Full wwPDB EM Validation Report ⓘ

Jun 25, 2023 – 01:07 AM JST

PDB ID	:	8H9U
EMDB ID	:	EMD-34582
Title	:	Human ATP synthase state 3a (combined)
Authors	:	Lai, Y.; Zhang, Y.; Liu, F.; Gao, Y.; Gong, H.; Rao, Z.
Deposited on	:	2022-10-25
Resolution	:	2.61 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

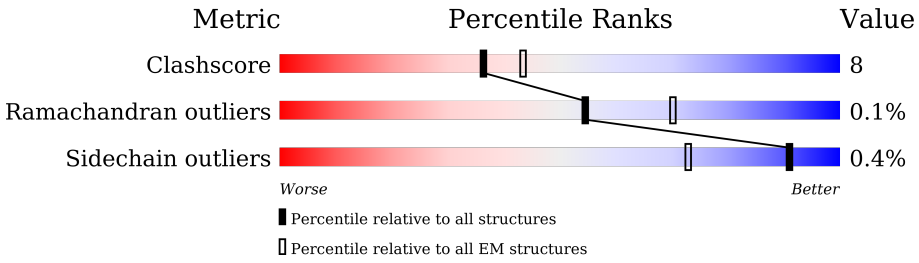
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

The reported resolution of this entry is 2.61 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	510	80% 15% 5%
1	B	510	79% 14% 6%
1	C	510	73% 19% 8%
2	D	482	80% 18%
2	E	482	76% 18% 5%
2	F	482	83% 14%
3	G	273	81% 18%
4	O	190	39% 64% 35%

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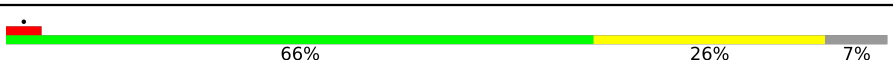
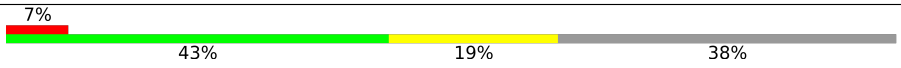
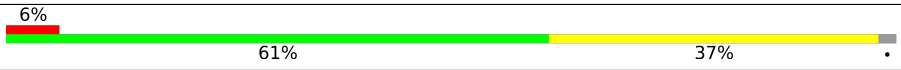
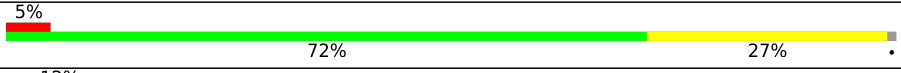
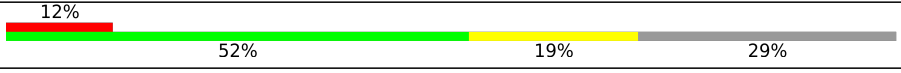
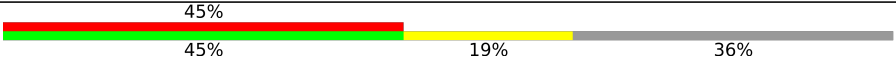
Mol	Chain	Length	Quality of chain
5	K	214	
6	L	108	
7	M	160	
8	1	75	
8	2	75	
8	3	75	
8	4	75	
8	5	75	
8	6	75	
8	7	75	
8	8	75	
9	H	146	
10	I	51	
11	N	226	
12	P	58	
13	Q	68	
14	R	93	
15	S	102	
16	T	69	
17	J	81	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 38481 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 ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	486	Total	C	N	O	S	0	0
			3706	2334	655	705	12		
1	B	477	Total	C	N	O	S	0	0
			3639	2290	645	692	12		
1	C	470	Total	C	N	O	S	0	0
			3587	2261	636	678	12		

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	456	Total	C	N	O	S	0	0
			3458	2192	588	666	12		
2	F	466	Total	C	N	O	S	0	0
			3529	2238	598	680	13		
2	D	470	Total	C	N	O	S	0	0
			3562	2257	604	688	13		

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	271	Total	C	N	O	S	0	0
			2103	1329	359	406	9		

- Molecule 4 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	187	Total	C	N	O	S	0	0
			1437	909	252	270	6		

- Molecule 5 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	198	Total	C	N	O	S	0	0
			1573	1013	270	285	5		

- Molecule 6 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	67	Total	C	N	O	S	0	0
			549	350	91	106	2		

- Molecule 7 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	156	Total	C	N	O	S	0	0
			1259	813	199	243	4		

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	4	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	5	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	6	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	7	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	8	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	1	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	2	75	Total	C	N	O	S	0	0
			534	353	83	94	4		

- Molecule 9 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	132	Total	C	N	O	S	0	0
			975	614	164	195	2		

- Molecule 10 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	45	Total	C	N	O	S	0	0
			354	225	64	64	1		

- Molecule 11 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	223	Total	C	N	O	S	0	0
			1718	1145	273	289	11		

- Molecule 12 is a protein called ATP synthase subunit ATP5MJ, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	41	Total	C	N	O	S	0	0
			344	234	53	54	3		

- Molecule 13 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	51	Total	C	N	O	S	0	0
			422	281	67	68	6		

- Molecule 14 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	74	Total	C	N	O	S	0	0
			621	411	104	103	3		

- Molecule 15 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	77	Total	C	N	O	S	0	0
			605	401	96	107	1		

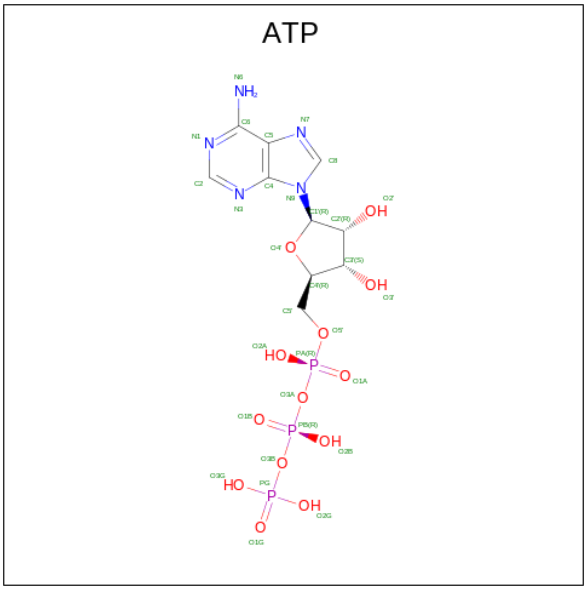
- Molecule 16 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	T	44	Total	C	N	O	0	0
			346	224	63	59		

- Molecule 17 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	J	35	Total	C	N	O	0	0
			270	163	54	53		

- Molecule 18 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).

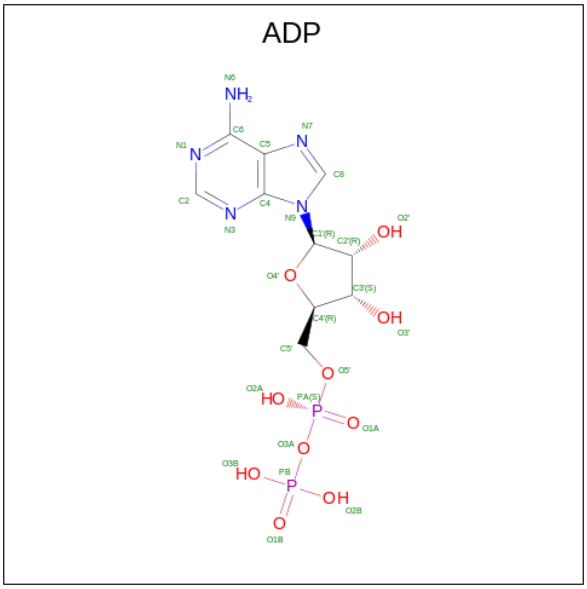


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



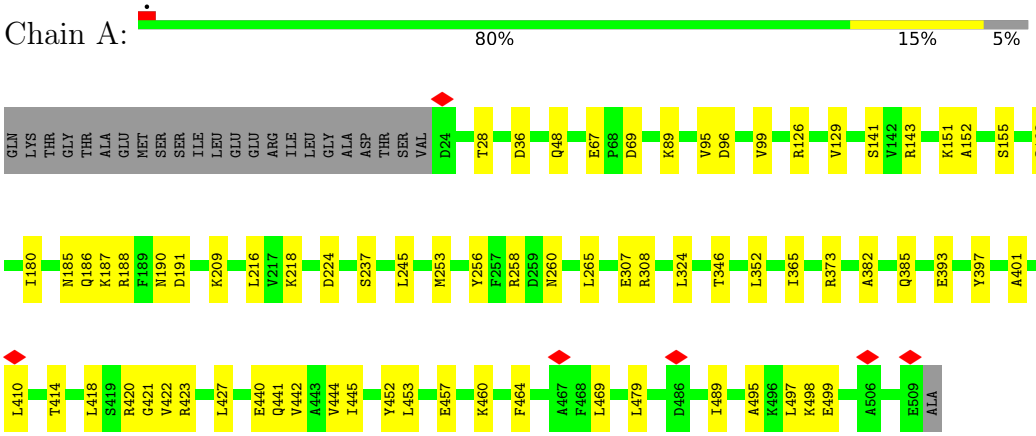
Mol	Chain	Residues	Atoms					AltConf
20	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

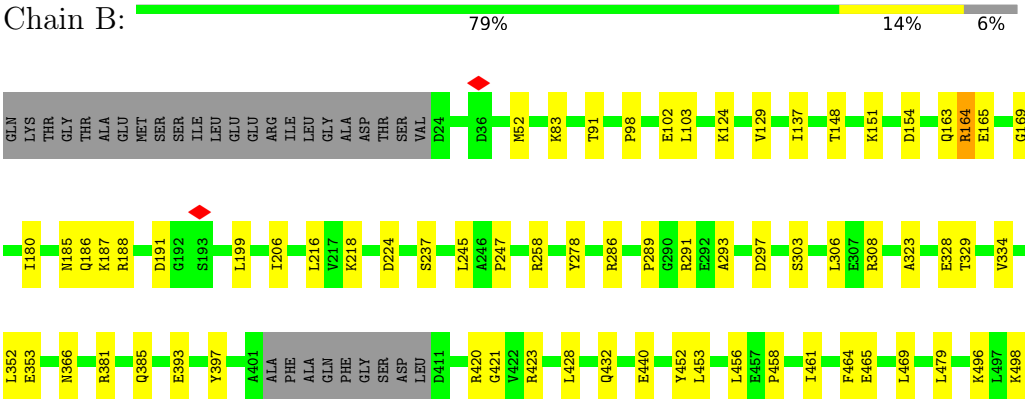
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain A:



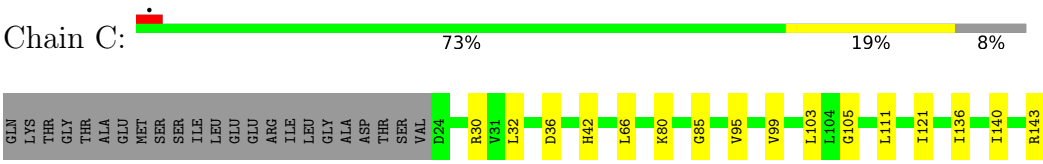
• Molecule 1: ATP synthase subunit alpha, mitochondrial

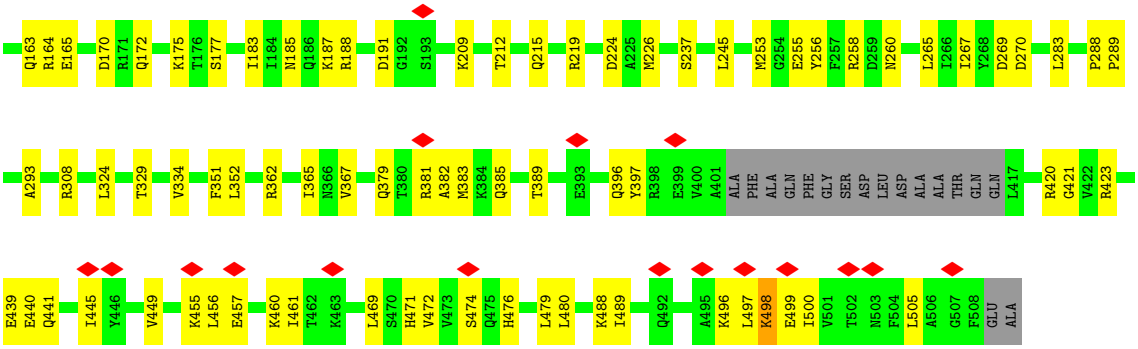
Chain B:



• Molecule 1: ATP synthase subunit alpha, mitochondrial

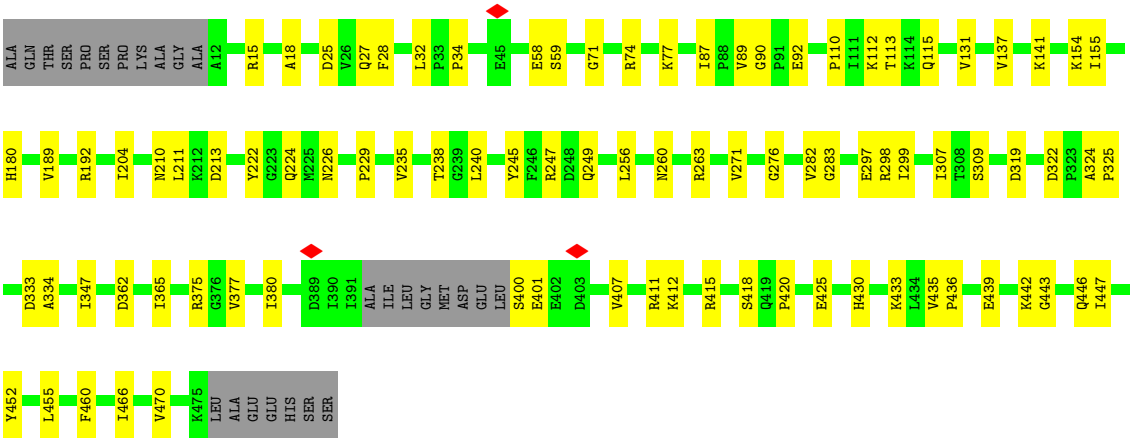
Chain C:





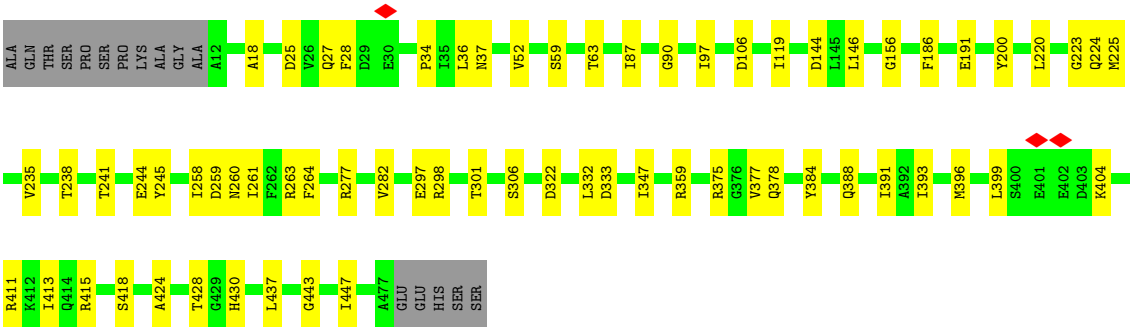
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain E:



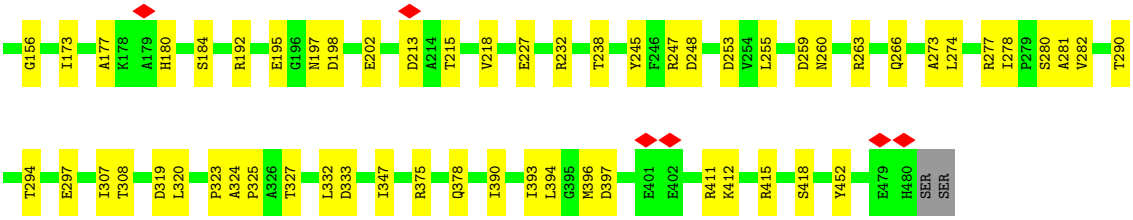
• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F:

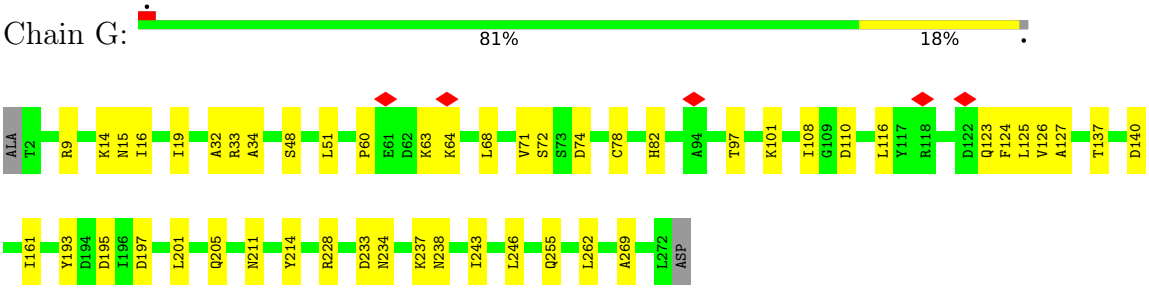


• Molecule 2: ATP synthase subunit beta, mitochondrial

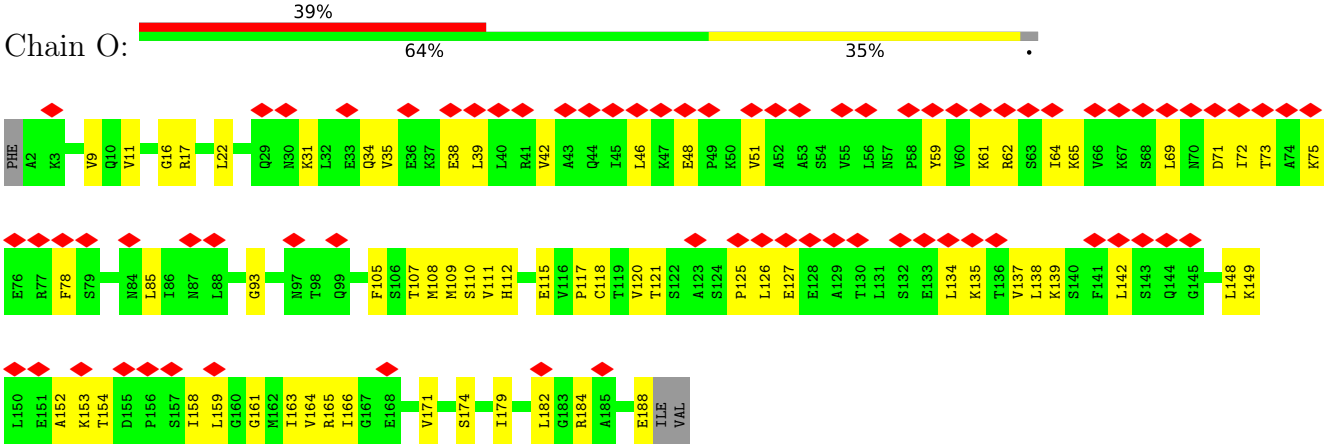
Chain D:



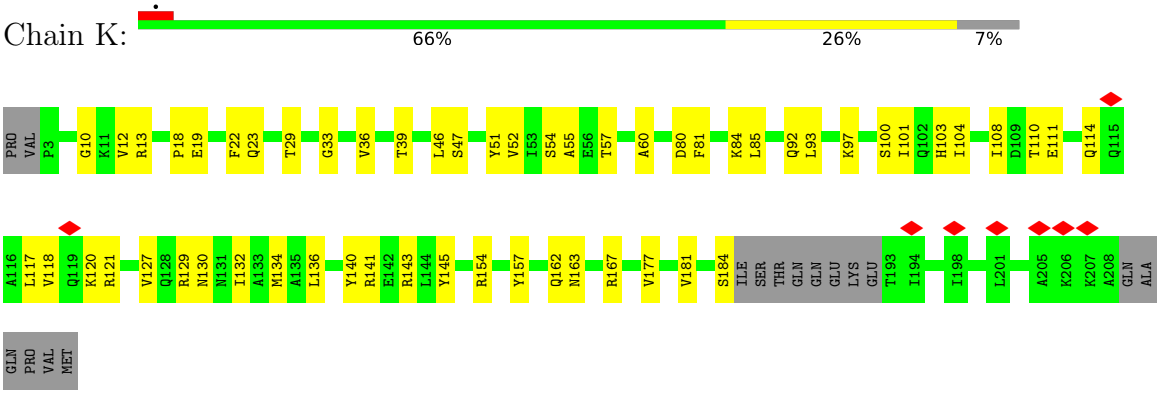
• Molecule 3: ATP synthase subunit gamma, mitochondrial



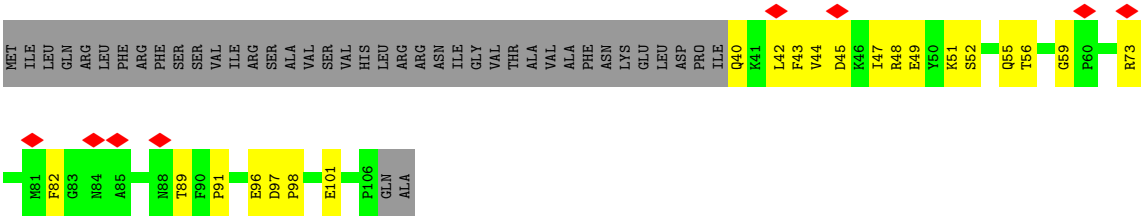
• Molecule 4: ATP synthase subunit O, mitochondrial



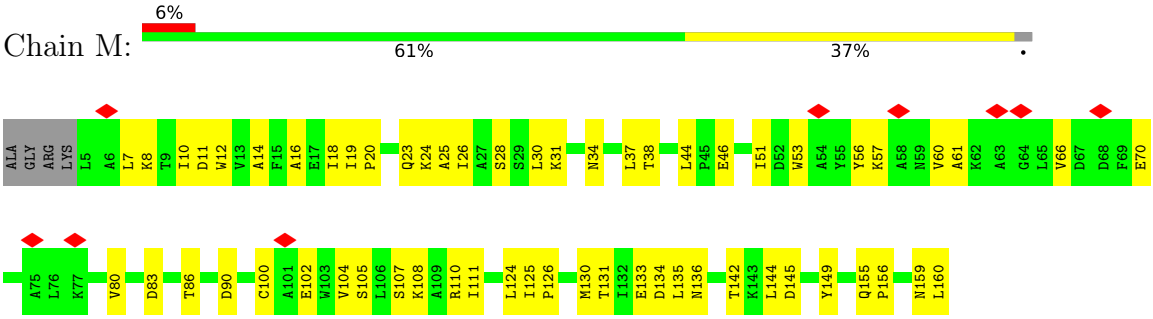
• Molecule 5: ATP synthase F(0) complex subunit B1, mitochondrial



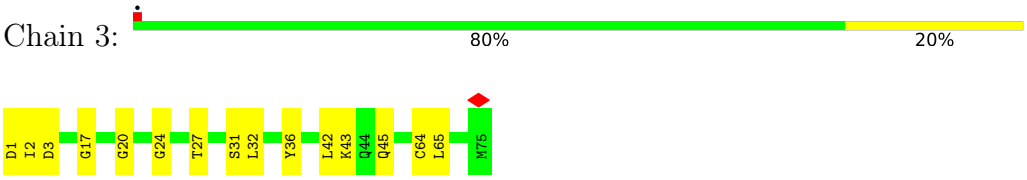
• Molecule 6: ATP synthase-coupling factor 6, mitochondrial



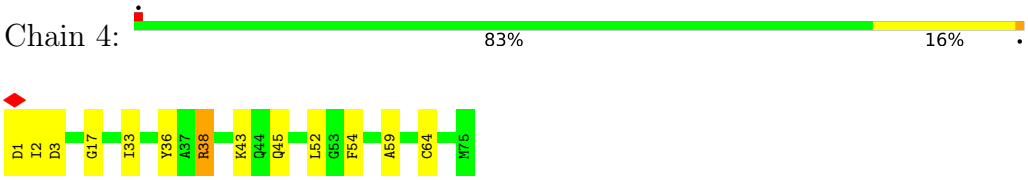
• Molecule 7: ATP synthase subunit d, mitochondrial



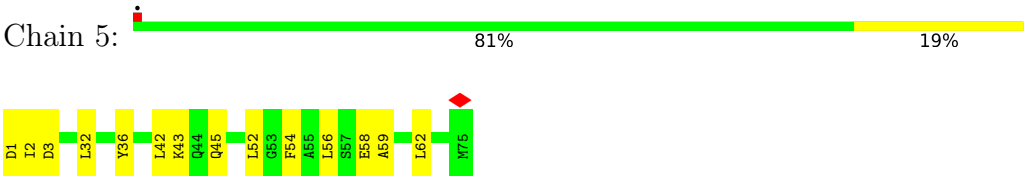
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



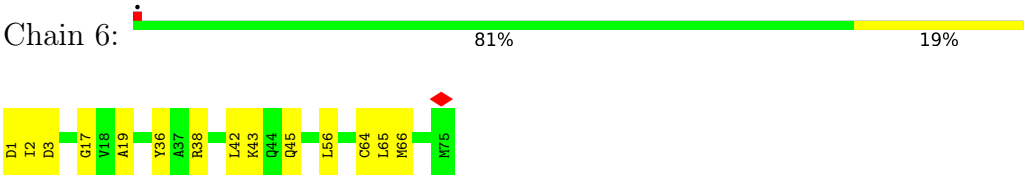
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

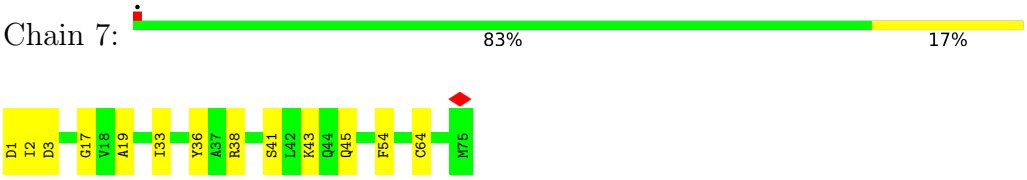


• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



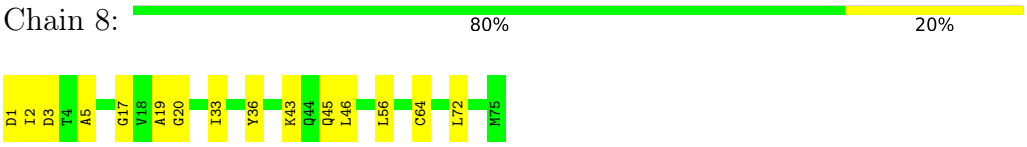
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 7:



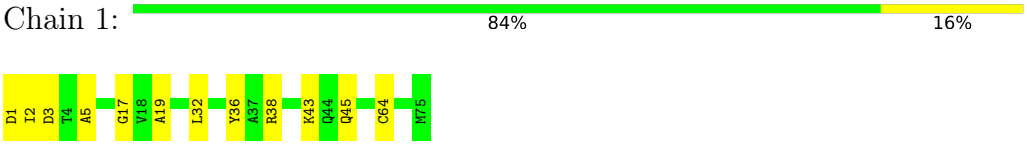
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 8:



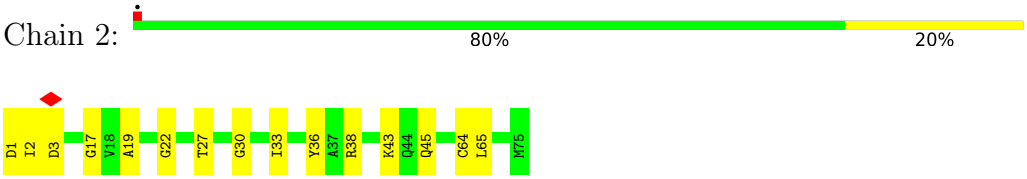
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 1:



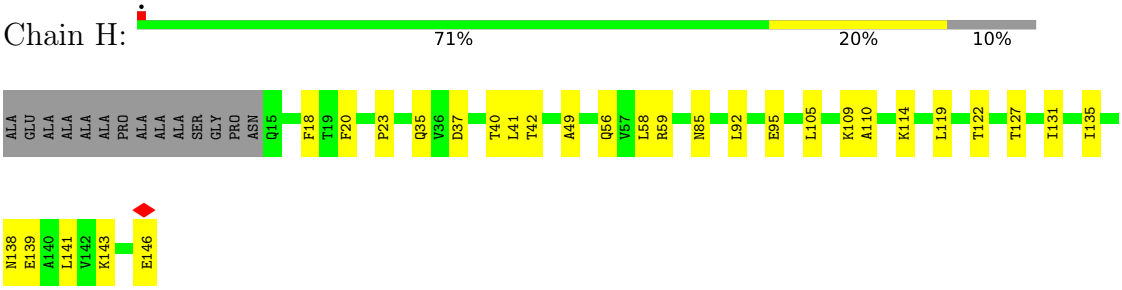
• Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial

Chain 2:



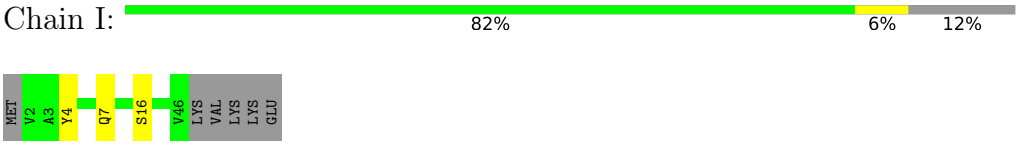
• Molecule 9: ATP synthase subunit delta, mitochondrial

Chain H:



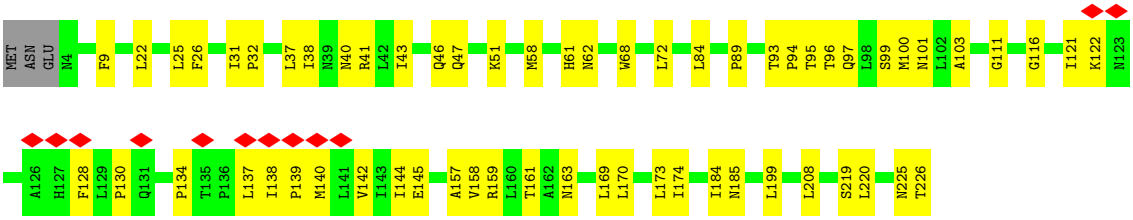
• Molecule 10: ATP synthase subunit epsilon, mitochondrial

Chain I:



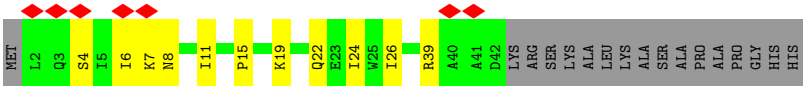
• Molecule 11: ATP synthase subunit a

Chain N:



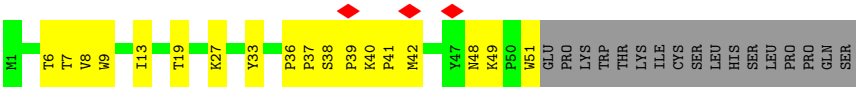
• Molecule 12: ATP synthase subunit ATP5MJ, mitochondrial

Chain P:



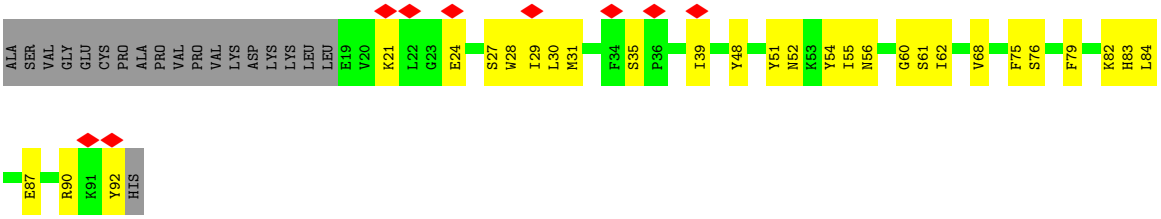
• Molecule 13: ATP synthase protein 8

Chain Q:



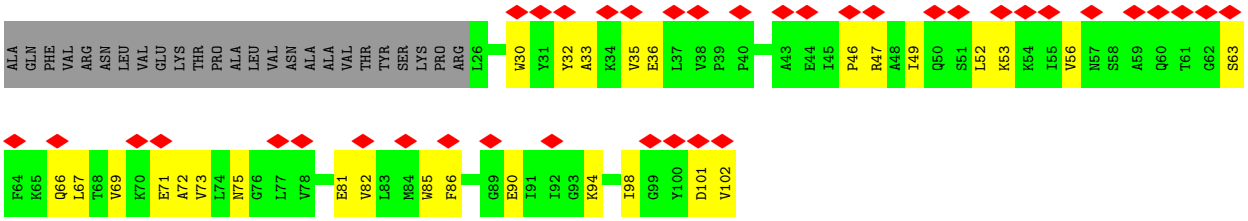
• Molecule 14: ATP synthase subunit f, mitochondrial

Chain R:



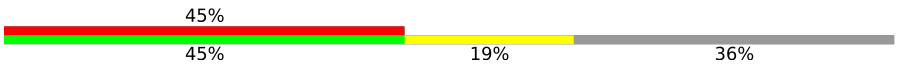
• Molecule 15: ATP synthase subunit g, mitochondrial

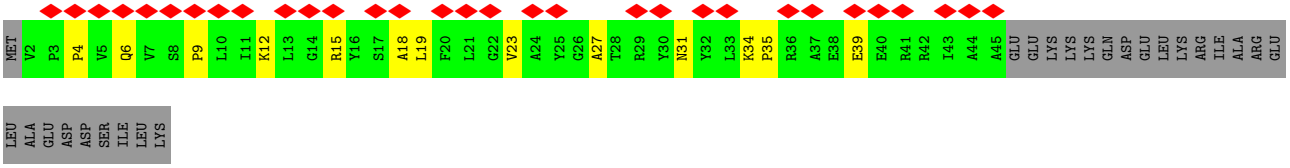
Chain S:



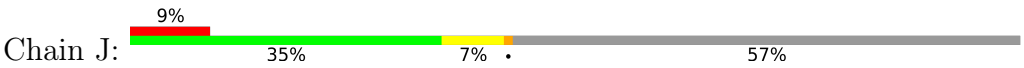
• Molecule 16: ATP synthase subunit e, mitochondrial

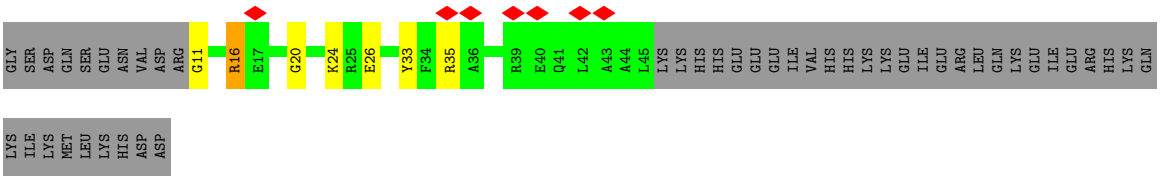
Chain T:





• Molecule 17: ATPase inhibitor, mitochondrial





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	37.850	Depositor
Minimum map value	-22.127	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.078	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/3757	0.45	0/5069
1	B	0.32	0/3687	0.45	0/4973
1	C	0.30	0/3635	0.45	0/4902
2	D	0.31	0/3621	0.46	0/4911
2	E	0.33	0/3515	0.45	0/4766
2	F	0.33	0/3587	0.45	0/4865
3	G	0.34	0/2129	0.43	0/2860
4	O	0.27	0/1453	0.48	0/1958
5	K	0.29	0/1605	0.40	0/2169
6	L	0.30	0/560	0.49	0/748
7	M	0.33	0/1291	0.44	0/1755
8	1	0.35	0/543	0.41	0/732
8	2	0.34	0/543	0.41	0/732
8	3	0.35	0/543	0.41	0/732
8	4	0.35	0/543	0.41	0/732
8	5	0.35	0/543	0.42	0/732
8	6	0.35	0/543	0.42	0/732
8	7	0.35	0/543	0.41	0/732
8	8	0.35	0/543	0.41	0/732
9	H	0.34	0/987	0.51	0/1344
10	I	0.36	0/359	0.41	0/482
11	N	0.31	0/1755	0.46	0/2403
12	P	0.31	0/354	0.43	0/478
13	Q	0.32	0/437	0.51	0/598
14	R	0.34	0/640	0.43	0/858
15	S	0.28	0/619	0.46	0/841
16	T	0.25	0/354	0.36	0/480
17	J	0.49	0/272	0.59	0/359
All	All	0.32	0/38961	0.45	0/52675

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	4	0	1
17	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	4	38	ARG	Sidechain
17	J	16	ARG	Sidechain

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	A	3706	0	3801	48	0
1	B	3639	0	3741	48	0
1	C	3587	0	3698	63	0
2	D	3562	0	3608	52	0
2	E	3458	0	3508	59	0
2	F	3529	0	3584	42	0
3	G	2103	0	2174	39	0
4	O	1437	0	1536	45	0
5	K	1573	0	1552	56	0
6	L	549	0	533	20	0
7	M	1259	0	1238	50	0
8	1	534	0	553	12	0
8	2	534	0	553	16	0
8	3	534	0	553	12	0
8	4	534	0	553	10	0
8	5	534	0	553	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	6	534	0	553	12	0
8	7	534	0	553	12	0
8	8	534	0	553	14	0
9	H	975	0	979	22	0
10	I	354	0	364	2	0
11	N	1718	0	1879	50	0
12	P	344	0	361	9	0
13	Q	422	0	450	23	0
14	R	621	0	618	26	0
15	S	605	0	631	28	0
16	T	346	0	355	13	0
17	J	270	0	257	5	0
18	A	31	0	12	0	0
18	B	31	0	12	0	0
18	C	31	0	12	2	0
19	A	1	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
20	D	27	0	12	0	0
20	F	27	0	12	0	0
All	All	38481	0	39351	652	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 (652) 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)
8:6:66:MET:HE3	11:N:169:LEU:HD22	1.59	0.85
4:O:22:LEU:HD22	4:O:85:LEU:HD22	1.60	0.84
9:H:40:THR:HG22	9:H:42:THR:H	1.40	0.84
5:K:121:ARG:HA	7:M:18:ILE:HG21	1.62	0.81
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.67	0.75
1:C:379:GLN:HE21	1:C:383:MET:HG3	1.51	0.75
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.20	0.74
3:G:193:TYR:OH	9:H:85:ASN:ND2	2.21	0.74
5:K:117:LEU:HB3	13:Q:49:LYS:HZ2	1.53	0.74
7:M:53:TRP:O	7:M:57:LYS:N	2.22	0.73
1:C:185:ASN:OD1	1:C:188:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:HD21	1:C:497:LEU:HB3	1.72	0.72
2:E:299:ILE:HG21	2:E:309:SER:HB2	1.71	0.71
4:O:134:LEU:HA	4:O:137:VAL:HG12	1.73	0.71
1:B:102:GLU:OE1	1:B:124:LYS:NZ	2.23	0.70
16:T:27:ALA:O	16:T:31:ASN:ND2	2.24	0.70
2:D:184:SER:HB2	2:D:218:VAL:HG22	1.74	0.70
8:6:38:ARG:HD2	8:7:38:ARG:HH12	1.55	0.69
13:Q:40:LYS:HG2	13:Q:42:MET:H	1.58	0.69
7:M:53:TRP:CZ2	7:M:70:GLU:HB3	2.28	0.69
3:G:78:CYS:SG	3:G:228:ARG:NH2	2.67	0.68
1:C:423:ARG:NH2	1:C:456:LEU:O	2.26	0.68
7:M:160:LEU:HD11	13:Q:33:TYR:CD2	2.29	0.68
12:P:4:SER:HA	12:P:7:LYS:HE3	1.75	0.68
11:N:97:GLN:O	11:N:101:ASN:ND2	2.26	0.67
11:N:37:LEU:HD23	11:N:38:ILE:HG13	1.77	0.67
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.28	0.67
1:C:209:LYS:NZ	2:F:333:ASP:OD1	2.28	0.67
5:K:117:LEU:HB3	13:Q:49:LYS:NZ	2.09	0.67
1:B:291:ARG:NH1	2:F:322:ASP:OD1	2.28	0.66
11:N:116:GLY:HA3	11:N:225:ASN:HD22	1.60	0.66
2:E:400:SER:OG	2:E:401:GLU:N	2.28	0.65
5:K:130:ASN:HD21	7:M:8:LYS:H	1.42	0.65
5:K:143:ARG:NH2	6:L:96:GLU:O	2.26	0.65
5:K:129:ARG:NH1	7:M:90:ASP:OD2	2.27	0.65
2:E:58:GLU:HG3	4:O:17:ARG:HH12	1.62	0.65
8:7:19:ALA:HB2	8:8:17:GLY:HA2	1.79	0.65
7:M:11:ASP:OD2	7:M:12:TRP:N	2.30	0.65
11:N:184:ILE:HG22	11:N:185:ASN:H	1.62	0.65
12:P:39:ARG:HG2	13:Q:6:THR:HB	1.79	0.65
11:N:31:ILE:HA	11:N:46:GLN:HE22	1.60	0.65
1:C:441:GLN:O	1:C:445:ILE:HG12	1.96	0.64
2:F:119:ILE:O	2:F:298:ARG:NH2	2.30	0.64
11:N:62:ASN:ND2	11:N:226:THR:O	2.28	0.64
7:M:108:LYS:HD3	7:M:111:ILE:HD12	1.78	0.64
1:B:381:ARG:HG3	1:B:385:GLN:HE21	1.63	0.64
2:D:248:ASP:O	6:L:73:ARG:NH2	2.26	0.64
2:E:412:LYS:NZ	2:E:452:TYR:O	2.27	0.64
4:O:121:THR:HG22	4:O:153:LYS:HB2	1.78	0.63
15:S:86:PHE:HB2	16:T:18:ALA:HB1	1.80	0.63
1:B:286:ARG:NH2	2:E:276:GLY:O	2.32	0.62
4:O:115:GLU:HB3	4:O:149:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:NZ	1:B:465:GLU:OE2	2.31	0.62
6:L:43:PHE:O	6:L:47:ILE:HG12	1.99	0.62
1:C:30:ARG:HH21	1:C:85:GLY:HA2	1.63	0.62
9:H:41:LEU:HD23	9:H:59:ARG:HB3	1.81	0.62
1:A:346:THR:O	1:A:373:ARG:NH2	2.33	0.62
1:A:479:LEU:HD21	1:A:497:LEU:HG	1.82	0.62
1:B:258:ARG:NH1	1:B:308:ARG:O	2.33	0.62
1:A:175:LYS:HG2	1:A:352:LEU:HD12	1.81	0.62
8:7:33:ILE:HG23	8:8:46:LEU:HD22	1.82	0.61
6:L:40:GLN:HB3	6:L:43:PHE:HB2	1.82	0.61
1:A:187:LYS:NZ	1:A:191:ASP:OD2	2.33	0.61
2:F:258:ILE:HG21	2:F:261:ILE:HD13	1.82	0.61
7:M:130:MET:HG3	7:M:134:ASP:HB2	1.81	0.61
1:C:237:SER:HB3	2:F:297:GLU:HG3	1.82	0.61
8:5:58:GLU:OE2	11:N:163:ASN:ND2	2.34	0.61
2:D:411:ARG:O	2:D:415:ARG:HG2	2.01	0.61
2:F:244:GLU:OE2	2:F:298:ARG:NH1	2.34	0.60
11:N:111:GLY:HA3	12:P:24:ILE:HD13	1.84	0.60
1:A:95:VAL:HG11	1:A:245:LEU:HD21	1.83	0.60
2:D:412:LYS:NZ	2:D:452:TYR:O	2.34	0.60
3:G:74:ASP:OD1	3:G:110:ASP:N	2.29	0.60
5:K:47:SER:O	14:R:92:TYR:OH	2.20	0.60
2:D:198:ASP:O	2:D:202:GLU:HG3	2.00	0.59
11:N:134:PRO:HG2	11:N:137:LEU:HB2	1.84	0.59
5:K:111:GLU:OE2	7:M:110:ARG:NH2	2.36	0.59
15:S:35:VAL:HG11	16:T:4:PRO:HB2	1.85	0.59
1:B:187:LYS:NZ	1:B:191:ASP:OD2	2.36	0.59
2:E:319:ASP:OD2	3:G:255:GLN:NE2	2.35	0.59
2:E:347:ILE:HG23	2:E:418:SER:HB3	1.85	0.58
3:G:72:SER:HB2	3:G:82:HIS:HD1	1.66	0.58
2:F:301:THR:HG23	2:F:306:SER:HA	1.85	0.58
1:B:423:ARG:NH2	1:B:456:LEU:O	2.33	0.58
15:S:32:TYR:HD1	16:T:4:PRO:HB3	1.67	0.58
1:A:495:ALA:O	1:A:499:GLU:HG2	2.04	0.58
1:C:36:ASP:OD1	2:F:277:ARG:NH1	2.36	0.58
2:E:240:LEU:HD21	2:E:298:ARG:HB2	1.85	0.58
1:C:30:ARG:CZ	4:O:59:TYR:HB3	2.34	0.58
8:3:27:THR:HG21	8:2:27:THR:HA	1.85	0.58
1:A:96:ASP:OD1	1:A:126:ARG:NE	2.29	0.58
4:O:179:ILE:HA	6:L:42:LEU:HD11	1.85	0.57
9:H:138:ASN:HA	9:H:141:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:SER:OG	1:B:432:GLN:NE2	2.37	0.57
1:C:258:ARG:NH1	1:C:308:ARG:O	2.37	0.57
2:F:87:ILE:HD13	2:F:238:THR:HG23	1.86	0.57
8:4:52:LEU:HD13	11:N:130:PRO:HG2	1.87	0.57
12:P:4:SER:HA	12:P:7:LYS:HB3	1.85	0.57
1:C:256:TYR:O	1:C:260:ASN:ND2	2.31	0.57
2:D:263:ARG:HH11	2:D:266:GLN:HE22	1.53	0.57
13:Q:9:TRP:O	13:Q:13:ILE:HG12	2.05	0.57
2:E:247:ARG:HD3	2:E:307:ILE:HG13	1.87	0.57
2:F:52:VAL:HA	2:F:63:THR:HG22	1.87	0.57
7:M:131:THR:HG22	7:M:133:GLU:H	1.70	0.57
2:D:192:ARG:HB2	2:D:195:GLU:HG3	1.87	0.57
2:E:322:ASP:HB3	2:E:325:PRO:HD2	1.87	0.56
7:M:34:ASN:O	7:M:38:THR:HG23	2.04	0.56
7:M:51:ILE:HG12	7:M:56:TYR:HE2	1.70	0.56
13:Q:7:THR:HG23	13:Q:8:VAL:HG13	1.87	0.56
15:S:69:VAL:HA	15:S:72:ALA:HB3	1.87	0.56
1:B:278:TYR:OH	1:B:297:ASP:OD2	2.23	0.56
1:B:218:LYS:HD2	2:E:131:VAL:HB	1.88	0.56
3:G:125:LEU:HG	3:G:126:VAL:HG23	1.87	0.56
2:F:18:ALA:HB3	2:F:25:ASP:HB2	1.88	0.56
15:S:63:SER:O	15:S:66:GLN:HG3	2.06	0.55
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.88	0.55
8:3:45:GLN:O	8:3:45:GLN:NE2	2.40	0.55
1:C:163:GLN:NE2	1:C:165:GLU:OE2	2.40	0.55
6:L:47:ILE:HG13	6:L:48:ARG:HD2	1.87	0.55
2:E:411:ARG:O	2:E:415:ARG:HG2	2.05	0.55
8:1:45:GLN:O	8:1:45:GLN:NE2	2.40	0.55
15:S:85:TRP:CD1	16:T:15:ARG:HD3	2.41	0.55
1:A:187:LYS:HE2	1:A:224:ASP:HB3	1.89	0.55
8:4:45:GLN:O	8:4:45:GLN:NE2	2.40	0.55
11:N:93:THR:HB	11:N:96:THR:HG23	1.89	0.55
1:C:334:VAL:HG11	1:C:351:PHE:HE1	1.70	0.55
2:E:92:GLU:HB2	2:E:113:THR:HG22	1.89	0.55
5:K:12:VAL:HA	5:K:18:PRO:HA	1.89	0.55
11:N:58:MET:HE1	11:N:72:LEU:HD12	1.88	0.55
1:A:385:GLN:HE22	1:A:489:ILE:H	1.54	0.54
2:D:255:LEU:HD23	2:D:308:THR:HB	1.89	0.54
5:K:54:SER:OG	5:K:55:ALA:N	2.40	0.54
1:C:140:ILE:HD13	1:C:143:ARG:HH12	1.72	0.54
8:2:45:GLN:O	8:2:45:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:45:GLN:O	8:8:45:GLN:NE2	2.40	0.54
11:N:103:ALA:HB2	13:Q:13:ILE:HD12	1.88	0.54
2:F:27:GLN:HE22	4:O:61:LYS:NZ	2.06	0.54
1:C:423:ARG:HG3	1:C:461:ILE:HD11	1.88	0.54
1:C:80:LYS:HD3	2:F:36:LEU:HD12	1.89	0.54
2:F:375:ARG:NH1	2:F:378:GLN:OE1	2.41	0.54
2:D:393:ILE:HD11	3:G:16:ILE:HG12	1.89	0.54
8:7:45:GLN:O	8:7:45:GLN:NE2	2.40	0.54
1:C:175:LYS:HG2	1:C:352:LEU:HD12	1.89	0.54
4:O:9:VAL:HG11	4:O:111:VAL:HG21	1.88	0.54
4:O:61:LYS:HB3	4:O:64:ILE:HD12	1.88	0.54
2:F:156:GLY:HA3	2:F:332:LEU:HD13	1.90	0.54
1:A:163:GLN:NE2	1:A:165:GLU:OE2	2.40	0.53
4:O:125:PRO:HD3	4:O:154:THR:HG21	1.90	0.53
1:B:137:ILE:HG13	2:F:106:ASP:HA	1.90	0.53
8:5:45:GLN:O	8:5:45:GLN:NE2	2.40	0.53
15:S:47:ARG:HB2	16:T:9:PRO:HG2	1.89	0.53
4:O:118:CYS:HB3	4:O:166:ILE:HA	1.91	0.53
2:E:189:VAL:HG22	2:E:235:VAL:HG13	1.88	0.53
3:G:233:ASP:O	3:G:237:LYS:HG2	2.08	0.53
4:O:62:ARG:HH21	4:O:93:GLY:HA3	1.74	0.53
14:R:28:TRP:HA	14:R:31:MET:HG3	1.90	0.53
5:K:36:VAL:HA	5:K:39:THR:HG22	1.91	0.53
2:D:115:GLN:NE2	2:D:245:TYR:OH	2.41	0.53
8:6:45:GLN:O	8:6:45:GLN:NE2	2.40	0.53
14:R:79:PHE:O	14:R:82:LYS:NZ	2.41	0.53
1:C:170:ASP:OD1	1:C:329:THR:OG1	2.27	0.53
8:5:62:LEU:HD13	11:N:159:ARG:HA	1.91	0.53
2:E:110:PRO:HG2	2:E:112:LYS:HE3	1.91	0.53
7:M:108:LYS:HA	7:M:111:ILE:HD12	1.90	0.53
1:B:237:SER:HB3	2:E:297:GLU:HG3	1.90	0.53
3:G:97:THR:HG21	3:G:123:GLN:HE22	1.72	0.53
3:G:124:PHE:HZ	3:G:127:ALA:HB2	1.73	0.53
14:R:27:SER:O	14:R:30:LEU:HG	2.09	0.53
1:A:307:GLU:HG3	2:E:226:ASN:HB3	1.91	0.52
1:C:66:LEU:HB3	2:D:74:ARG:HD3	1.89	0.52
4:O:34:GLN:O	4:O:38:GLU:HG3	2.09	0.52
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.44	0.52
2:F:28:PHE:O	2:F:59:SER:HB3	2.08	0.52
7:M:25:ALA:O	7:M:28:SER:OG	2.24	0.52
14:R:76:SER:HA	14:R:79:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:NZ	2:D:333:ASP:OD1	2.41	0.52
1:B:289:PRO:HB2	1:B:293:ALA:HA	1.91	0.52
1:C:420:ARG:NH1	1:C:449:VAL:O	2.43	0.52
13:Q:49:LYS:O	13:Q:51:TRP:N	2.37	0.52
9:H:127:THR:O	9:H:131:ILE:HG12	2.09	0.52
9:H:58:LEU:HD11	9:H:92:LEU:HD11	1.92	0.52
1:B:453:LEU:HD11	1:B:464:PHE:CE1	2.44	0.52
2:E:455:LEU:HD11	2:E:470:VAL:HG12	1.92	0.52
13:Q:40:LYS:HE3	13:Q:42:MET:O	2.09	0.52
2:E:229:PRO:HB2	2:E:271:VAL:HG23	1.91	0.52
2:F:411:ARG:O	2:F:415:ARG:HG2	2.09	0.52
8:3:32:LEU:HA	8:2:33:ILE:HG21	1.91	0.52
1:A:256:TYR:O	1:A:260:ASN:ND2	2.33	0.52
1:C:136:ILE:O	2:D:197:ASN:ND2	2.41	0.52
1:C:456:LEU:HD21	1:C:505:LEU:HD11	1.92	0.52
5:K:36:VAL:HG13	15:S:81:GLU:OE1	2.10	0.52
4:O:118:CYS:HA	4:O:165:ARG:O	2.11	0.51
9:H:138:ASN:O	9:H:141:LEU:HB2	2.10	0.51
5:K:127:VAL:HG22	7:M:10:ILE:HD13	1.93	0.51
6:L:40:GLN:O	6:L:44:VAL:HG23	2.10	0.51
11:N:128:PHE:HA	11:N:145:GLU:OE1	2.10	0.51
1:B:170:ASP:O	1:B:175:LYS:NZ	2.43	0.51
2:D:96:ARG:NH2	2:D:109:GLY:O	2.35	0.51
11:N:140:MET:O	11:N:144:ILE:HG12	2.11	0.51
15:S:72:ALA:HA	15:S:75:ASN:HD21	1.76	0.51
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.45	0.51
3:G:201:LEU:O	3:G:205:GLN:HG2	2.11	0.51
6:L:56:THR:OG1	6:L:59:GLY:O	2.27	0.51
5:K:103:HIS:HD2	5:K:104:ILE:HG23	1.76	0.51
3:G:197:ASP:OD1	3:G:197:ASP:N	2.42	0.51
7:M:125:ILE:HD12	7:M:126:PRO:HD2	1.92	0.51
8:1:19:ALA:HB2	8:2:17:GLY:HA2	1.93	0.51
1:C:187:LYS:NZ	1:C:191:ASP:OD2	2.44	0.51
2:D:87:ILE:HG21	2:D:238:THR:HG23	1.92	0.51
8:8:19:ALA:HB2	8:1:17:GLY:HA2	1.93	0.51
4:O:161:GLY:HA3	4:O:174:SER:HA	1.92	0.51
8:5:59:ALA:HB2	11:N:159:ARG:HH21	1.75	0.51
1:A:441:GLN:O	1:A:445:ILE:HG12	2.11	0.50
2:D:34:PRO:HD2	2:D:37:ASN:ND2	2.26	0.50
2:D:52:VAL:HA	2:D:63:THR:HG22	1.93	0.50
2:D:390:ILE:HD13	3:G:19:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:ASP:HB3	2:E:365:ILE:HD12	1.92	0.50
3:G:137:THR:OG1	3:G:140:ASP:OD1	2.27	0.50
4:O:164:VAL:HB	4:O:171:VAL:HG22	1.93	0.50
5:K:130:ASN:ND2	7:M:7:LEU:HB2	2.27	0.50
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.93	0.50
1:C:397:TYR:CG	1:C:421:GLY:HA3	2.46	0.50
3:G:234:ASN:O	3:G:238:ASN:ND2	2.45	0.50
1:B:52:MET:O	1:B:91:THR:OG1	2.22	0.50
2:D:142:VAL:HG23	2:D:146:LEU:HD12	1.92	0.50
12:P:15:PRO:HA	12:P:19:LYS:HE2	1.93	0.50
1:C:289:PRO:HB2	1:C:293:ALA:HA	1.94	0.50
2:E:415:ARG:O	2:E:418:SER:OG	2.29	0.50
3:G:48:SER:OG	3:G:211:ASN:ND2	2.44	0.50
7:M:107:SER:O	7:M:111:ILE:HG13	2.10	0.50
8:2:36:TYR:HE1	8:2:43:LYS:HB2	1.77	0.50
1:A:141:SER:HB2	1:A:143:ARG:HH21	1.77	0.50
2:D:51:GLU:OE2	2:D:120:HIS:NE2	2.37	0.50
3:G:14:LYS:HA	3:G:243:ILE:HD11	1.94	0.50
8:8:36:TYR:HE1	8:8:43:LYS:HB2	1.77	0.50
2:E:15:ARG:NH1	2:E:27:GLN:OE1	2.41	0.50
5:K:51:TYR:HH	5:K:57:THR:HG1	1.58	0.50
8:4:54:PHE:CE1	8:5:56:LEU:HD13	2.47	0.50
5:K:108:ILE:HG23	7:M:111:ILE:HG23	1.94	0.49
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.93	0.49
1:B:334:VAL:HG11	1:B:351:PHE:HE1	1.77	0.49
2:E:420:PRO:HG2	2:E:433:LYS:HG2	1.93	0.49
2:D:290:THR:O	2:D:294:THR:HG23	2.11	0.49
7:M:155:GLN:NE2	13:Q:33:TYR:O	2.43	0.49
8:7:36:TYR:HE1	8:7:43:LYS:HB2	1.77	0.49
8:3:36:TYR:HE1	8:3:43:LYS:HB2	1.77	0.49
8:2:36:TYR:CE1	8:2:43:LYS:HB2	2.48	0.49
8:4:36:TYR:CE1	8:4:43:LYS:HB2	2.48	0.49
8:6:36:TYR:HE1	8:6:43:LYS:HB2	1.77	0.49
8:8:36:TYR:CE1	8:8:43:LYS:HB2	2.48	0.49
3:G:214:TYR:OH	9:H:23:PRO:O	2.24	0.49
4:O:39:LEU:HA	4:O:42:VAL:HG12	1.94	0.49
1:A:151:LYS:O	1:A:155:SER:OG	2.20	0.49
1:B:164:ARG:NH1	1:B:306:LEU:O	2.41	0.49
1:B:453:LEU:HD23	1:B:461:ILE:HD12	1.95	0.49
4:O:120:VAL:HG23	4:O:152:ALA:HA	1.94	0.49
8:5:36:TYR:CE1	8:5:43:LYS:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:36:TYR:CE1	8:7:43:LYS:HB2	2.48	0.49
1:C:215:GLN:O	1:C:219:ARG:HG2	2.13	0.48
8:1:36:TYR:CE1	8:1:43:LYS:HB2	2.48	0.48
2:F:428:THR:HG23	2:F:430:HIS:H	1.78	0.48
3:G:63:LYS:O	3:G:101:LYS:NZ	2.34	0.48
8:4:36:TYR:HE1	8:4:43:LYS:HB2	1.77	0.48
11:N:22:LEU:HD22	14:R:75:PHE:CE2	2.48	0.48
1:B:329:THR:HG21	1:B:334:VAL:HG12	1.95	0.48
2:D:92:GLU:HB2	2:D:113:THR:HG22	1.96	0.48
2:D:173:ILE:O	2:D:177:ALA:HB3	2.13	0.48
8:6:36:TYR:CE1	8:6:43:LYS:HB2	2.48	0.48
9:H:40:THR:HG23	9:H:56:GLN:HB3	1.94	0.48
15:S:35:VAL:O	16:T:6:GLN:NE2	2.47	0.48
5:K:120:LYS:HD3	7:M:14:ALA:HB1	1.95	0.48
8:3:36:TYR:CE1	8:3:43:LYS:HB2	2.48	0.48
8:5:36:TYR:HE1	8:5:43:LYS:HB2	1.77	0.48
8:1:36:TYR:HE1	8:1:43:LYS:HB2	1.77	0.48
15:S:46:PRO:HB2	15:S:47:ARG:NH2	2.28	0.48
11:N:68:TRP:CH2	12:P:24:ILE:HD11	2.49	0.48
12:P:6:ILE:O	12:P:11:ILE:HG13	2.14	0.48
1:A:452:TYR:OH	1:A:498:LYS:HD2	2.14	0.48
2:D:227:GLU:O	2:D:232:ARG:NH1	2.46	0.48
4:O:48:GLU:OE1	4:O:51:VAL:N	2.34	0.48
5:K:100:SER:O	5:K:104:ILE:HG12	2.14	0.48
1:A:410:LEU:HD22	1:A:414:THR:HG21	1.96	0.48
2:E:18:ALA:HB3	2:E:25:ASP:HB2	1.95	0.48
2:F:391:ILE:HG12	2:F:399:LEU:HD11	1.96	0.48
3:G:9:ARG:HG2	3:G:246:LEU:HD11	1.96	0.48
4:O:139:LYS:HA	4:O:142:LEU:HD23	1.94	0.48
2:E:32:LEU:HD11	2:E:59:SER:HA	1.96	0.48
2:E:210:ASN:ND2	2:E:213:ASP:OD1	2.47	0.48
4:O:73:THR:HG23	4:O:78:PHE:CD2	2.49	0.48
4:O:31:LYS:O	4:O:35:VAL:HG23	2.13	0.48
5:K:154:ARG:NH1	6:L:89:THR:O	2.47	0.48
5:K:162:GLN:NE2	7:M:61:ALA:H	2.12	0.48
7:M:136:ASN:OD1	7:M:142:THR:OG1	2.26	0.48
8:6:1:ASP:OD1	8:6:2:ILE:N	2.47	0.48
9:H:18:PHE:CE2	9:H:20:PHE:HB2	2.49	0.48
14:R:29:ILE:HD12	14:R:29:ILE:H	1.79	0.48
1:B:479:LEU:HD13	1:B:496:LYS:HD2	1.94	0.48
2:F:259:ASP:HA	2:F:260:ASN:HA	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:182:LEU:HB2	6:L:42:LEU:HG	1.95	0.48
7:M:20:PRO:HB3	13:Q:51:TRP:HD1	1.78	0.48
7:M:145:ASP:OD1	7:M:145:ASP:N	2.45	0.48
8:1:5:ALA:HB2	8:2:2:ILE:HG23	1.95	0.48
8:5:1:ASP:OD1	8:5:2:ILE:N	2.47	0.47
8:8:1:ASP:OD1	8:8:2:ILE:N	2.47	0.47
1:A:28:THR:HG22	1:A:89:LYS:HG3	1.96	0.47
1:A:393:GLU:OE1	1:A:420:ARG:NH1	2.47	0.47
2:E:87:ILE:HG21	2:E:238:THR:HG23	1.97	0.47
2:E:89:VAL:HG23	2:E:115:GLN:HG2	1.95	0.47
5:K:80:ASP:OD1	5:K:81:PHE:N	2.48	0.47
8:2:1:ASP:OD1	8:2:2:ILE:N	2.47	0.47
1:A:406:PHE:HE1	2:D:394:LEU:HD21	1.79	0.47
2:E:141:LYS:HD3	2:E:435:VAL:HG21	1.95	0.47
2:F:144:ASP:HB3	2:F:437:LEU:HD13	1.96	0.47
3:G:60:PRO:HB2	3:G:63:LYS:HG2	1.95	0.47
4:O:184:ARG:O	4:O:188:GLU:N	2.46	0.47
8:4:1:ASP:OD1	8:4:2:ILE:N	2.47	0.47
8:7:1:ASP:OD1	8:7:2:ILE:N	2.47	0.47
1:C:498:LYS:NZ	1:C:499:GLU:OE2	2.33	0.47
2:D:397:ASP:OD1	2:D:397:ASP:N	2.44	0.47
8:3:1:ASP:OD1	8:3:2:ILE:N	2.47	0.47
8:5:36:TYR:CE2	8:6:42:LEU:HD13	2.50	0.47
8:1:1:ASP:OD1	8:1:2:ILE:N	2.47	0.47
9:H:105:LEU:HB3	9:H:109:LYS:NZ	2.29	0.47
11:N:84:LEU:HD11	11:N:208:LEU:HD21	1.96	0.47
14:R:48:TYR:O	14:R:52:ASN:ND2	2.48	0.47
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.96	0.47
1:C:32:LEU:HG	1:C:42:HIS:HB2	1.96	0.47
2:F:223:GLY:N	2:F:235:VAL:HG21	2.29	0.47
2:D:280:SER:OG	2:D:281:ALA:N	2.47	0.47
15:S:30:TRP:HA	15:S:33:ALA:HB3	1.97	0.47
2:D:324:ALA:HB3	2:D:325:PRO:HD3	1.96	0.47
3:G:15:ASN:ND2	17:J:11:GLY:O	2.48	0.47
1:A:440:GLU:HB3	1:A:469:LEU:HD11	1.96	0.46
2:E:90:GLY:HA2	2:E:245:TYR:CE1	2.50	0.46
2:E:260:ASN:HB3	2:E:263:ARG:HG3	1.97	0.46
9:H:135:ILE:O	9:H:139:GLU:HG3	2.15	0.46
14:R:82:LYS:HG3	14:R:83:HIS:CD2	2.51	0.46
2:E:245:TYR:CD2	2:E:249:GLN:HG3	2.50	0.46
3:G:68:LEU:HD11	3:G:161:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:29:THR:HG23	5:K:33:GLY:HA3	1.96	0.46
11:N:94:PRO:HB2	11:N:100:MET:SD	2.55	0.46
14:R:51:TYR:CD1	14:R:55:ILE:HB	2.50	0.46
1:A:427:LEU:HD11	1:A:444:VAL:HG13	1.97	0.46
1:C:99:VAL:HG12	1:C:253:MET:HA	1.98	0.46
2:F:34:PRO:HD2	2:F:37:ASN:ND2	2.30	0.46
7:M:53:TRP:HB3	7:M:57:LYS:HE3	1.97	0.46
11:N:170:LEU:HG	11:N:199:LEU:HD21	1.98	0.46
1:C:105:GLY:HA2	1:C:226:MET:O	2.15	0.46
1:C:270:ASP:N	1:C:270:ASP:OD1	2.47	0.46
3:G:124:PHE:CZ	3:G:127:ALA:HB2	2.50	0.46
5:K:80:ASP:O	5:K:84:LYS:N	2.36	0.46
4:O:118:CYS:SG	4:O:148:LEU:HD22	2.56	0.46
8:3:24:GLY:HA3	8:2:22:GLY:O	2.16	0.46
8:3:31:SER:HB3	8:2:30:GLY:O	2.15	0.46
11:N:9:PHE:O	11:N:97:GLN:NE2	2.43	0.46
14:R:51:TYR:HD1	14:R:55:ILE:HB	1.79	0.46
2:F:186:PHE:HB3	2:F:220:LEU:HD23	1.97	0.46
2:F:191:GLU:O	2:F:224:GLN:HB3	2.16	0.46
2:D:101:ILE:HG13	2:D:103:GLU:HG3	1.98	0.46
2:D:213:ASP:O	2:D:215:THR:HG23	2.16	0.46
7:M:60:VAL:HG11	7:M:66:VAL:HB	1.98	0.46
11:N:41:ARG:NH1	14:R:60:GLY:O	2.45	0.46
1:B:148:THR:OG1	1:B:154:ASP:OD1	2.34	0.46
2:E:87:ILE:HD13	2:E:238:THR:HG23	1.96	0.46
2:E:299:ILE:HG23	2:E:307:ILE:HG22	1.98	0.46
5:K:97:LYS:O	5:K:101:ILE:HG13	2.16	0.46
5:K:157:TYR:HB2	6:L:82:PHE:CD2	2.51	0.46
17:J:16:ARG:HD2	17:J:26:GLU:OE1	2.16	0.46
2:E:324:ALA:HB3	2:E:325:PRO:HD3	1.98	0.46
16:T:35:PRO:O	16:T:39:GLU:HG2	2.16	0.46
2:E:28:PHE:O	2:E:59:SER:HB3	2.15	0.46
3:G:32:ALA:O	3:G:33:ARG:HG2	2.16	0.46
1:A:423:ARG:HH21	1:A:457:GLU:HA	1.81	0.45
7:M:20:PRO:HB3	13:Q:51:TRP:CD1	2.51	0.45
7:M:156:PRO:HD2	7:M:159:ASN:HD22	1.81	0.45
1:C:265:LEU:HD11	1:C:324:LEU:HD12	1.98	0.45
3:G:71:VAL:HG22	3:G:108:ILE:HD12	1.98	0.45
3:G:195:ASP:HB3	9:H:56:GLN:HE22	1.81	0.45
2:F:261:ILE:O	2:F:264:PHE:HB3	2.16	0.45
5:K:134:MET:HB2	7:M:37:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:36:TYR:OH	8:2:45:GLN:HG2	2.16	0.45
2:F:90:GLY:HA2	2:F:245:TYR:CE2	2.51	0.45
3:G:15:ASN:O	3:G:19:ILE:HG13	2.16	0.45
7:M:102:GLU:O	7:M:105:SER:OG	2.26	0.45
12:P:7:LYS:HD2	12:P:8:ASN:OD1	2.17	0.45
15:S:67:LEU:HD21	15:S:71:GLU:HB3	1.97	0.45
1:A:457:GLU:OE2	1:A:460:LYS:HG2	2.16	0.45
1:C:288:PRO:HB2	2:D:273:ALA:HB1	1.97	0.45
2:E:283:GLY:HA2	3:G:262:LEU:CD1	2.46	0.45
7:M:26:ILE:O	7:M:30:LEU:HG	2.16	0.45
8:4:36:TYR:CE2	8:5:42:LEU:HD13	2.52	0.45
2:E:204:ILE:HD13	2:E:211:LEU:HD11	1.99	0.45
11:N:157:ALA:O	11:N:161:THR:HG22	2.17	0.45
5:K:60:ALA:HA	11:N:89:PRO:HG3	1.98	0.45
7:M:20:PRO:HG2	7:M:23:GLN:HG2	1.98	0.45
8:7:54:PHE:CE1	8:8:56:LEU:HD13	2.52	0.45
11:N:40:ASN:HD22	14:R:56:ASN:HA	1.82	0.45
15:S:102:VAL:HG11	16:T:34:LYS:HD3	1.99	0.45
2:D:259:ASP:HA	2:D:260:ASN:HA	1.71	0.45
12:P:22:GLN:O	12:P:26:ILE:HG12	2.17	0.45
1:A:265:LEU:HD11	1:A:324:LEU:HG	1.99	0.45
2:D:180:HIS:HE1	2:D:253:ASP:O	1.99	0.45
2:D:396:MET:HG2	17:J:33:TYR:CG	2.52	0.45
4:O:158:ILE:C	4:O:159:LEU:HD23	2.36	0.45
15:S:49:ILE:HA	15:S:52:LEU:HB3	1.98	0.45
2:F:87:ILE:HD11	2:F:241:THR:HB	1.99	0.44
2:D:156:GLY:HA3	2:D:332:LEU:HD13	1.99	0.44
4:O:69:LEU:HA	4:O:72:ILE:HG22	1.99	0.44
8:4:59:ALA:HB1	11:N:144:ILE:HD12	1.99	0.44
9:H:119:LEU:O	9:H:122:THR:HG22	2.17	0.44
11:N:174:ILE:HD12	11:N:199:LEU:HD22	1.98	0.44
17:J:20:GLY:C	17:J:24:LYS:HE2	2.38	0.44
1:C:152:ALA:HB3	1:C:365:ILE:HD12	1.98	0.44
2:E:155:ILE:HG13	2:E:334:ALA:HB3	1.98	0.44
1:C:103:LEU:HD23	1:C:121:ILE:HD13	1.98	0.44
5:K:129:ARG:HG2	7:M:86:THR:HG23	1.98	0.44
5:K:132:ILE:O	5:K:136:LEU:HG	2.17	0.44
5:K:154:ARG:HH21	6:L:91:PRO:HB3	1.81	0.44
15:S:32:TYR:CD1	16:T:4:PRO:HB3	2.51	0.44
1:A:99:VAL:HG12	1:A:253:MET:HA	1.99	0.44
3:G:63:LYS:C	3:G:64:LYS:HD2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:84:LYS:HE2	5:K:84:LYS:HB2	1.87	0.44
8:8:36:TYR:OH	8:1:45:GLN:HG2	2.18	0.44
10:I:4:TYR:HA	10:I:7:GLN:OE1	2.17	0.44
13:Q:48:ASN:ND2	13:Q:51:TRP:O	2.50	0.44
1:C:472:VAL:HA	1:C:476:HIS:CD2	2.52	0.44
2:F:261:ILE:HD12	2:F:261:ILE:HA	1.85	0.44
5:K:177:VAL:HB	6:L:49:GLU:HB3	1.99	0.44
8:5:62:LEU:CD1	11:N:159:ARG:HA	2.47	0.44
11:N:43:ILE:HG22	11:N:47:GLN:HG3	1.99	0.44
1:B:381:ARG:O	1:B:385:GLN:HG3	2.18	0.44
2:E:442:LYS:HE3	2:E:446:GLN:HE21	1.82	0.44
1:A:186:GLN:O	1:A:190:ASN:ND2	2.37	0.44
1:B:83:LYS:HD3	2:E:34:PRO:HG3	2.00	0.44
2:E:137:VAL:O	2:E:180:HIS:NE2	2.31	0.44
7:M:16:ALA:HA	7:M:19:ILE:HD12	2.00	0.44
9:H:95:GLU:OE1	10:I:16:SER:HB2	2.18	0.44
15:S:72:ALA:HA	15:S:75:ASN:ND2	2.32	0.44
1:A:237:SER:HB3	2:D:297:GLU:HG3	1.99	0.44
1:A:397:TYR:O	1:A:401:ALA:HB2	2.17	0.44
11:N:99:SER:OG	11:N:100:MET:N	2.51	0.44
14:R:35:SER:O	14:R:39:ILE:HG12	2.17	0.44
14:R:61:SER:OG	14:R:62:ILE:N	2.50	0.44
1:A:218:LYS:HD2	2:D:131:VAL:HG21	2.00	0.44
1:B:187:LYS:HE2	1:B:224:ASP:HB3	1.99	0.44
2:D:77:LYS:HA	2:D:77:LYS:HD3	1.79	0.44
14:R:24:GLU:OE2	15:S:69:VAL:HG13	2.17	0.44
15:S:69:VAL:O	15:S:73:VAL:HG23	2.17	0.44
1:C:471:HIS:O	1:C:474:SER:OG	2.29	0.43
8:4:33:ILE:HG21	8:5:32:LEU:HA	2.00	0.43
9:H:35:GLN:NE2	9:H:37:ASP:OD1	2.50	0.43
14:R:87:GLU:N	14:R:87:GLU:OE1	2.51	0.43
15:S:53:LYS:HA	15:S:56:VAL:HG12	2.01	0.43
1:C:381:ARG:HG3	1:C:385:GLN:HE21	1.82	0.43
1:C:489:ILE:HG13	1:C:489:ILE:O	2.18	0.43
2:E:460:PHE:HE1	2:E:466:ILE:HD11	1.84	0.43
5:K:92:GLN:HE22	13:Q:36:PRO:HB3	1.83	0.43
8:8:5:ALA:HB2	8:1:2:ILE:HG23	1.99	0.43
11:N:61:HIS:HE1	11:N:219:SER:OG	2.01	0.43
16:T:19:LEU:O	16:T:23:VAL:HG23	2.17	0.43
1:B:452:TYR:OH	1:B:498:LYS:HG3	2.19	0.43
2:F:377:VAL:HG13	2:F:413:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD1	1:A:69:ASP:N	2.50	0.43
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.81	0.43
2:F:393:ILE:HD13	3:G:16:ILE:HG21	1.99	0.43
3:G:195:ASP:HA	8:2:38:ARG:HH11	1.84	0.43
4:O:48:GLU:OE1	4:O:51:VAL:HG23	2.18	0.43
4:O:138:LEU:HB2	4:O:148:LEU:HD11	2.00	0.43
5:K:10:GLY:HA3	14:R:54:TYR:CE2	2.53	0.43
6:L:48:ARG:HH12	6:L:51:LYS:HE2	1.83	0.43
8:3:42:LEU:HD13	8:2:36:TYR:CE2	2.53	0.43
8:7:19:ALA:O	8:8:20:GLY:HA3	2.19	0.43
8:7:41:SER:HB3	9:H:49:ALA:O	2.17	0.43
1:A:48:GLN:HB3	2:E:71:GLY:HA2	2.01	0.43
3:G:51:LEU:HD12	9:H:85:ASN:HD21	1.83	0.43
6:L:97:ASP:OD1	6:L:98:PRO:HD2	2.19	0.43
4:O:126:LEU:HD12	4:O:127:GLU:H	1.84	0.43
5:K:52:VAL:HG11	14:R:84:LEU:O	2.18	0.43
11:N:169:LEU:HD23	11:N:173:LEU:HG	1.99	0.43
1:B:206:ILE:HD11	1:B:247:PRO:HG3	1.99	0.43
1:C:389:THR:OG1	1:C:449:VAL:HG21	2.19	0.43
7:M:144:LEU:HD21	13:Q:33:TYR:O	2.19	0.43
8:6:66:MET:HG3	11:N:170:LEU:HD13	2.00	0.43
1:A:129:VAL:HG21	1:A:245:LEU:HD11	2.01	0.43
1:A:453:LEU:HD21	1:A:464:PHE:CE1	2.54	0.43
1:C:95:VAL:HG11	1:C:245:LEU:HD21	2.01	0.43
1:C:183:ILE:HD11	1:C:267:ILE:HD13	2.01	0.43
1:C:212:THR:OG1	2:F:359:ARG:NH1	2.40	0.43
2:F:146:LEU:HD22	2:F:378:GLN:HG3	2.01	0.43
5:K:97:LYS:HE2	7:M:124:LEU:HD23	2.00	0.43
5:K:127:VAL:CG2	7:M:10:ILE:HD13	2.48	0.43
7:M:149:TYR:CE2	7:M:156:PRO:HD3	2.54	0.43
14:R:90:ARG:HH21	15:S:98:ILE:HG23	1.82	0.43
1:A:180:ILE:HD11	1:A:216:LEU:HD11	2.00	0.43
1:C:172:GLN:NE2	18:C:601:ATP:O3G	2.52	0.43
5:K:145:TYR:HE2	7:M:44:LEU:HB2	1.83	0.43
1:C:397:TYR:HB2	1:C:421:GLY:HA3	2.01	0.43
2:E:425:GLU:HG2	2:E:430:HIS:O	2.18	0.43
2:D:375:ARG:NH1	2:D:378:GLN:OE1	2.49	0.43
5:K:46:LEU:O	15:S:98:ILE:HD12	2.19	0.43
1:C:187:LYS:HE2	1:C:224:ASP:HB3	2.00	0.42
1:C:439:GLU:HG2	1:C:440:GLU:N	2.34	0.42
2:F:260:ASN:HB3	2:F:263:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:142:LEU:HD21	4:O:148:LEU:HD21	2.01	0.42
5:K:118:VAL:HG23	13:Q:49:LYS:HE3	2.01	0.42
5:K:181:VAL:HG21	6:L:45:ASP:OD2	2.19	0.42
11:N:95:THR:O	11:N:101:ASN:ND2	2.41	0.42
1:A:67:GLU:O	2:E:74:ARG:NH1	2.47	0.42
2:F:384:TYR:O	2:F:388:GLN:HG2	2.20	0.42
2:F:396:MET:HE3	2:F:404:LYS:HG2	2.00	0.42
1:B:303:SER:HB2	2:F:225:MET:HB2	2.00	0.42
2:E:407:VAL:O	2:E:411:ARG:HG2	2.18	0.42
2:E:442:LYS:HA	2:E:442:LYS:HD2	1.94	0.42
4:O:107:THR:O	4:O:110:SER:OG	2.27	0.42
9:H:143:LYS:HB2	9:H:143:LYS:HE3	1.77	0.42
2:E:77:LYS:HA	2:E:77:LYS:HD3	1.87	0.42
11:N:31:ILE:O	13:Q:27:LYS:HD3	2.19	0.42
1:B:164:ARG:HG3	1:B:323:ALA:HB3	2.00	0.42
1:B:458:PRO:HA	1:B:461:ILE:HG12	2.01	0.42
1:C:30:ARG:NH1	1:C:32:LEU:HD23	2.34	0.42
2:F:347:ILE:HG23	2:F:418:SER:HB3	2.01	0.42
2:D:35:ILE:HG22	2:D:36:LEU:HG	2.00	0.42
5:K:117:LEU:C	13:Q:49:LYS:HZ1	2.22	0.42
5:K:163:ASN:O	5:K:167:ARG:HG2	2.20	0.42
8:2:65:LEU:HD23	8:2:65:LEU:HA	1.85	0.42
13:Q:37:PRO:C	13:Q:39:PRO:HD3	2.39	0.42
1:C:457:GLU:HB2	1:C:460:LYS:HG2	2.01	0.42
2:D:247:ARG:HD3	2:D:307:ILE:HG13	2.02	0.42
4:O:121:THR:OG1	4:O:163:ILE:HB	2.20	0.42
11:N:122:LYS:HE3	11:N:122:LYS:HA	2.01	0.42
1:A:36:ASP:OD1	2:D:277:ARG:NH2	2.52	0.42
3:G:195:ASP:HB3	9:H:56:GLN:NE2	2.34	0.42
7:M:135:LEU:HD22	11:N:37:LEU:HD11	2.02	0.42
14:R:90:ARG:CZ	15:S:101:ASP:HA	2.49	0.42
15:S:46:PRO:HA	15:S:49:ILE:HG12	2.02	0.42
1:B:334:VAL:HG11	1:B:351:PHE:CE1	2.54	0.42
4:O:65:LYS:HB2	4:O:65:LYS:HE3	1.88	0.42
4:O:182:LEU:HD23	4:O:182:LEU:HA	1.95	0.42
11:N:25:LEU:HD23	13:Q:19:THR:OG1	2.20	0.42
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.90	0.42
2:D:28:PHE:HB2	2:D:32:LEU:HD12	2.01	0.42
4:O:73:THR:HG23	4:O:78:PHE:HD2	1.85	0.42
8:6:65:LEU:HD23	8:6:65:LEU:HA	1.85	0.42
1:A:152:ALA:HB3	1:A:365:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:NH1	1:A:308:ARG:O	2.53	0.42
2:F:97:ILE:HD11	2:F:200:TYR:CD2	2.55	0.42
2:D:90:GLY:HA2	2:D:245:TYR:CE1	2.54	0.42
4:O:105:PHE:O	4:O:108:MET:HB2	2.20	0.42
8:5:52:LEU:HD13	11:N:220:LEU:HD12	2.02	0.42
8:5:54:PHE:CE1	8:6:56:LEU:HD13	2.55	0.42
9:H:110:ALA:O	9:H:114:LYS:HG3	2.20	0.42
15:S:82:VAL:HG23	16:T:15:ARG:HA	2.02	0.42
1:B:169:GLY:O	1:B:328:GLU:HA	2.20	0.41
1:C:255:GLU:OE1	1:C:258:ARG:NH2	2.53	0.41
1:C:382:ALA:HB2	1:C:488:LYS:HA	2.02	0.41
2:E:222:TYR:HB3	2:E:224:GLN:OE1	2.19	0.41
2:D:50:LEU:HD23	2:D:65:ALA:HA	2.01	0.41
3:G:116:LEU:HD23	3:G:116:LEU:HA	1.88	0.41
8:3:65:LEU:HD23	8:3:65:LEU:HA	1.85	0.41
1:B:163:GLN:NE2	1:B:165:GLU:OE2	2.53	0.41
1:B:206:ILE:CD1	1:B:247:PRO:HG3	2.49	0.41
2:F:424:ALA:O	2:F:428:THR:HG22	2.20	0.41
7:M:160:LEU:HG	11:N:51:LYS:HG3	2.02	0.41
8:4:17:GLY:HA3	8:4:64:CYS:SG	2.61	0.41
8:6:17:GLY:HA3	8:6:64:CYS:SG	2.61	0.41
14:R:21:LYS:HA	15:S:69:VAL:HG23	2.02	0.41
1:B:338:ILE:O	1:B:342:VAL:HG23	2.20	0.41
1:C:381:ARG:O	1:C:385:GLN:HG3	2.20	0.41
2:E:256:LEU:O	2:E:309:SER:HA	2.20	0.41
2:D:23:VAL:HG21	2:D:274:LEU:HB3	2.02	0.41
4:O:135:LYS:O	4:O:139:LYS:HG2	2.21	0.41
5:K:19:GLU:O	5:K:23:GLN:HG2	2.20	0.41
5:K:163:ASN:OD1	5:K:167:ARG:NH1	2.53	0.41
7:M:100:CYS:O	7:M:104:VAL:HG23	2.19	0.41
8:8:17:GLY:HA3	8:8:64:CYS:SG	2.61	0.41
1:A:418:LEU:O	1:A:422:VAL:HG13	2.21	0.41
1:B:393:GLU:OE2	1:B:420:ARG:NH1	2.53	0.41
2:E:377:VAL:O	2:E:380:ILE:HG22	2.21	0.41
2:D:323:PRO:O	2:D:327:THR:OG1	2.22	0.41
2:D:347:ILE:HG23	2:D:418:SER:HB2	2.02	0.41
5:K:13:ARG:HD3	5:K:22:PHE:CE1	2.55	0.41
15:S:90:GLU:O	15:S:94:LYS:HE3	2.20	0.41
2:E:375:ARG:HA	2:E:375:ARG:HD3	1.85	0.41
2:F:443:GLY:O	2:F:447:ILE:HG13	2.21	0.41
5:K:141:ARG:HD3	7:M:46:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:160:LEU:HD12	7:M:160:LEU:HA	1.92	0.41
8:2:17:GLY:HA3	8:2:64:CYS:SG	2.61	0.41
13:Q:38:SER:N	13:Q:39:PRO:HD3	2.35	0.41
1:A:164:ARG:HH22	2:E:192:ARG:HD3	1.85	0.41
2:D:278:ILE:HG23	3:G:269:ALA:HB2	2.03	0.41
5:K:85:LEU:HD23	5:K:85:LEU:HA	1.89	0.41
5:K:103:HIS:HB2	13:Q:41:PRO:HA	2.02	0.41
9:H:105:LEU:HD21	9:H:146:GLU:HB2	2.01	0.41
11:N:26:PHE:HZ	14:R:68:VAL:HG12	1.84	0.41
2:E:283:GLY:CA	3:G:262:LEU:HD11	2.50	0.41
2:D:319:ASP:O	2:D:320:LEU:HB2	2.21	0.41
5:K:93:LEU:CD1	11:N:37:LEU:HD21	2.50	0.41
2:E:154:LYS:O	2:E:333:ASP:N	2.50	0.41
2:E:283:GLY:HA2	3:G:262:LEU:HD11	2.02	0.41
1:B:98:PRO:O	1:B:103:LEU:HD11	2.21	0.41
1:B:124:LYS:HE2	1:B:124:LYS:HB2	1.88	0.41
1:B:186:GLN:HG3	1:B:199:LEU:HD23	2.03	0.41
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.86	0.41
1:C:177:SER:OG	18:C:601:ATP:O1A	2.20	0.41
1:C:439:GLU:HG3	1:C:480:LEU:HB3	2.03	0.41
1:C:476:HIS:CD2	1:C:500:ILE:HD12	2.56	0.41
2:E:436:PRO:HD2	2:E:439:GLU:HG3	2.02	0.41
2:D:390:ILE:HG23	2:D:394:LEU:HD13	2.02	0.41
4:O:42:VAL:O	4:O:46:LEU:HG	2.21	0.41
4:O:71:ASP:O	4:O:75:LYS:HG3	2.20	0.41
8:3:20:GLY:HA3	8:2:19:ALA:HA	2.02	0.41
8:8:33:ILE:HG21	8:1:32:LEU:HA	2.03	0.41
8:8:72:LEU:HD12	8:8:72:LEU:HA	1.94	0.41
11:N:134:PRO:O	11:N:138:ILE:HG12	2.21	0.41
1:C:396:GLN:HG2	17:J:35:ARG:HH12	1.86	0.41
4:O:117:PRO:HA	4:O:149:LYS:HB2	2.02	0.41
6:L:40:GLN:HB3	6:L:43:PHE:HD2	1.86	0.41
7:M:12:TRP:CH2	7:M:31:LYS:HA	2.57	0.41
14:R:52:ASN:HA	14:R:56:ASN:HB3	2.03	0.41
15:S:36:GLU:O	16:T:12:LYS:NZ	2.46	0.41
2:D:87:ILE:HD13	2:D:238:THR:HG23	2.04	0.40
6:L:47:ILE:O	6:L:51:LYS:HD3	2.21	0.40
8:7:17:GLY:HA3	8:7:64:CYS:SG	2.61	0.40
11:N:158:VAL:HA	11:N:161:THR:HG22	2.03	0.40
4:O:31:LYS:HE2	4:O:31:LYS:HB3	1.85	0.40
5:K:110:THR:O	5:K:114:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:101:GLU:N	6:L:101:GLU:OE1	2.53	0.40
8:1:17:GLY:HA3	8:1:64:CYS:SG	2.61	0.40
11:N:32:PRO:HG2	11:N:43:ILE:HG12	2.03	0.40
14:R:76:SER:HA	14:R:79:PHE:CZ	2.56	0.40
1:A:164:ARG:NH1	1:A:307:GLU:OE1	2.55	0.40
1:A:180:ILE:HD13	1:A:180:ILE:HA	1.89	0.40
1:A:393:GLU:OE1	1:A:420:ARG:HG2	2.22	0.40
1:C:269:ASP:HA	1:C:270:ASP:HA	1.86	0.40
1:C:496:LYS:O	1:C:500:ILE:HG12	2.21	0.40
4:O:11:VAL:O	4:O:16:GLY:HA3	2.22	0.40
5:K:52:VAL:HG11	14:R:84:LEU:HB3	2.04	0.40
8:3:17:GLY:HA3	8:3:64:CYS:SG	2.61	0.40
11:N:121:ILE:HG23	11:N:122:LYS:HD2	2.03	0.40
1:A:382:ALA:HB1	1:A:442:VAL:HG11	2.03	0.40
5:K:136:LEU:HD11	7:M:83:ASP:HA	2.03	0.40
5:K:140:TYR:CE1	7:M:80:VAL:HG22	2.55	0.40
5:K:181:VAL:O	5:K:184:SER:OG	2.24	0.40
8:6:19:ALA:HB2	8:7:17:GLY:HA2	2.04	0.40
1:B:129:VAL:HG21	1:B:245:LEU:HD11	2.02	0.40
1:C:156:LEU:HD13	1:C:367:VAL:HG11	2.04	0.40
2:E:443:GLY:O	2:E:447:ILE:HG13	2.22	0.40
3:G:32:ALA:C	3:G:34:ALA:H	2.24	0.40
4:O:109:MET:HE3	4:O:112:HIS:HB3	2.03	0.40
6:L:52:SER:HA	6:L:55:GLN:OE1	2.21	0.40
7:M:19:ILE:HB	7:M:24:LYS:HZ2	1.86	0.40
11:N:139:PRO:O	11:N:142:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/510 (95%)	477 (99%)	7 (1%)	0	100	100
1	B	473/510 (93%)	463 (98%)	10 (2%)	0	100	100
1	C	466/510 (91%)	454 (97%)	12 (3%)	0	100	100
2	D	468/482 (97%)	446 (95%)	21 (4%)	1 (0%)	47	69
2	E	452/482 (94%)	439 (97%)	12 (3%)	1 (0%)	47	69
2	F	464/482 (96%)	448 (97%)	15 (3%)	1 (0%)	47	69
3	G	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
4	O	185/190 (97%)	177 (96%)	8 (4%)	0	100	100
5	K	194/214 (91%)	187 (96%)	7 (4%)	0	100	100
6	L	65/108 (60%)	57 (88%)	8 (12%)	0	100	100
7	M	154/160 (96%)	143 (93%)	11 (7%)	0	100	100
8	1	73/75 (97%)	73 (100%)	0	0	100	100
8	2	73/75 (97%)	73 (100%)	0	0	100	100
8	3	73/75 (97%)	73 (100%)	0	0	100	100
8	4	73/75 (97%)	73 (100%)	0	0	100	100
8	5	73/75 (97%)	73 (100%)	0	0	100	100
8	6	73/75 (97%)	73 (100%)	0	0	100	100
8	7	73/75 (97%)	73 (100%)	0	0	100	100
8	8	73/75 (97%)	73 (100%)	0	0	100	100
9	H	130/146 (89%)	124 (95%)	6 (5%)	0	100	100
10	I	43/51 (84%)	43 (100%)	0	0	100	100
11	N	221/226 (98%)	209 (95%)	12 (5%)	0	100	100
12	P	39/58 (67%)	37 (95%)	2 (5%)	0	100	100
13	Q	49/68 (72%)	45 (92%)	4 (8%)	0	100	100
14	R	72/93 (77%)	68 (94%)	4 (6%)	0	100	100
15	S	75/102 (74%)	73 (97%)	2 (3%)	0	100	100
16	T	42/69 (61%)	41 (98%)	1 (2%)	0	100	100
17	J	33/81 (41%)	32 (97%)	1 (3%)	0	100	100
All	All	4962/5415 (92%)	4808 (97%)	151 (3%)	3 (0%)	54	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	282	VAL
2	D	282	VAL
2	F	282	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/412 (95%)	393 (100%)	0	100	100
1	B	387/412 (94%)	386 (100%)	1 (0%)	92	97
1	C	382/412 (93%)	378 (99%)	4 (1%)	76	89
2	D	379/388 (98%)	379 (100%)	0	100	100
2	E	369/388 (95%)	369 (100%)	0	100	100
2	F	376/388 (97%)	376 (100%)	0	100	100
3	G	228/229 (100%)	228 (100%)	0	100	100
4	O	162/165 (98%)	162 (100%)	0	100	100
5	K	160/187 (86%)	160 (100%)	0	100	100
6	L	60/98 (61%)	60 (100%)	0	100	100
7	M	135/139 (97%)	135 (100%)	0	100	100
8	1	51/51 (100%)	49 (96%)	2 (4%)	32	56
8	2	51/51 (100%)	50 (98%)	1 (2%)	55	77
8	3	51/51 (100%)	50 (98%)	1 (2%)	55	77
8	4	51/51 (100%)	49 (96%)	2 (4%)	32	56
8	5	51/51 (100%)	50 (98%)	1 (2%)	55	77
8	6	51/51 (100%)	50 (98%)	1 (2%)	55	77
8	7	51/51 (100%)	50 (98%)	1 (2%)	55	77
8	8	51/51 (100%)	50 (98%)	1 (2%)	55	77
9	H	103/108 (95%)	103 (100%)	0	100	100
10	I	36/42 (86%)	36 (100%)	0	100	100
11	N	196/199 (98%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	P	36/48 (75%)	36 (100%)	0	100	100
13	Q	51/68 (75%)	51 (100%)	0	100	100
14	R	65/82 (79%)	65 (100%)	0	100	100
15	S	64/85 (75%)	64 (100%)	0	100	100
16	T	34/58 (59%)	34 (100%)	0	100	100
17	J	23/68 (34%)	23 (100%)	0	100	100
All	All	4047/4384 (92%)	4032 (100%)	15 (0%)	91	97

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	ARG
1	C	164	ARG
1	C	362	ARG
1	C	455	LYS
1	C	498	LYS
8	3	3	ASP
8	4	3	ASP
8	4	38	ARG
8	5	3	ASP
8	6	3	ASP
8	7	3	ASP
8	8	3	ASP
8	1	3	ASP
8	1	38	ARG
8	2	3	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	385	GLN
1	A	396	GLN
1	A	405	GLN
1	A	475	GLN
1	A	477	GLN
1	A	503	ASN
1	B	48	GLN
1	B	385	GLN

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Mol	Chain	Res	Type
1	B	432	GLN
1	C	208	GLN
1	C	379	GLN
2	E	370	HIS
2	E	388	GLN
2	F	27	GLN
2	F	180	HIS
2	F	197	ASN
2	F	249	GLN
2	F	296	GLN
2	F	331	HIS
2	D	115	GLN
2	D	180	HIS
2	D	266	GLN
3	G	120	HIS
4	O	57	ASN
4	O	84	ASN
4	O	92	ASN
4	O	97	ASN
5	K	86	ASN
5	K	92	GLN
5	K	102	GLN
5	K	130	ASN
5	K	180	HIS
5	K	183	GLN
7	M	34	ASN
7	M	159	ASN
9	H	85	ASN
9	H	111	ASN
11	N	46	GLN
11	N	61	HIS
11	N	127	HIS
11	N	163	ASN
11	N	172	HIS
11	N	225	ASN
13	Q	46	ASN
14	R	83	HIS
16	T	31	ASN
17	J	27	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
18	ATP	B	601	19	26,33,33	2.23	7 (26%)	31,52,52	1.65	6 (19%)
18	ATP	C	601	19	26,33,33	2.20	6 (23%)	31,52,52	1.65	7 (22%)
20	ADP	D	501	19	24,29,29	2.37	8 (33%)	29,45,45	1.58	5 (17%)
20	ADP	F	501	19	24,29,29	2.35	8 (33%)	29,45,45	1.51	5 (17%)
18	ATP	A	601	19	26,33,33	2.20	6 (23%)	31,52,52	1.63	7 (22%)

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
18	ATP	B	601	19	-	7/18/38/38	0/3/3/3
18	ATP	C	601	19	-	6/18/38/38	0/3/3/3
20	ADP	D	501	19	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ADP	F	501	19	-	6/12/32/32	0/3/3/3
18	ATP	A	601	19	-	3/18/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	601	ATP	O4'-C1'	7.71	1.51	1.41
18	A	601	ATP	O4'-C1'	7.55	1.51	1.41
18	C	601	ATP	O4'-C1'	7.51	1.51	1.41
20	D	501	ADP	O4'-C1'	6.51	1.50	1.41
20	F	501	ADP	O4'-C1'	6.51	1.50	1.41
20	F	501	ADP	C6-N6	4.48	1.50	1.34
20	D	501	ADP	C6-N6	4.46	1.50	1.34
18	C	601	ATP	C2'-C1'	-4.29	1.47	1.53
18	B	601	ATP	C2'-C1'	-4.26	1.47	1.53
18	A	601	ATP	C2'-C1'	-4.23	1.47	1.53
20	D	501	ADP	C2'-C1'	-4.19	1.47	1.53
20	F	501	ADP	C2'-C1'	-4.11	1.47	1.53
20	F	501	ADP	O4'-C4'	3.43	1.52	1.45
18	C	601	ATP	C6-N6	3.42	1.46	1.34
20	D	501	ADP	O4'-C4'	3.40	1.52	1.45
18	A	601	ATP	C6-N6	3.36	1.46	1.34
18	B	601	ATP	C6-N6	3.36	1.46	1.34
18	B	601	ATP	C2'-C3'	-3.16	1.44	1.53
18	C	601	ATP	C2'-C3'	-3.11	1.44	1.53
18	A	601	ATP	C2'-C3'	-3.01	1.45	1.53
20	F	501	ADP	C2'-C3'	-2.83	1.45	1.53
20	D	501	ADP	C2'-C3'	-2.77	1.45	1.53
20	F	501	ADP	C3'-C4'	-2.60	1.46	1.53
20	D	501	ADP	C3'-C4'	-2.57	1.46	1.53
18	A	601	ATP	O4'-C4'	2.43	1.50	1.45
18	C	601	ATP	O4'-C4'	2.37	1.50	1.45
18	B	601	ATP	O4'-C4'	2.32	1.50	1.45
18	A	601	ATP	C4-N3	-2.32	1.32	1.35
18	B	601	ATP	C4-N3	-2.30	1.32	1.35
18	C	601	ATP	C4-N3	-2.21	1.32	1.35
20	D	501	ADP	PA-O5'	2.16	1.68	1.59
20	F	501	ADP	PA-O5'	2.15	1.68	1.59
20	F	501	ADP	C6-C5	-2.09	1.35	1.43
18	B	601	ATP	C3'-C4'	-2.04	1.47	1.53
20	D	501	ADP	C6-C5	-2.01	1.35	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	601	ATP	N3-C2-N1	-4.17	122.16	128.68
18	B	601	ATP	C3'-C2'-C1'	4.16	107.24	100.98
20	D	501	ADP	N3-C2-N1	-4.10	122.28	128.68
18	C	601	ATP	N3-C2-N1	-4.09	122.28	128.68
18	A	601	ATP	N3-C2-N1	-4.07	122.31	128.68
20	F	501	ADP	N3-C2-N1	-4.07	122.31	128.68
18	C	601	ATP	C4-C5-N7	-3.90	105.34	109.40
18	B	601	ATP	C4-C5-N7	-3.87	105.36	109.40
18	A	601	ATP	C4-C5-N7	-3.79	105.45	109.40
20	D	501	ADP	C4-C5-N7	-3.78	105.46	109.40
18	C	601	ATP	C3'-C2'-C1'	3.75	106.63	100.98
20	D	501	ADP	C3'-C2'-C1'	3.71	106.57	100.98
20	F	501	ADP	C4-C5-N7	-3.65	105.60	109.40
18	A	601	ATP	C3'-C2'-C1'	3.64	106.46	100.98
20	F	501	ADP	C3'-C2'-C1'	3.51	106.27	100.98
18	C	601	ATP	PA-O3A-PB	-2.89	122.90	132.83
18	A	601	ATP	PB-O3B-PG	-2.83	123.11	132.83
18	B	601	ATP	PB-O3B-PG	-2.80	123.23	132.83
20	D	501	ADP	PA-O3A-PB	-2.57	124.00	132.83
18	B	601	ATP	C1'-N9-C4	-2.57	122.12	126.64
18	A	601	ATP	C2'-C3'-C4'	2.56	107.61	102.64
20	D	501	ADP	C1'-N9-C4	-2.48	122.28	126.64
20	F	501	ADP	C1'-N9-C4	-2.43	122.37	126.64
18	C	601	ATP	C1'-N9-C4	-2.36	122.49	126.64
18	C	601	ATP	PB-O3B-PG	-2.34	124.79	132.83
18	C	601	ATP	C2'-C3'-C4'	2.20	106.92	102.64
18	A	601	ATP	C1'-N9-C4	-2.20	122.78	126.64
18	A	601	ATP	PA-O3A-PB	-2.13	125.53	132.83
20	F	501	ADP	PA-O3A-PB	-2.13	125.53	132.83
18	B	601	ATP	PA-O3A-PB	-2.11	125.58	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	601	ATP	PB-O3B-PG-O3G
18	B	601	ATP	PB-O3B-PG-O2G
18	B	601	ATP	PB-O3B-PG-O3G
18	B	601	ATP	C5'-O5'-PA-O1A
18	B	601	ATP	C5'-O5'-PA-O2A
18	C	601	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
18	C	601	ATP	C5'-O5'-PA-O1A
20	F	501	ADP	PA-O3A-PB-O2B
20	F	501	ADP	C5'-O5'-PA-O3A
18	C	601	ATP	O4'-C4'-C5'-O5'
18	C	601	ATP	C3'-C4'-C5'-O5'
20	F	501	ADP	O4'-C4'-C5'-O5'
20	F	501	ADP	C3'-C4'-C5'-O5'
20	F	501	ADP	C5'-O5'-PA-O1A
20	F	501	ADP	C5'-O5'-PA-O2A
18	A	601	ATP	PB-O3B-PG-O1G
18	C	601	ATP	PB-O3A-PA-O2A
18	B	601	ATP	C5'-O5'-PA-O3A
18	A	601	ATP	PB-O3A-PA-O2A
18	B	601	ATP	PB-O3A-PA-O1A
18	C	601	ATP	PB-O3A-PA-O1A
18	B	601	ATP	PB-O3B-PG-O1G

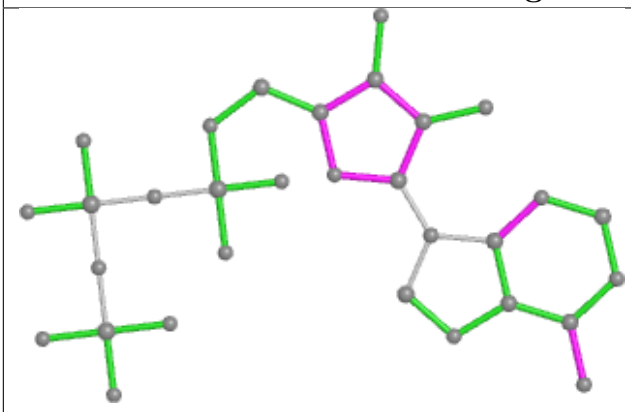
There are no ring outliers.

1 monomer is involved in 2 short contacts:

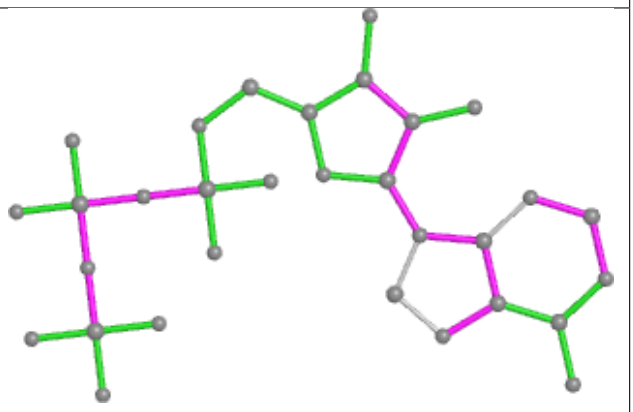
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	601	ATP	2	0

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

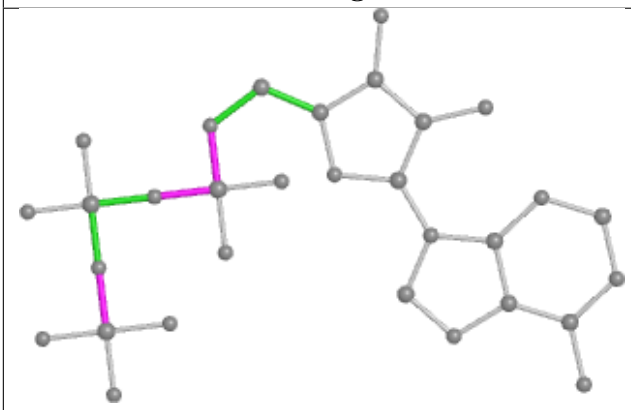
Ligand ATP B 601



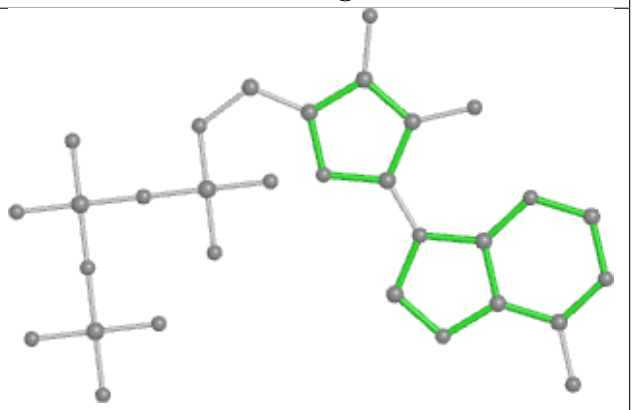
Bond lengths



Bond angles

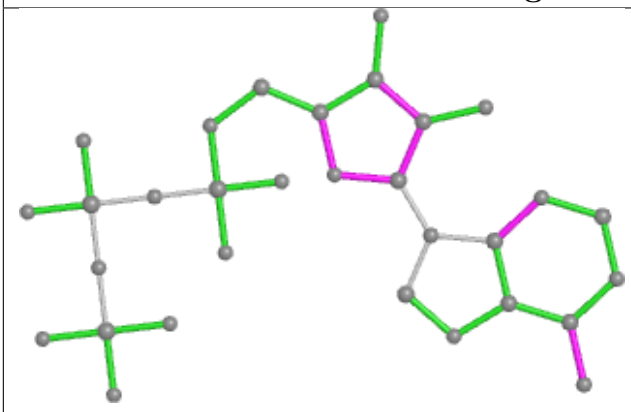


Torsions

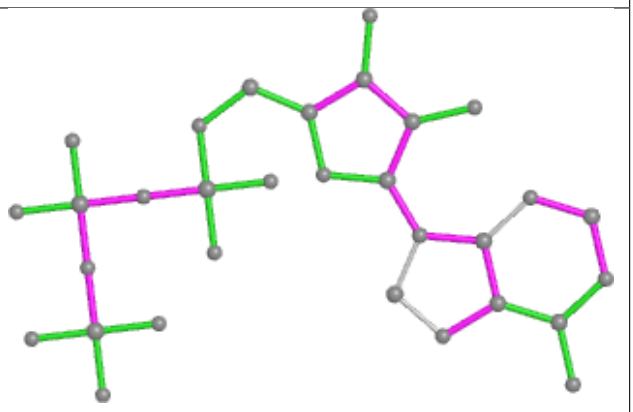


Rings

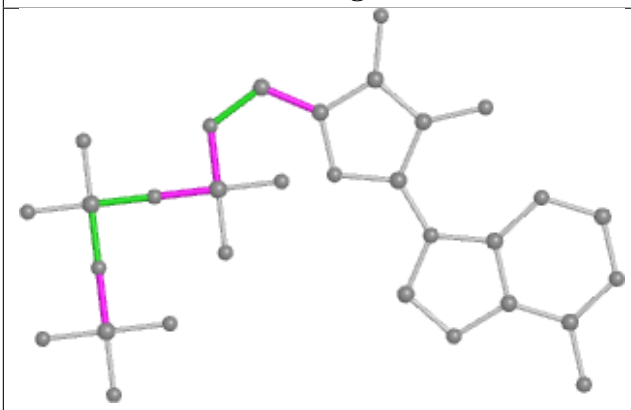
Ligand ATP C 601



Bond lengths



Bond angles



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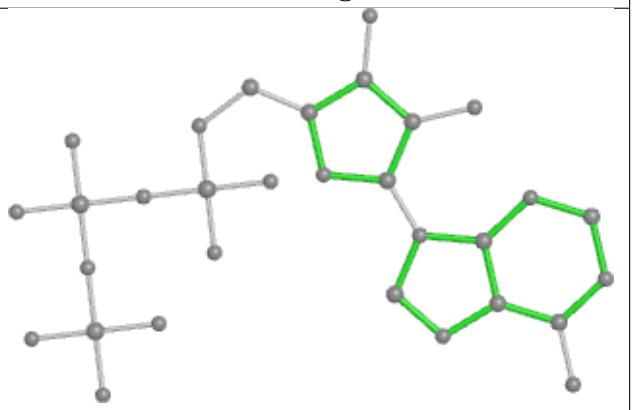
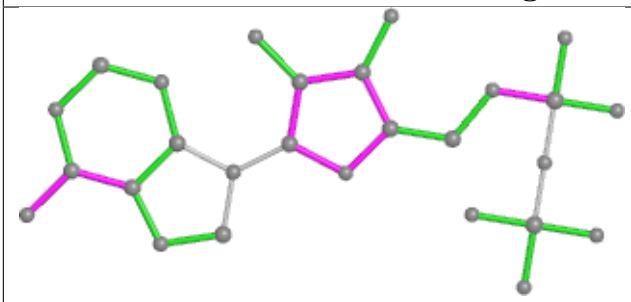
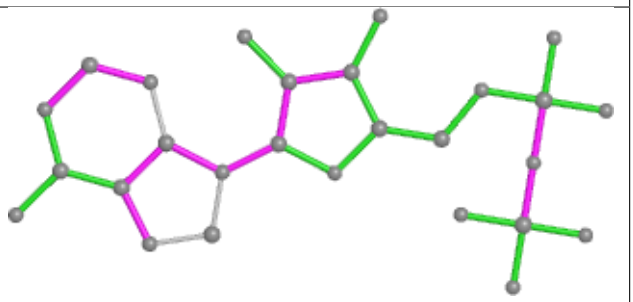


Rings

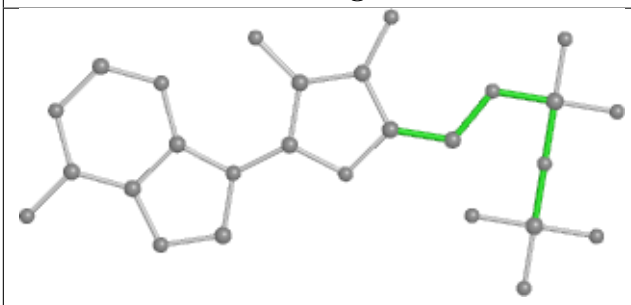
Ligand ADP D 501



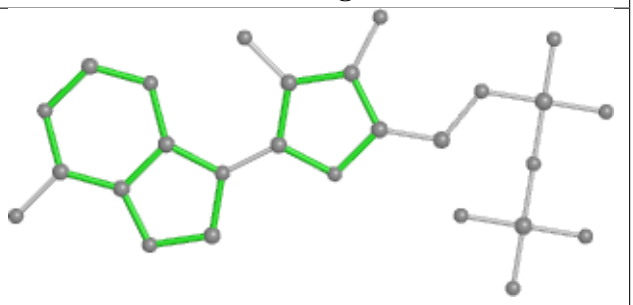
Bond lengths



Bond angles

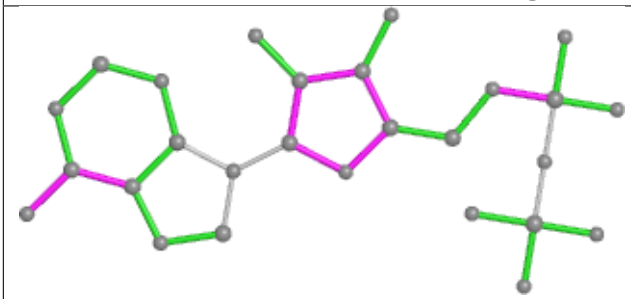


Torsions

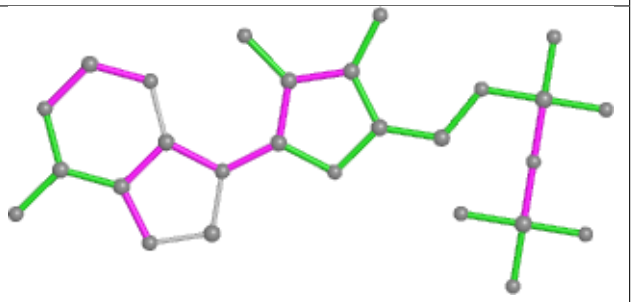


Rings

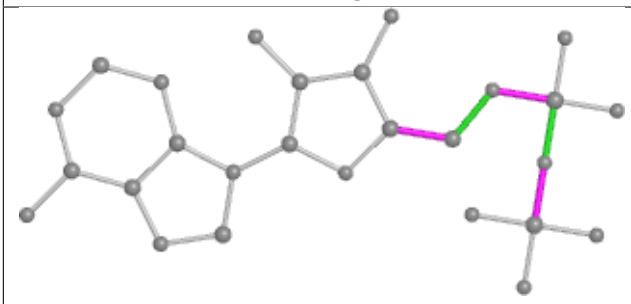
Ligand ADP F 501



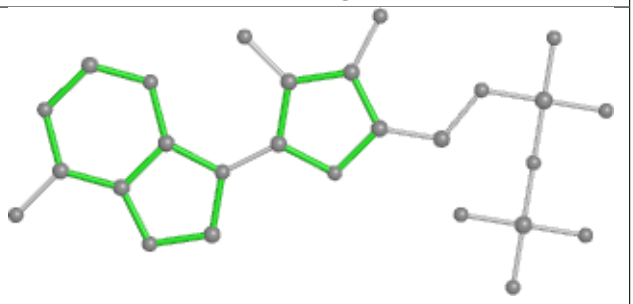
Bond lengths



Bond angles

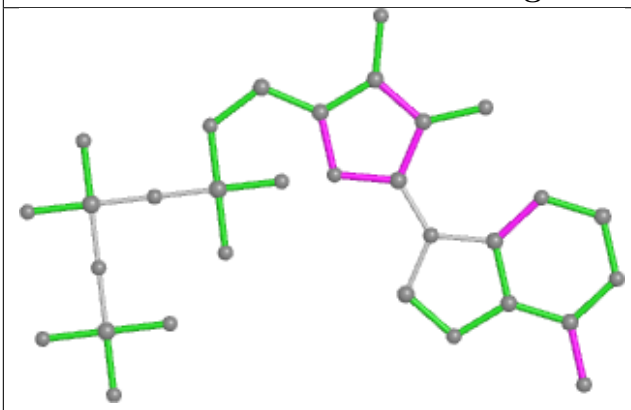


Torsions

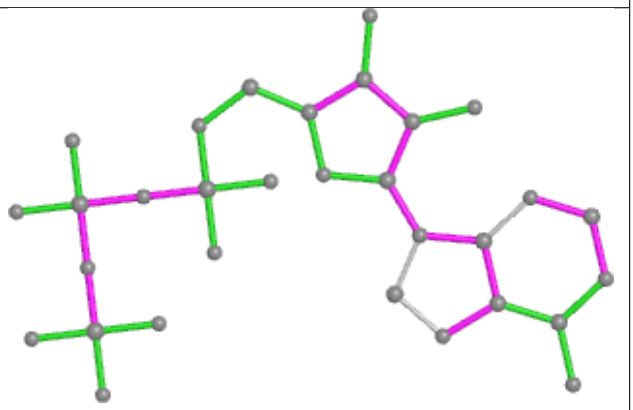


Rings

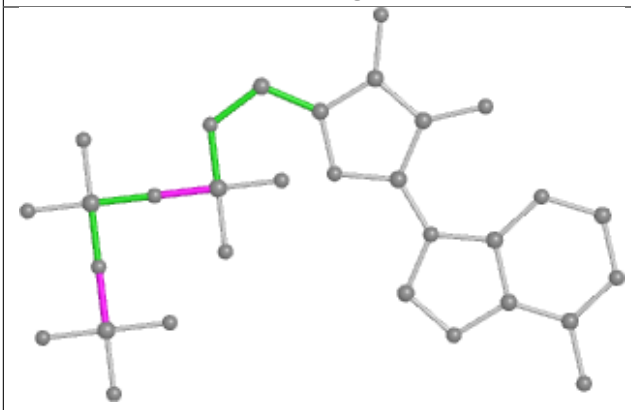
Ligand ATP A 601



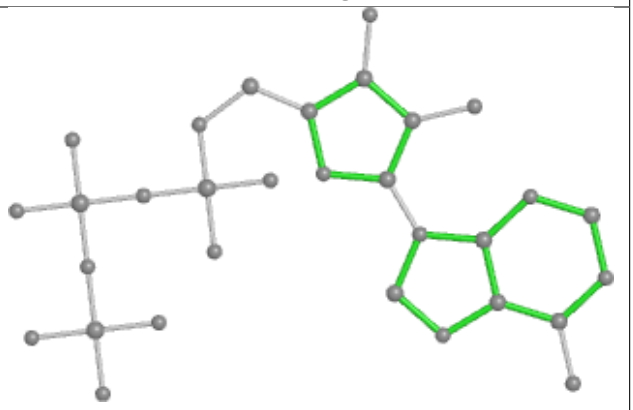
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

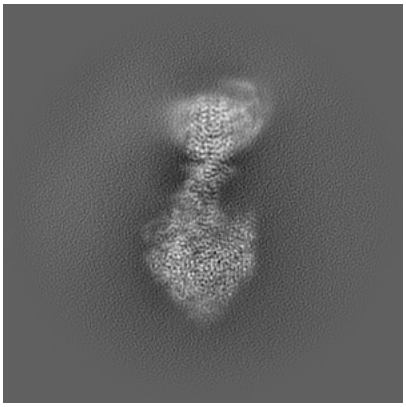
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34582. These allow visual inspection of the internal detail of the map and identification of artifacts.

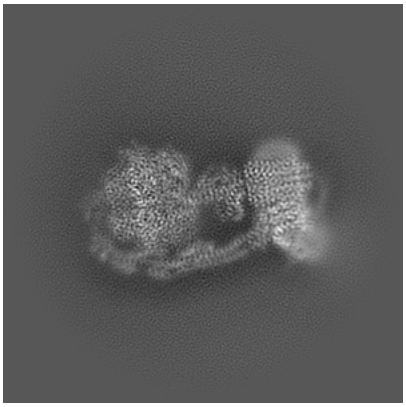
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

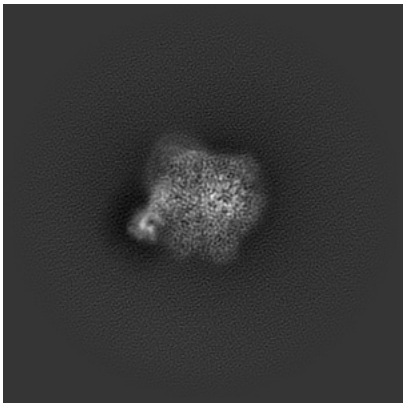
6.1.1 Primary map



X



Y

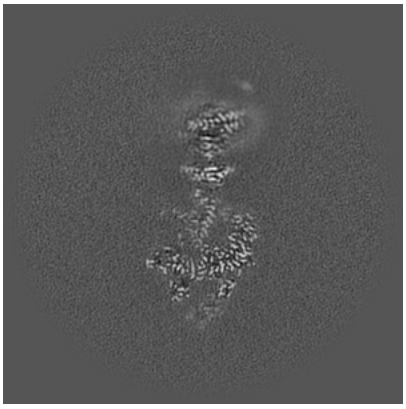


Z

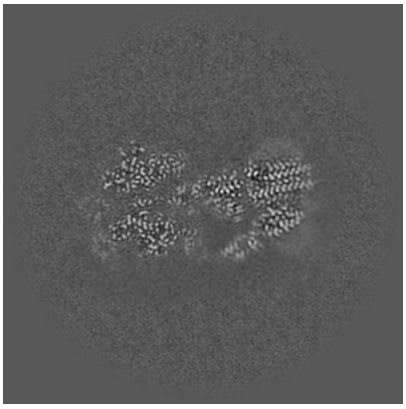
The images above show the map projected in three orthogonal directions.

6.2 Central slices

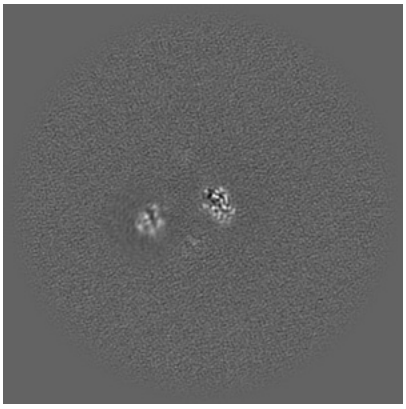
6.2.1 Primary map



X Index: 256



Y Index: 256



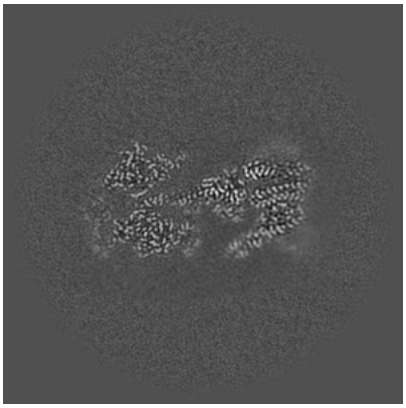
Z Index: 256

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

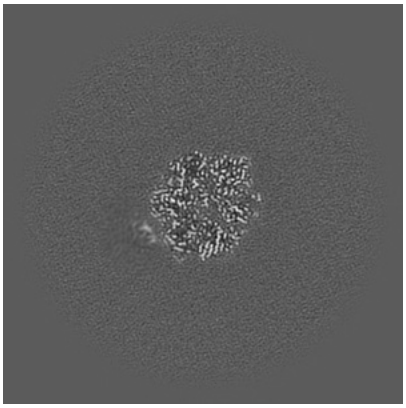
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 267



Y Index: 260

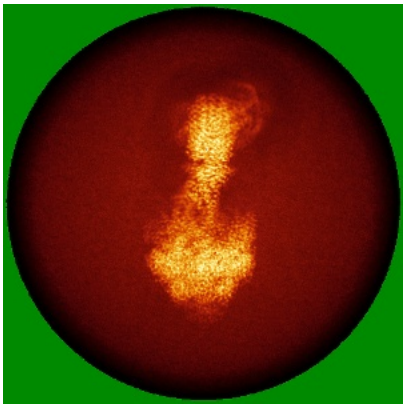


Z Index: 182

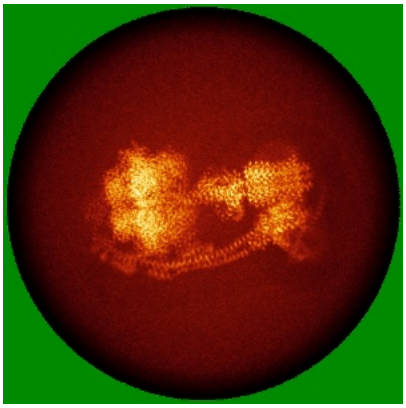
The images above show the largest variance slices of the map in three orthogonal directions.

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

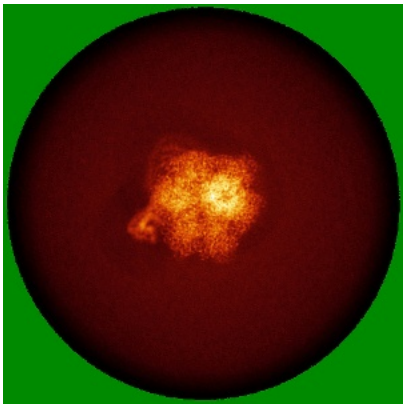
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

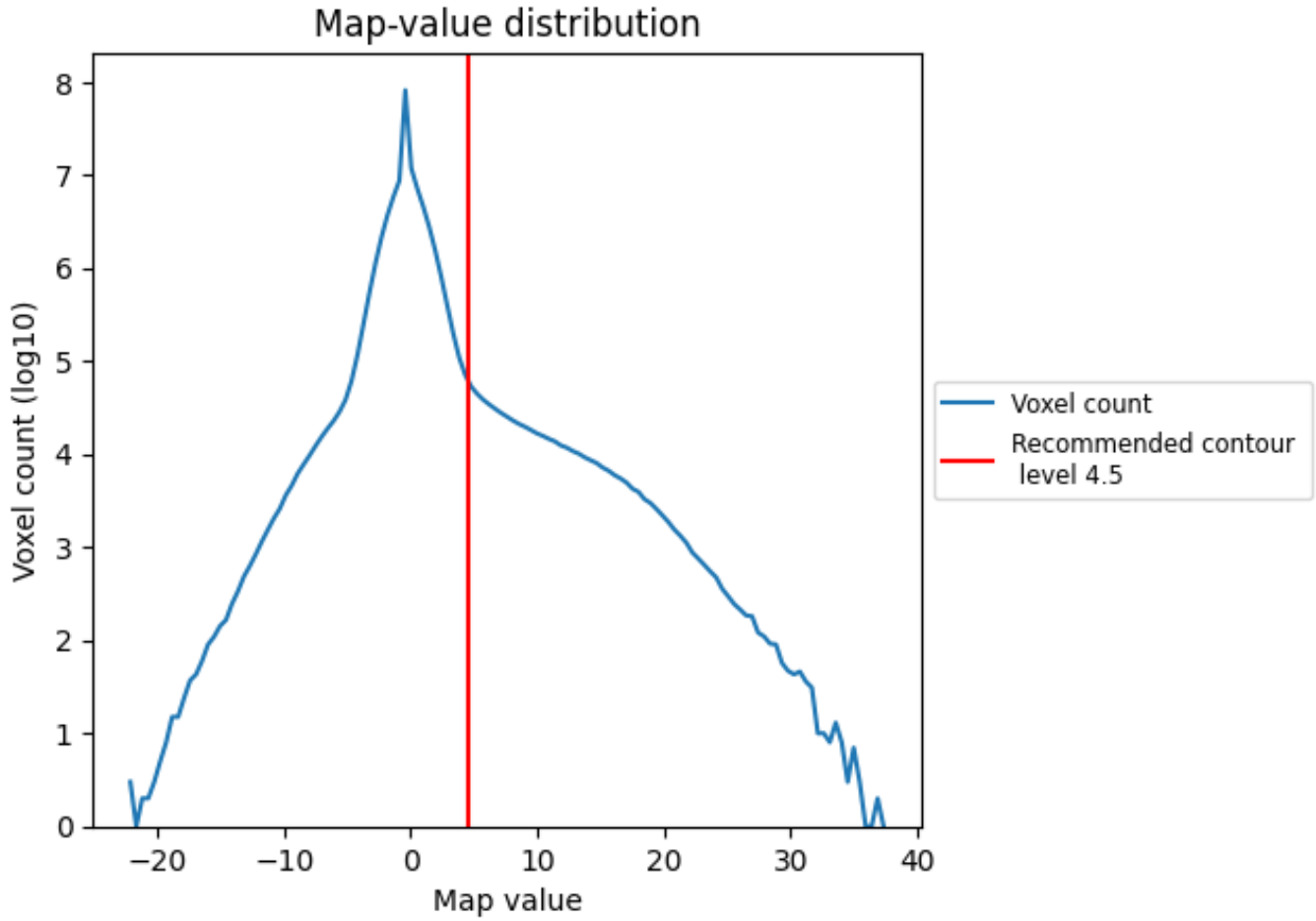
6.6 Mask visualisation (i)

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

7 Map analysis

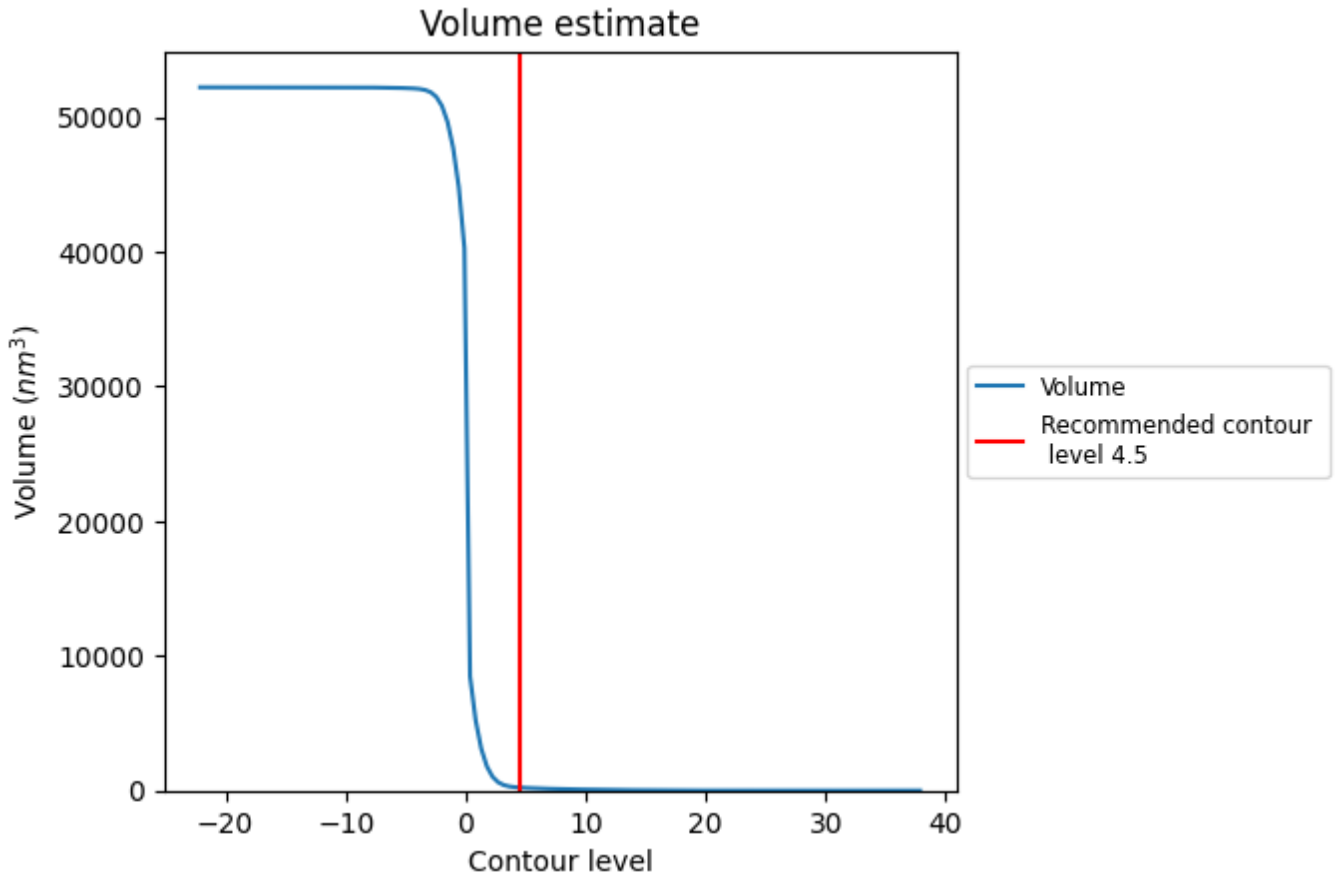
This section contains the results of statistical analysis of the map.

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.

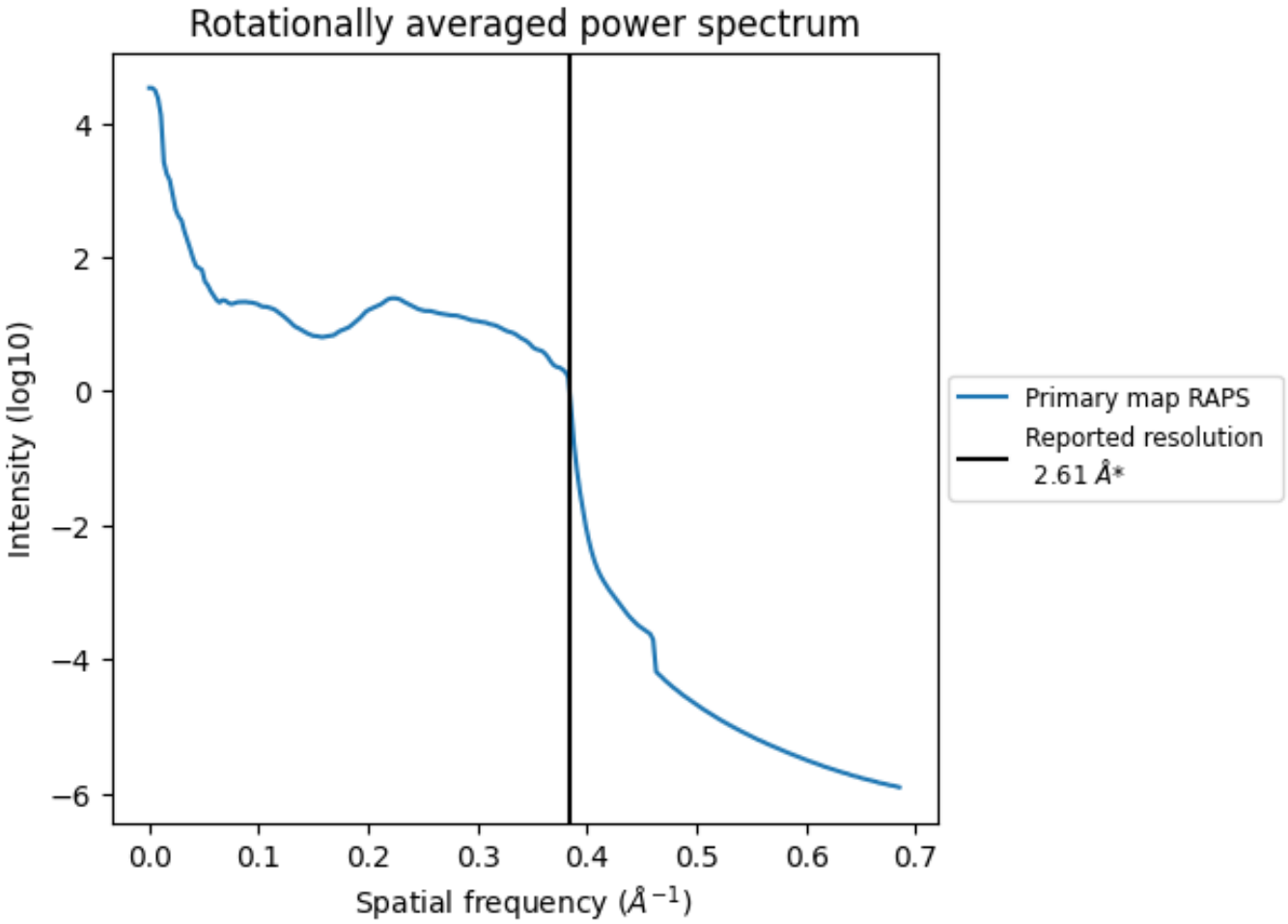
7.2 Volume estimate



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 201 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 0.383 Å^{-1}

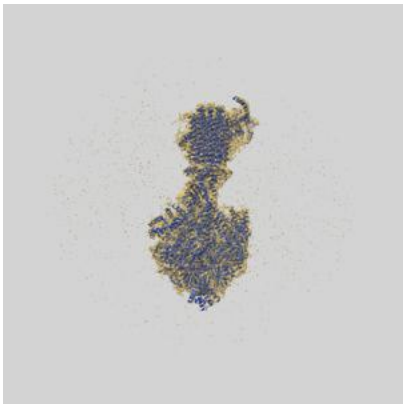
8 Fourier-Shell correlation

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

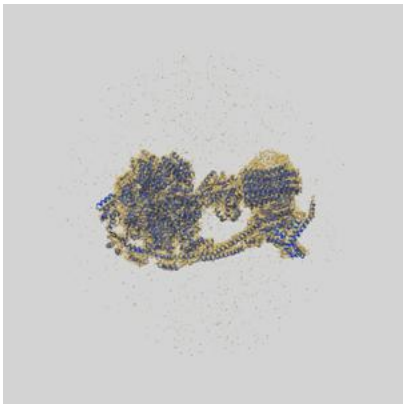
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34582 and PDB model 8H9U. Per-residue inclusion information can be found in section 3 on page 9.

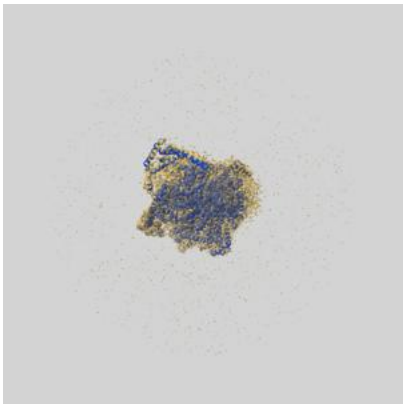
9.1 Map-model overlay



X



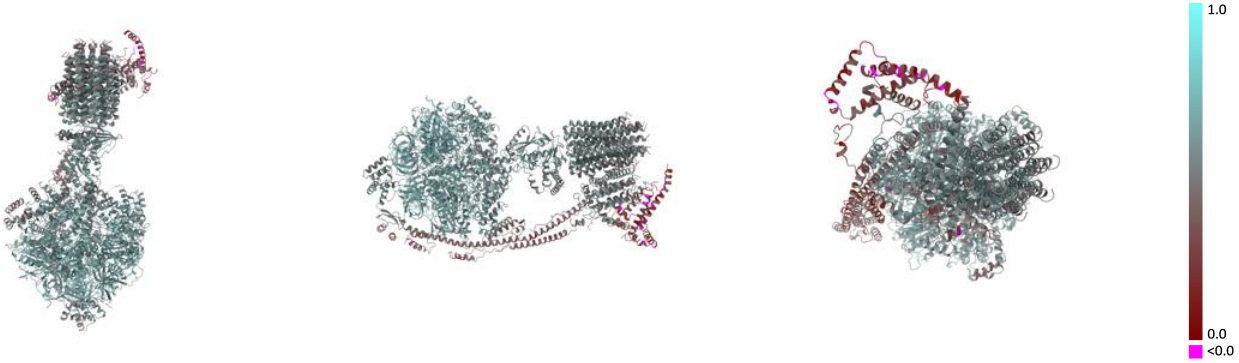
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

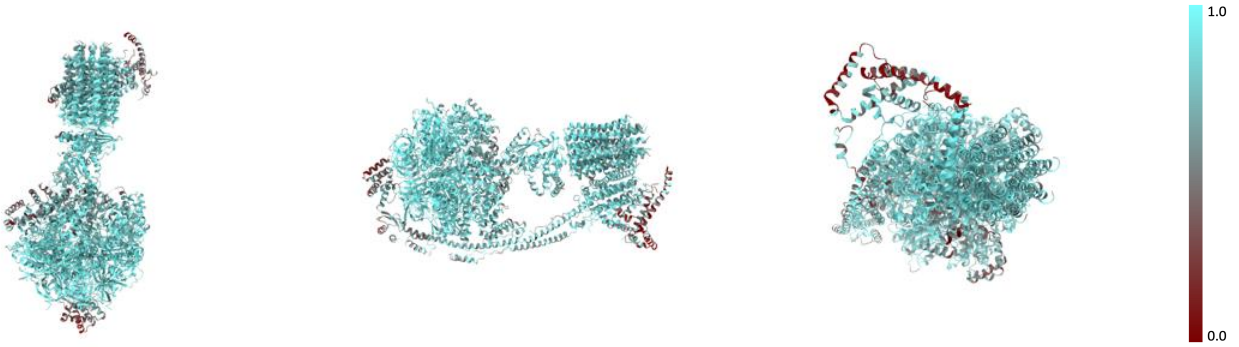
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

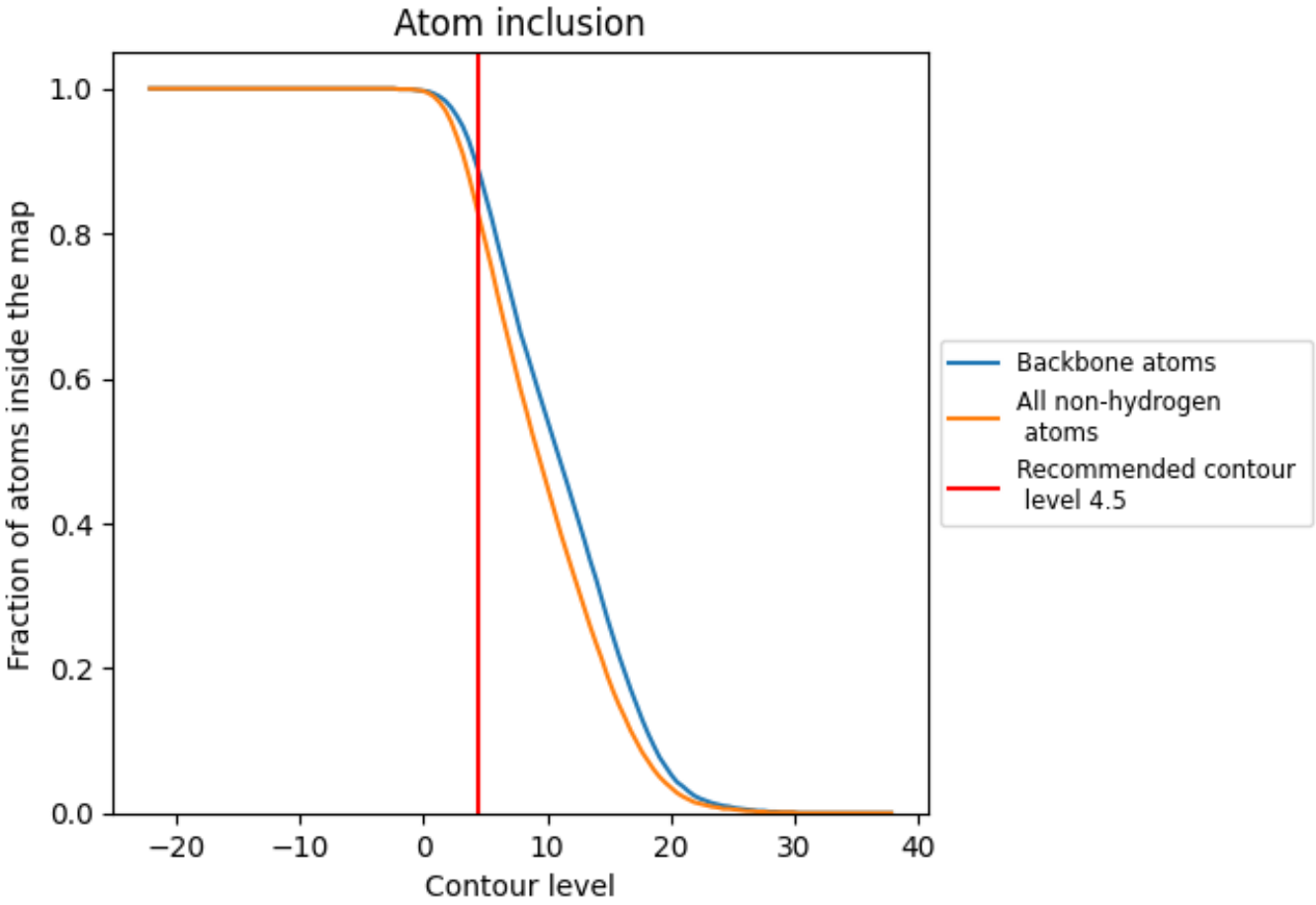
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.5530
1	0.8530	0.5240
2	0.8400	0.5200
3	0.7980	0.5100
4	0.8320	0.5170
5	0.8150	0.5060
6	0.8300	0.5170
7	0.8250	0.5120
8	0.8490	0.5140
A	0.8800	0.6220
B	0.9010	0.6240
C	0.8420	0.6000
D	0.8790	0.6250
E	0.9040	0.6270
F	0.9090	0.6290
G	0.8290	0.5620
H	0.8700	0.5440
I	0.8660	0.5400
J	0.6250	0.5690
K	0.7790	0.3970
L	0.6970	0.3000
M	0.7290	0.3600
N	0.7970	0.5000
O	0.4500	0.4870
P	0.6610	0.3990
Q	0.7630	0.4370
R	0.7470	0.4190
S	0.4020	0.2120
T	0.2800	0.2050