4 (2%)	49 69
4	P	164/217 (76%)	159 (97%)	5 (3%)	41 64
4	R	164/217 (76%)	160 (98%)	4 (2%)	49 69
4	S	164/217 (76%)	159 (97%)	5 (3%)	41 64
4	U	171/217 (79%)	166 (97%)	5 (3%)	42 65
4	V	164/217 (76%)	161 (98%)	3 (2%)	59 77
4	W	171/217 (79%)	167 (98%)	4 (2%)	50 70
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 60
All	All	7044/9353 (75%)	6850 (97%)	194 (3%)	46 65

All (194) 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	14	ARG
1	2	33	LEU
1	2	73	ASN
1	2	74	LEU
1	2	182	ARG
1	2	203	LEU
1	2	234	LEU
1	4	11	GLN
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	22	LYS
1	6	33	LEU
1	6	73	ASN
1	6	74	LEU
1	6	123	CYS
1	6	182	ARG
1	6	203	LEU
1	6	234	LEU
1	8	14	ARG
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	243	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	355	ARG
2	A	430	ARG
2	B	165	ARG
2	B	505	LYS
2	B	605	LEU
2	C	212	ARG
2	C	232	ARG
2	D	430	ARG
2	E	235	LYS
2	E	238	VAL
2	F	609	LEU
3	G	1	MET
4	H	330	ASP
4	H	345	ILE
4	H	444	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	b	412	SER
4	b	433	GLU
4	b	444	LEU
4	b	465	ARG
4	b	512	GLU
1	d	9	PRO
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
1	d	234	LEU
1	f	8	SER
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 (97) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	354	GLN
2	A	502	ASN
2	A	529	ASN
2	B	263	GLN
2	B	331	ASN
2	B	395	GLN
2	B	460	HIS
2	B	502	ASN
2	B	566	ASN
2	C	460	HIS
2	C	529	ASN
2	C	558	ASN
2	C	566	ASN
2	C	607	GLN
2	D	339	ASN
2	D	395	GLN
2	D	416	ASN
2	E	408	ASN
2	E	529	ASN
2	F	348	HIS
2	F	395	GLN
2	F	416	ASN
2	F	502	ASN
2	F	520	GLN
2	F	607	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 12 ligands modelled in this entry, 6 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	B	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.52	5 (16%)
5	ATP	D	701	6	26,33,33	0.91	1 (3%)	31,52,52	1.64	5 (16%)
5	ATP	A	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.53	5 (16%)
5	ATP	E	701	6	26,33,33	0.92	1 (3%)	31,52,52	1.49	5 (16%)
5	ATP	C	701	6	26,33,33	0.93	1 (3%)	31,52,52	1.51	5 (16%)
5	ATP	F	701	6	26,33,33	0.68	0	31,52,52	0.89	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	701	6	-	1/18/38/38	0/3/3/3
5	ATP	D	701	6	-	7/18/38/38	0/3/3/3
5	ATP	A	701	6	-	1/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	E	701	6	-	1/18/38/38	0/3/3/3
5	ATP	C	701	6	-	2/18/38/38	0/3/3/3
5	ATP	F	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	E	701	ATP	C5-C4	2.50	1.47	1.40
5	C	701	ATP	C5-C4	2.46	1.47	1.40
5	A	701	ATP	C5-C4	2.45	1.47	1.40
5	B	701	ATP	C5-C4	2.43	1.47	1.40
5	D	701	ATP	C5-C4	2.43	1.47	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	701	ATP	PA-O3A-PB	-4.31	118.03	132.83
5	B	701	ATP	PA-O3A-PB	-4.26	118.22	132.83
5	C	701	ATP	PA-O3A-PB	-4.21	118.38	132.83
5	D	701	ATP	PB-O3B-PG	-4.14	118.62	132.83
5	E	701	ATP	PA-O3A-PB	-4.10	118.77	132.83
5	D	701	ATP	PA-O3A-PB	-3.90	119.44	132.83
5	D	701	ATP	C3'-C2'-C1'	3.15	105.73	100.98
5	D	701	ATP	N3-C2-N1	-3.15	123.75	128.68
5	B	701	ATP	N3-C2-N1	-3.13	123.78	128.68
5	C	701	ATP	N3-C2-N1	-3.13	123.79	128.68
5	E	701	ATP	PB-O3B-PG	-3.12	122.13	132.83
5	B	701	ATP	PB-O3B-PG	-3.10	122.20	132.83
5	A	701	ATP	PB-O3B-PG	-3.04	122.39	132.83
5	E	701	ATP	N3-C2-N1	-3.01	123.98	128.68
5	C	701	ATP	C3'-C2'-C1'	2.91	105.36	100.98
5	A	701	ATP	C3'-C2'-C1'	2.89	105.32	100.98
5	A	701	ATP	N3-C2-N1	-2.89	124.17	128.68
5	C	701	ATP	PB-O3B-PG	-2.85	123.05	132.83
5	B	701	ATP	C3'-C2'-C1'	2.82	105.22	100.98
5	E	701	ATP	C3'-C2'-C1'	2.74	105.11	100.98
5	F	701	ATP	O4'-C1'-C2'	-2.65	103.06	106.93
5	D	701	ATP	C4-C5-N7	-2.60	106.69	109.40
5	C	701	ATP	C4-C5-N7	-2.58	106.71	109.40
5	A	701	ATP	C4-C5-N7	-2.55	106.74	109.40
5	E	701	ATP	C4-C5-N7	-2.49	106.81	109.40
5	B	701	ATP	C4-C5-N7	-2.44	106.86	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	701	ATP	C5-C6-N6	2.17	123.65	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	ATP	C5'-O5'-PA-O1A
5	D	701	ATP	C5'-O5'-PA-O3A
5	A	701	ATP	PA-O3A-PB-O1B
5	B	701	ATP	PA-O3A-PB-O1B
5	D	701	ATP	PA-O3A-PB-O1B
5	E	701	ATP	PA-O3A-PB-O1B
5	D	701	ATP	C5'-O5'-PA-O2A
5	D	701	ATP	C4'-C5'-O5'-PA
5	C	701	ATP	PA-O3A-PB-O1B
5	C	701	ATP	PA-O3A-PB-O2B
5	D	701	ATP	PA-O3A-PB-O2B
5	D	701	ATP	O4'-C4'-C5'-O5'

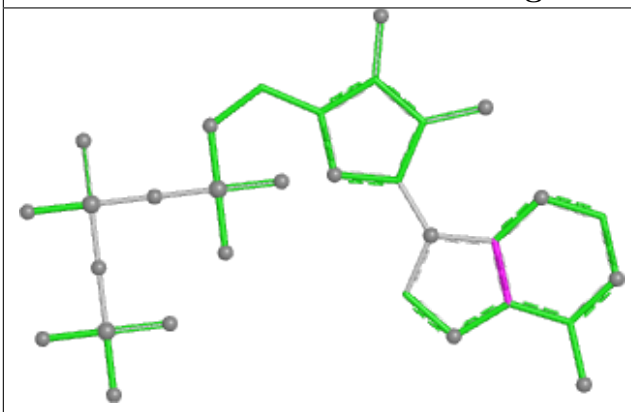
There are no ring outliers.

6 monomers are involved in 20 short contacts:

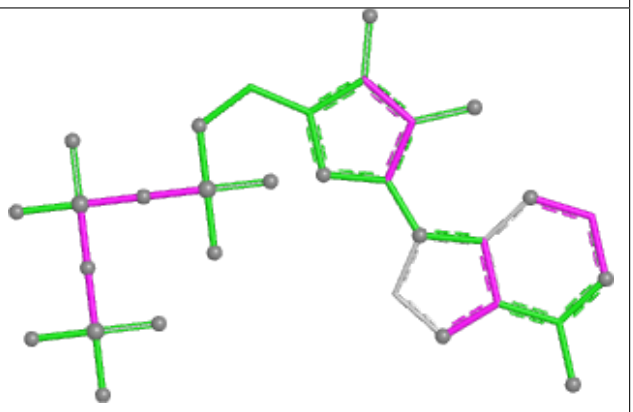
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	ATP	2	0
5	D	701	ATP	1	0
5	A	701	ATP	2	0
5	E	701	ATP	2	0
5	C	701	ATP	6	0
5	F	701	ATP	7	0

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.

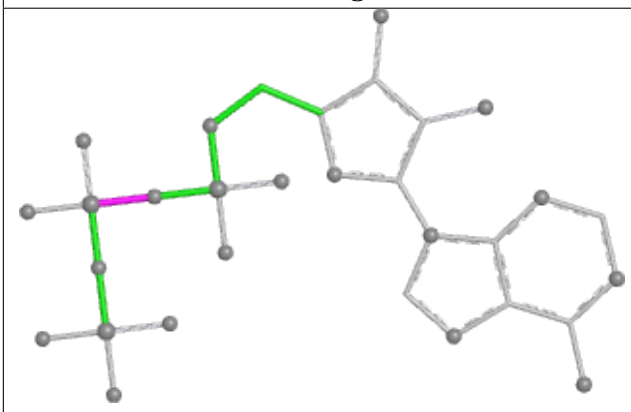
Ligand ATP B 701



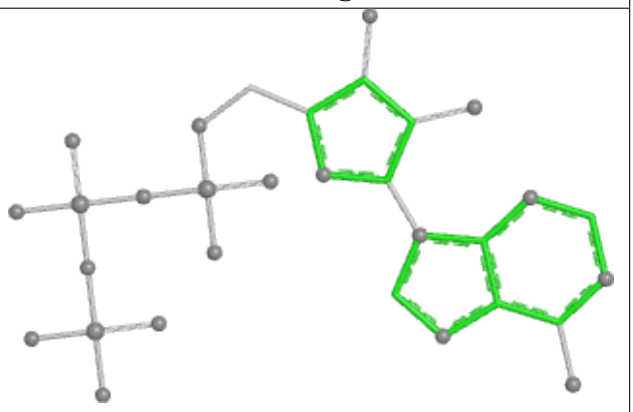
Bond lengths



Bond angles

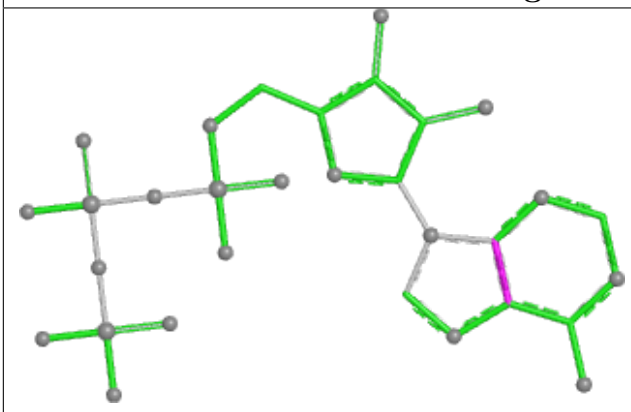


Torsions

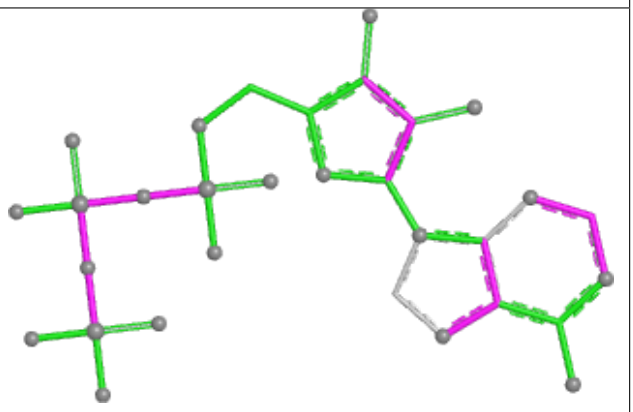


Rings

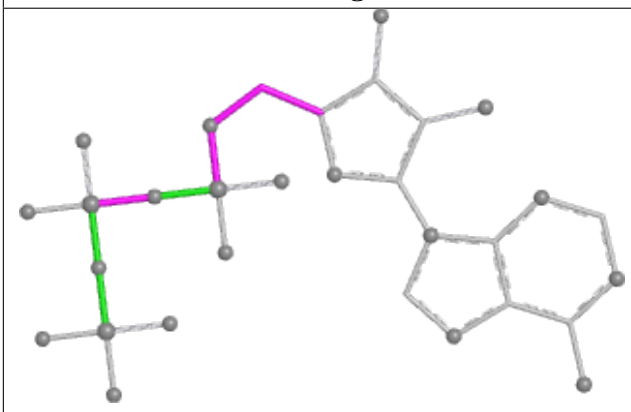
Ligand ATP D 701



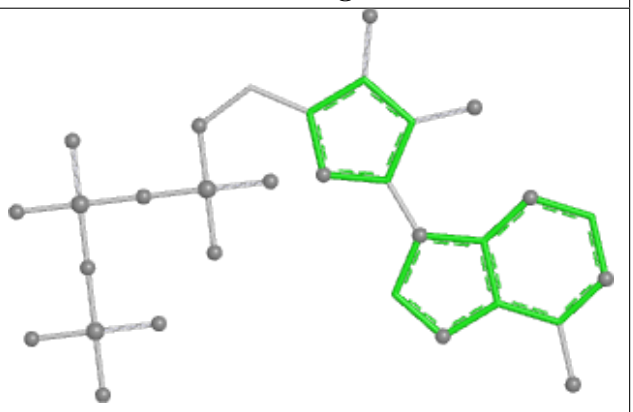
Bond lengths



Bond angles

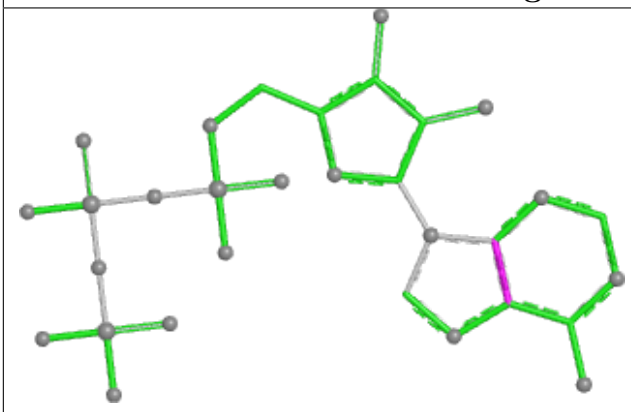


Torsions

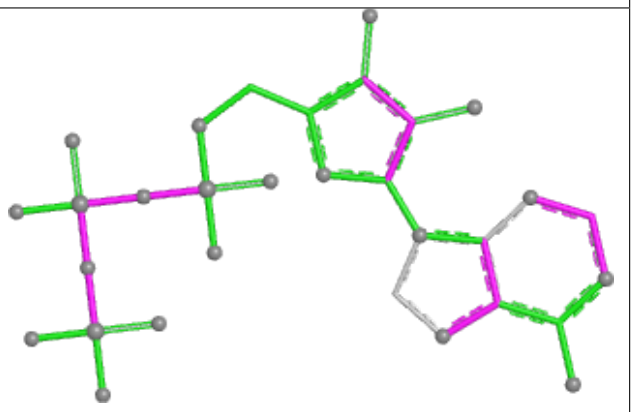


Rings

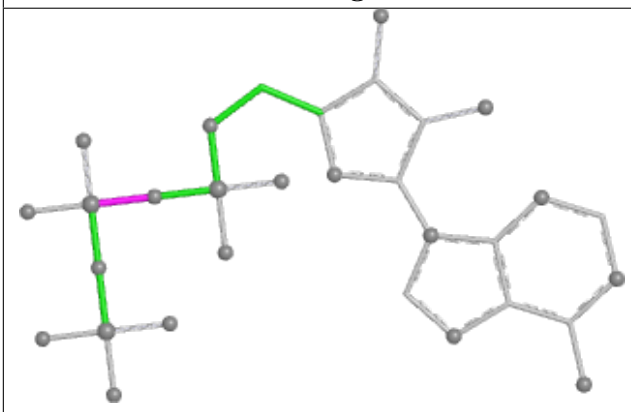
Ligand ATP A 701



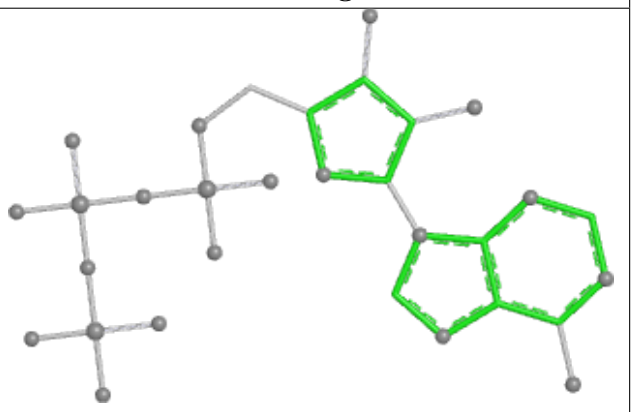
Bond lengths



Bond angles

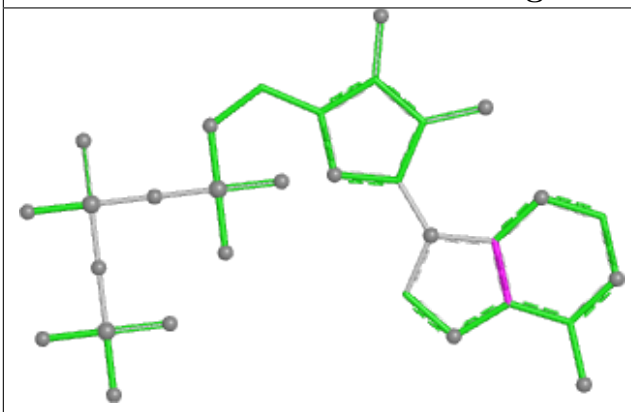


Torsions

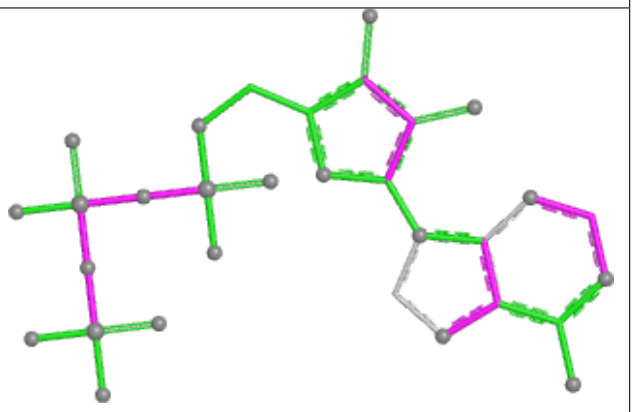


Rings

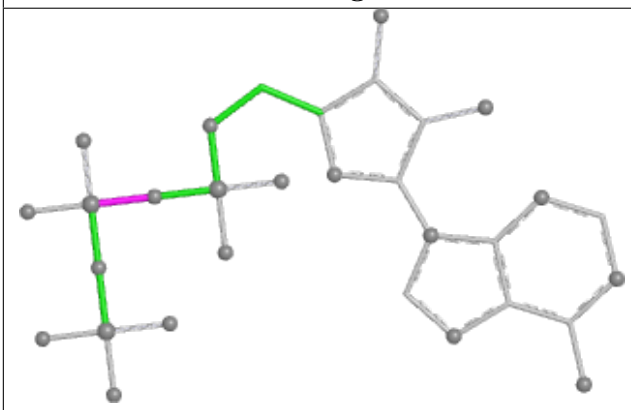
Ligand ATP E 701



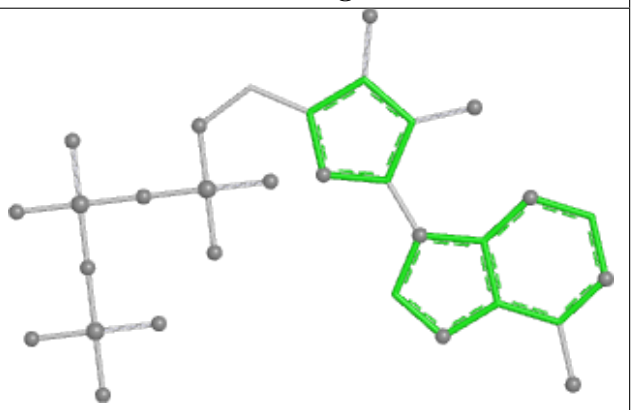
Bond lengths



Bond angles

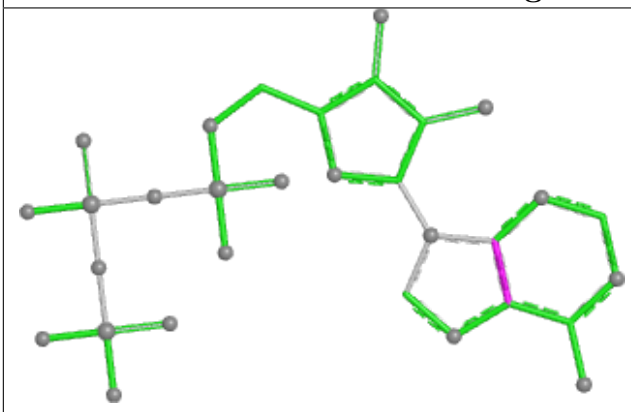


Torsions

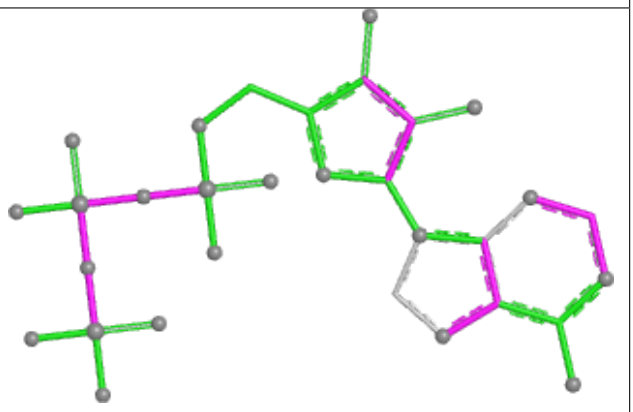


Rings

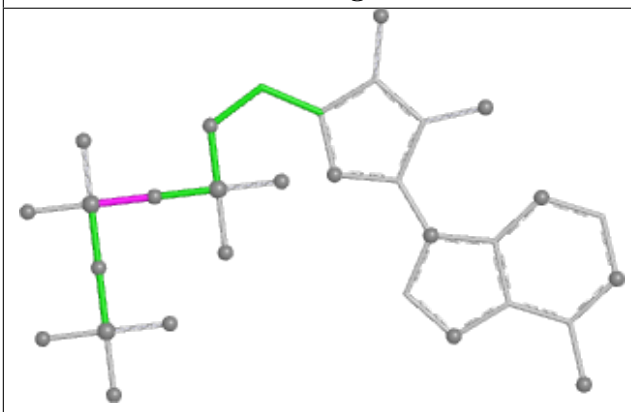
Ligand ATP C 701



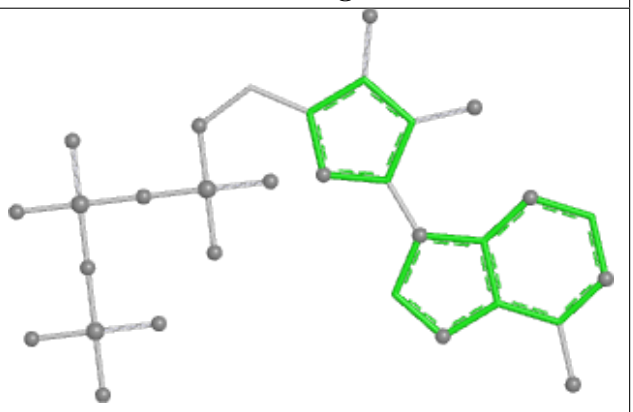
Bond lengths



Bond angles

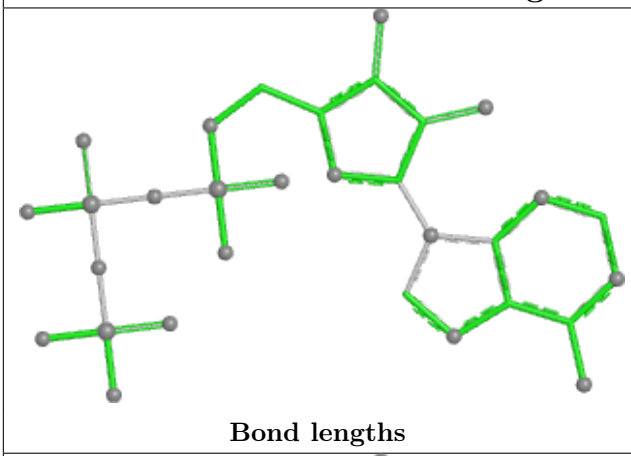


Torsions

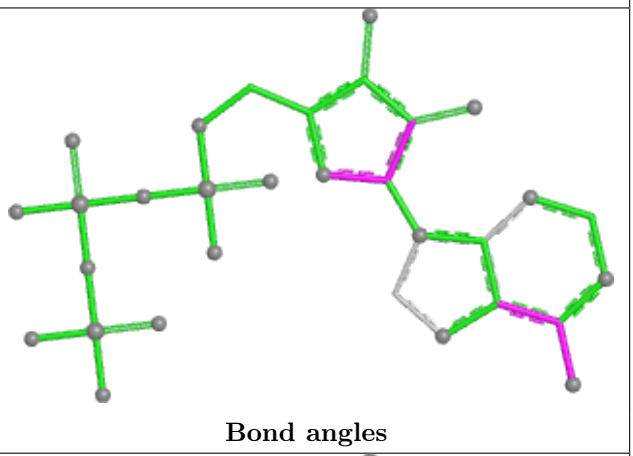


Rings

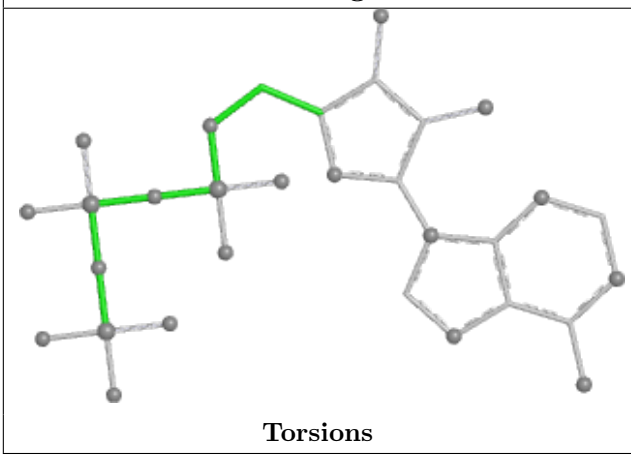
Ligand ATP F 701



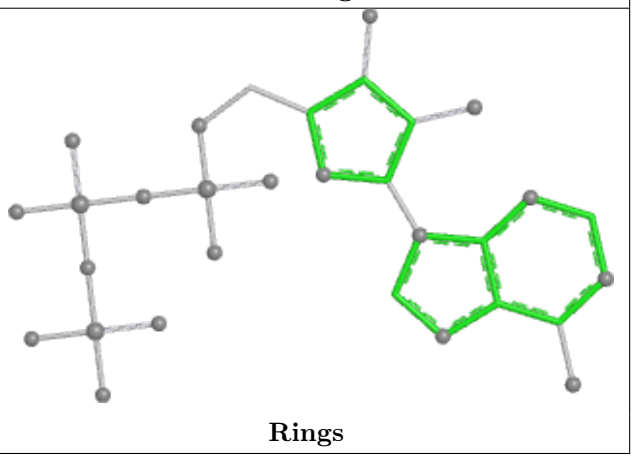
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

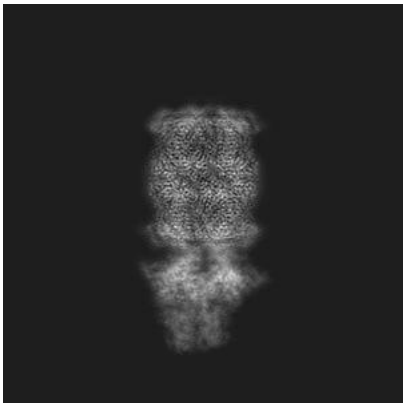
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13698. These allow visual inspection of the internal detail of the map and identification of artifacts.

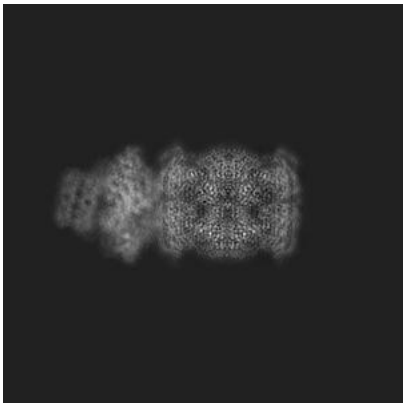
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

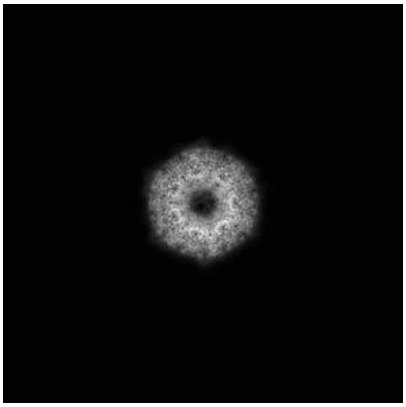
6.1.1 Primary map



X



Y



Z

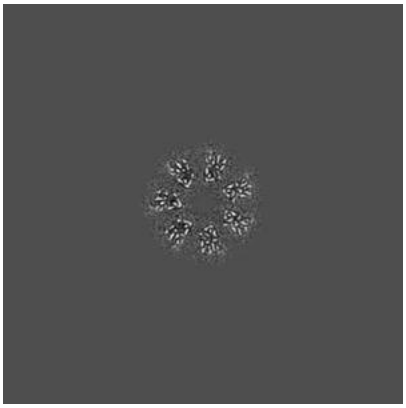
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 176

Y Index: 176

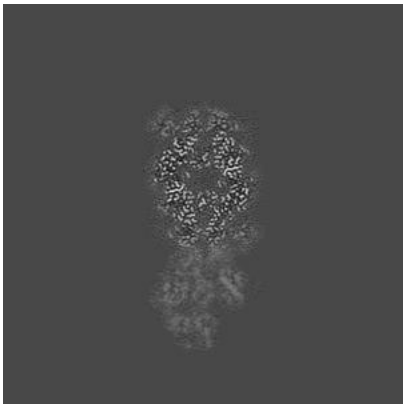


Z Index: 176

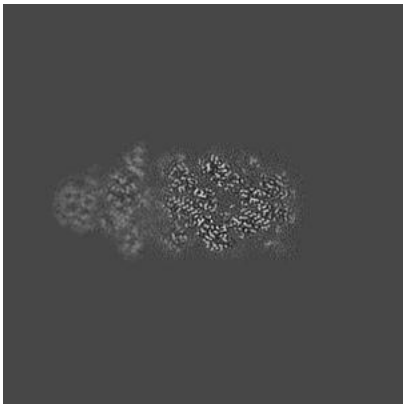
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

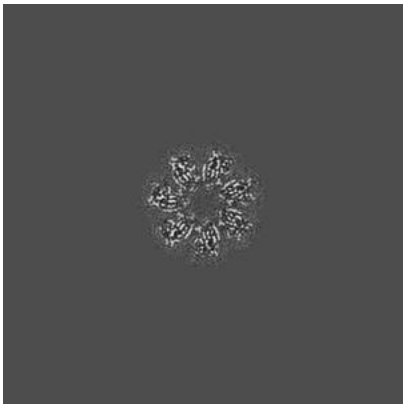
6.3.1 Primary map



X Index: 155



Y Index: 152

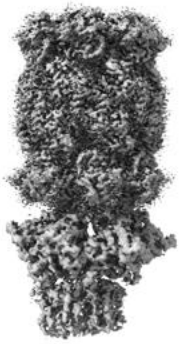


Z Index: 182

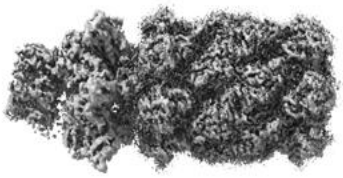
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0177. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

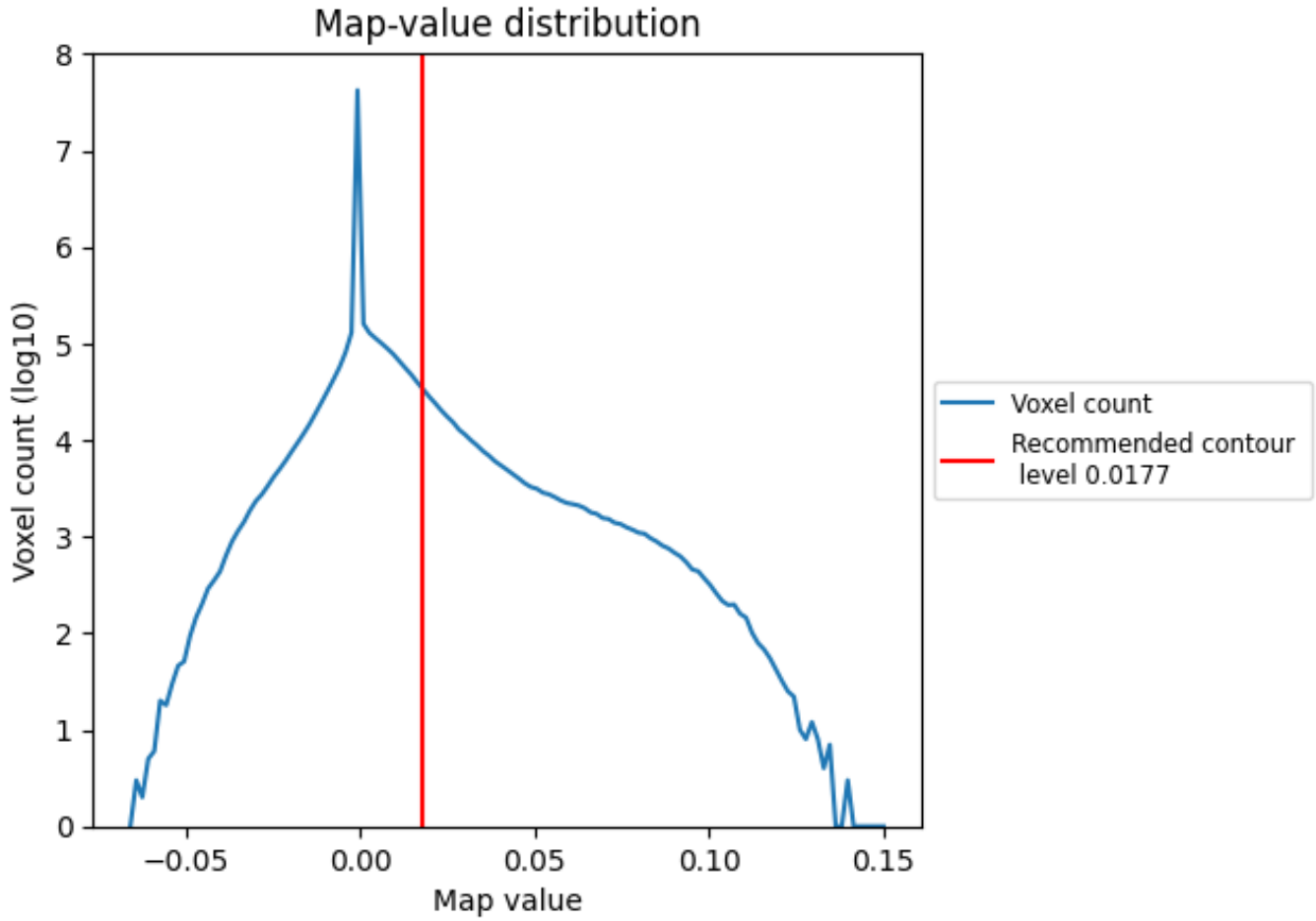
6.5 Mask visualisation (i)

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

7 Map analysis

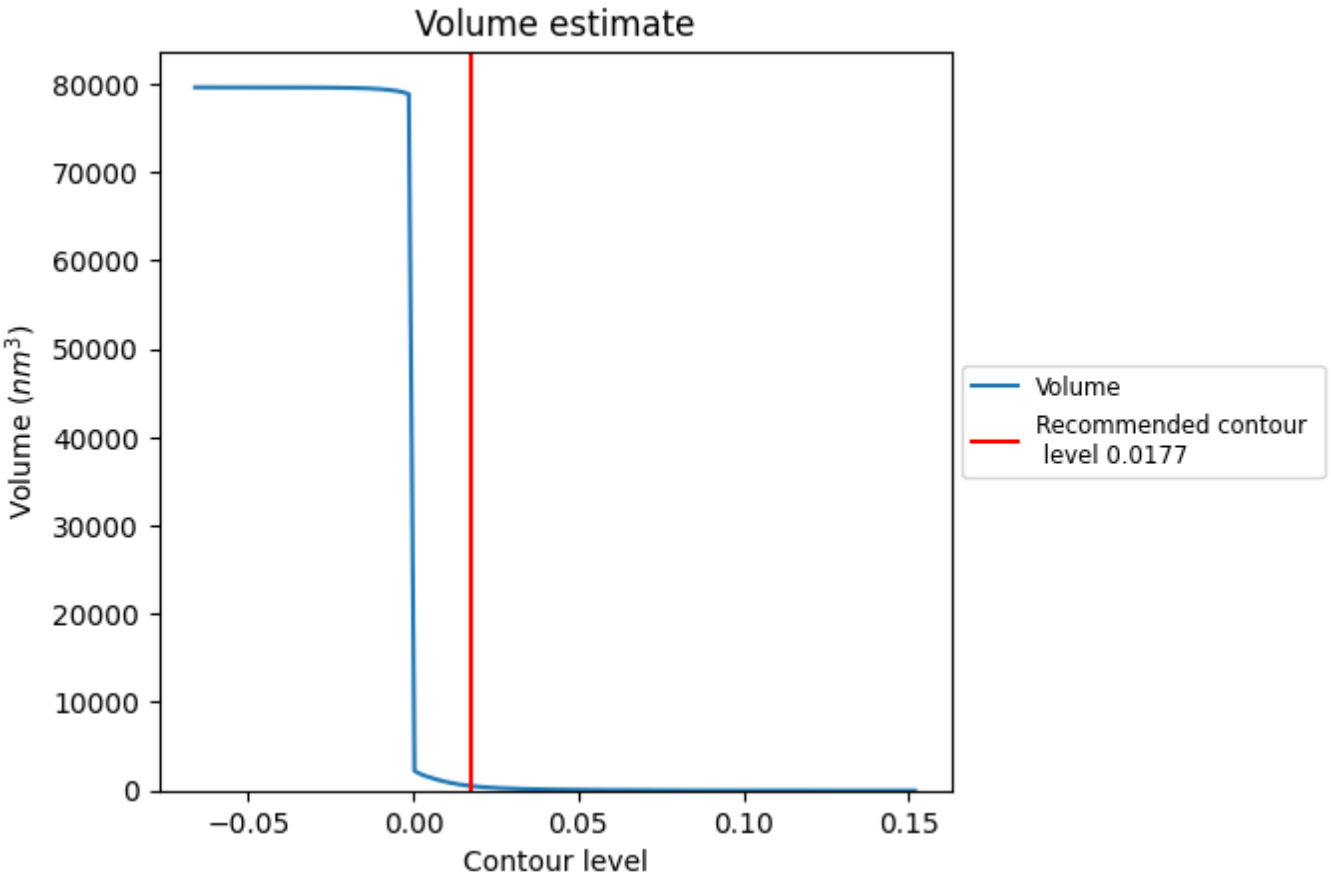
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

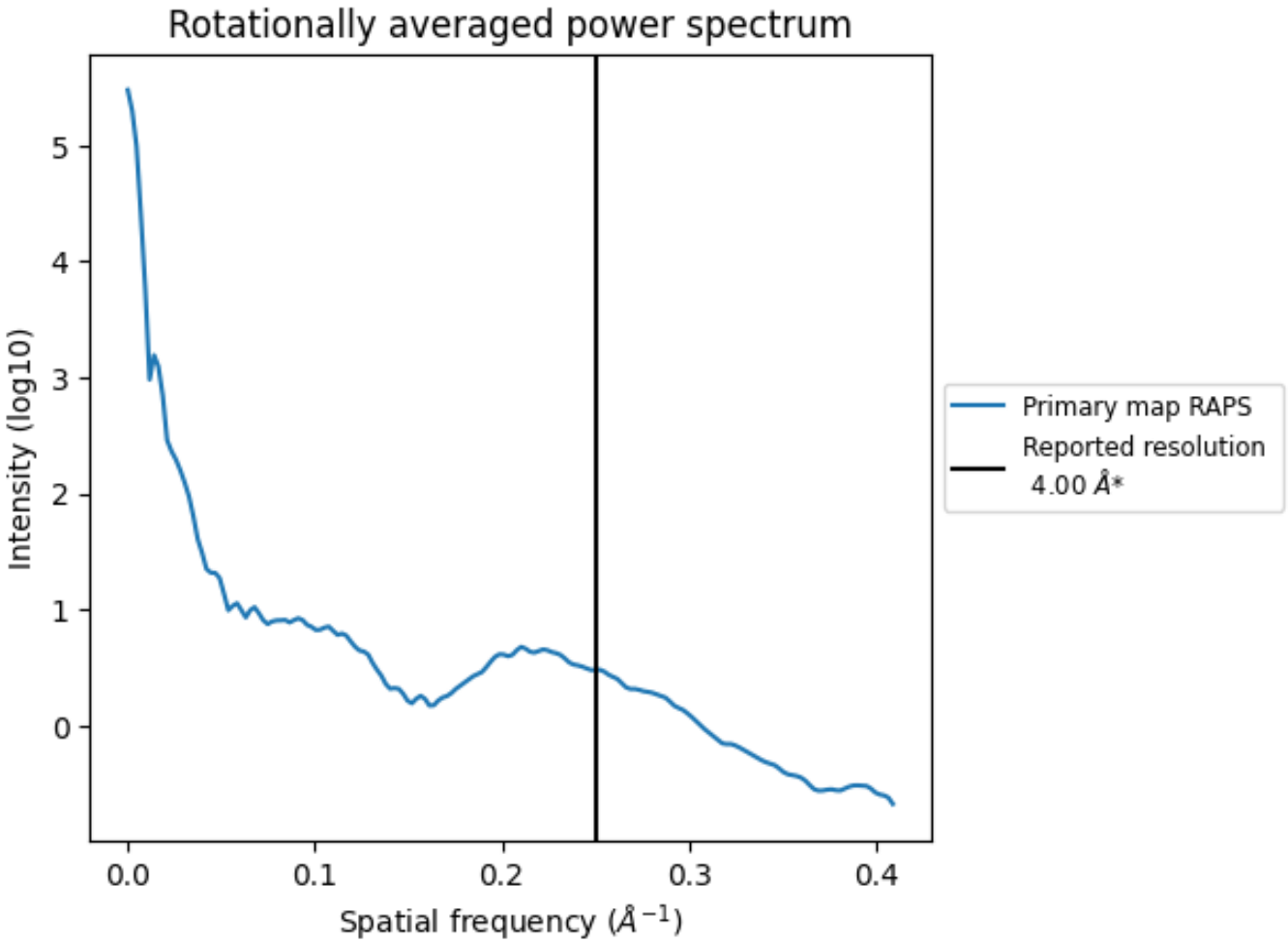
7.2 Volume estimate



The volume at the recommended contour level is 512 nm^3; this corresponds to an approximate mass of 463 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 0.250 Å^{-1}

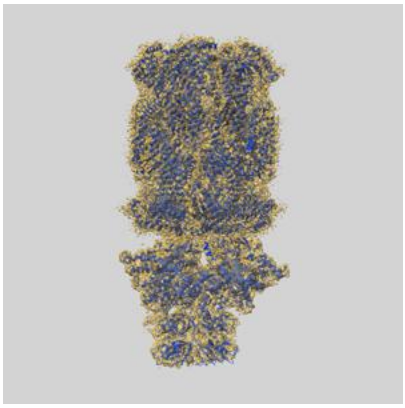
8 Fourier-Shell correlation (i)

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

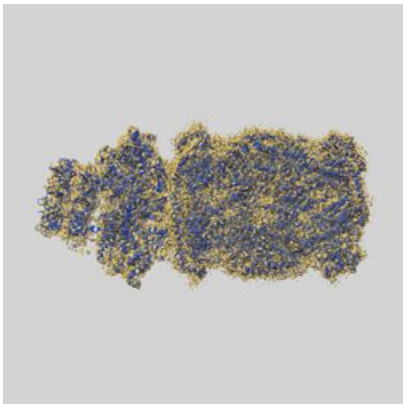
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13698 and PDB model 7PXD. Per-residue inclusion information can be found in section 3 on page 9.

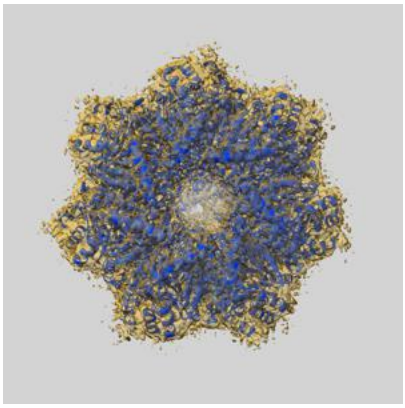
9.1 Map-model overlay



X



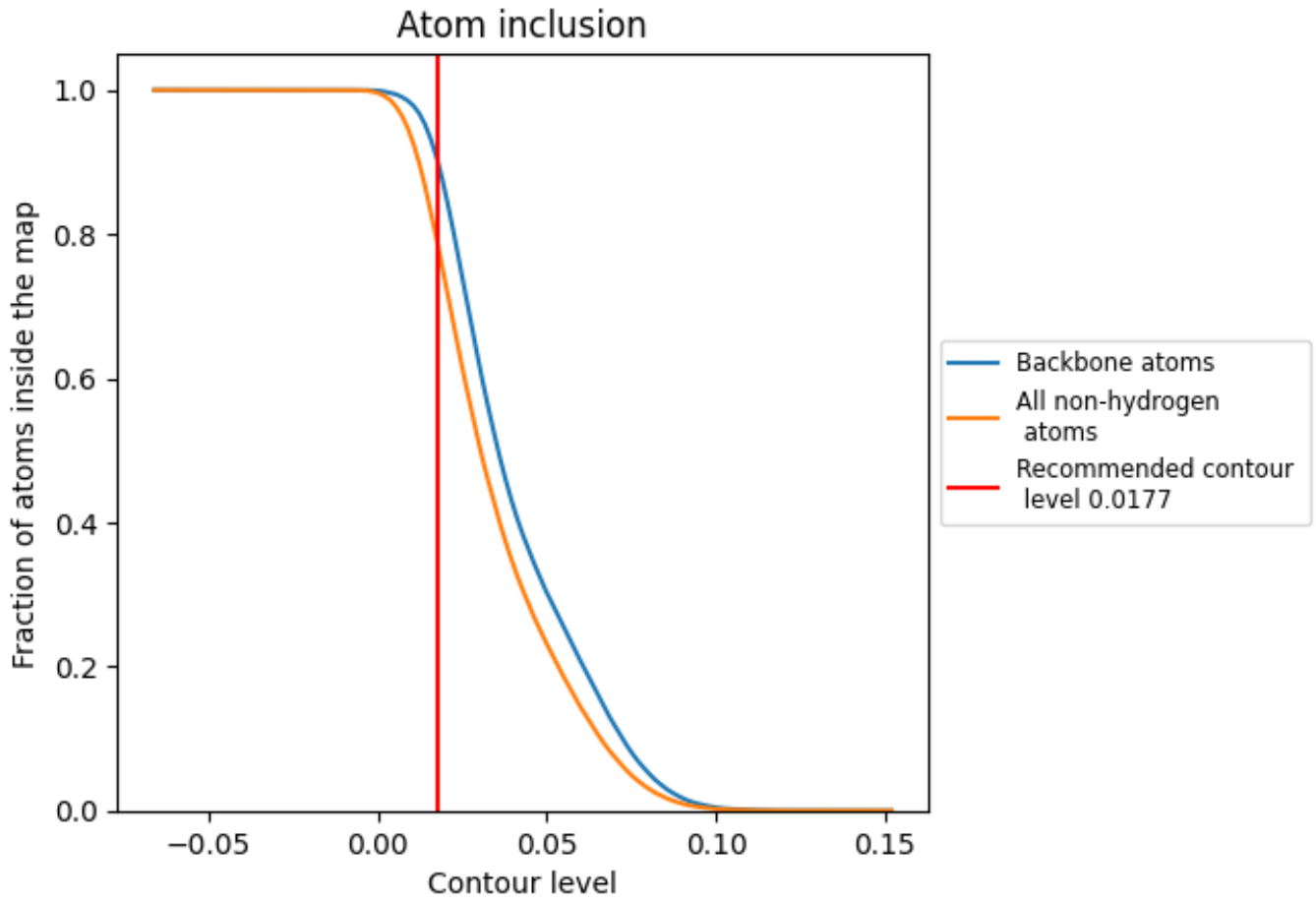
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0177 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 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.