Full wwPDB EM Validation Report (i)

Mar 17, 2022 – 03:47 am GMT

PDB ID	:	7NYZ
EMDB ID	:	EMD-12659
Title	:	Cryo-EM structure of the MukBEF-MatP-DNA monomer (partially open conformation)
Authors	:	Buermann, F.; Lowe, J.
Deposited on	:	2021-03-23
Resolution	:	6.50 Å(reported)

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

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

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

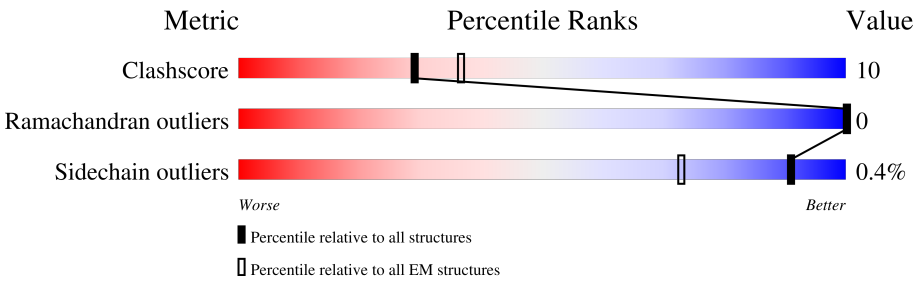
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 6.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1482	8% 76% 22% •
1	B	1482	7% 76% 23% •
2	C	440	20% 55% 21% 24%
2	D	440	• 13% 8% 79%
3	E	240	28% 61% 27% 12%
3	F	240	27% 65% 17% • 18%
4	G	78	14% 62% 31% 8%
4	H	78	5% 67% 26% 8%

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Mol	Chain	Length	Quality of chain
5	I	151	6% 72% 17% 11%
5	J	151	62% 28% 11%
6	K	80	18% 10% 72%
7	L	80	24% 72%
8	M	30	83% 17%
8	N	30	57% 43%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 70851 atoms, of which 34755 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1467	23552	7298	11712	2189	2313	40	0	0
1	B	1467	23553	7298	11713	2189	2313	40	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2
B	1407	GLN	GLU	engineered mutation	UNP A0A0F7LRY2

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	335	5330	1702	2626	470	524	8	0	0
2	D	94	1469	461	736	125	143	4	0	0

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	212	3441	1090	1719	301	322	9	0	0
3	F	198	3246	1029	1627	284	298	8	0	0

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	G	72	1105	349	543	85	127	1	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	H	72	1105	349	543	85	127	1	0	0

- Molecule 5 is a protein called Macrodomain Ter protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	I	134	2272	714	1137	215	202	4	0	0
5	J	135	2288	719	1144	217	204	4	0	0

- Molecule 6 is a DNA chain called matS2 DNA 80 b, oligo FBA769.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	K	22	694	214	249	80	130	21	0	0

- Molecule 7 is a DNA chain called matS2 DNA 80 b, oligo FBA770.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	L	22	702	216	248	84	132	22	0	0

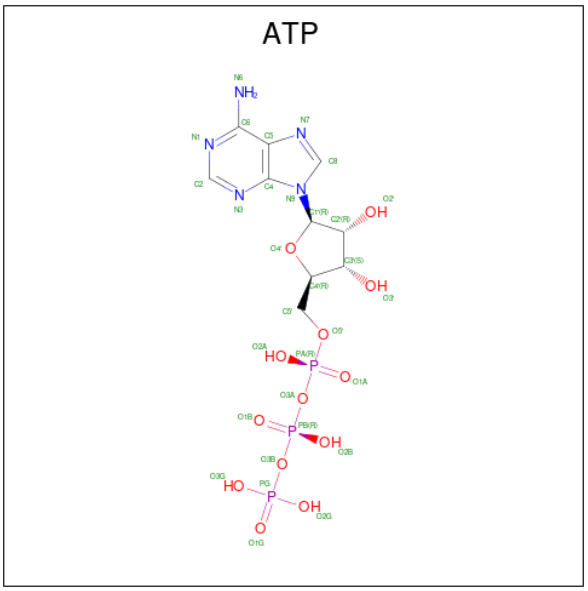
- Molecule 8 is a DNA chain called DNA 80 b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	M	30	961	300	346	105	180	30	0	0
8	N	30	961	300	346	105	180	30	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

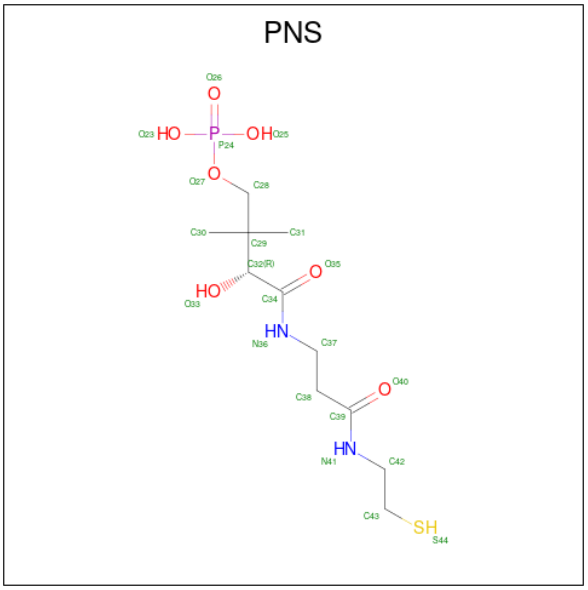
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	A	1	1	1	0
9	B	1	1	1	0

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
10	A	1	43	10	12	5	13	3	0
			Total	C	H	N	O	P	
10	B	1	43	10	12	5	13	3	0

- Molecule 11 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



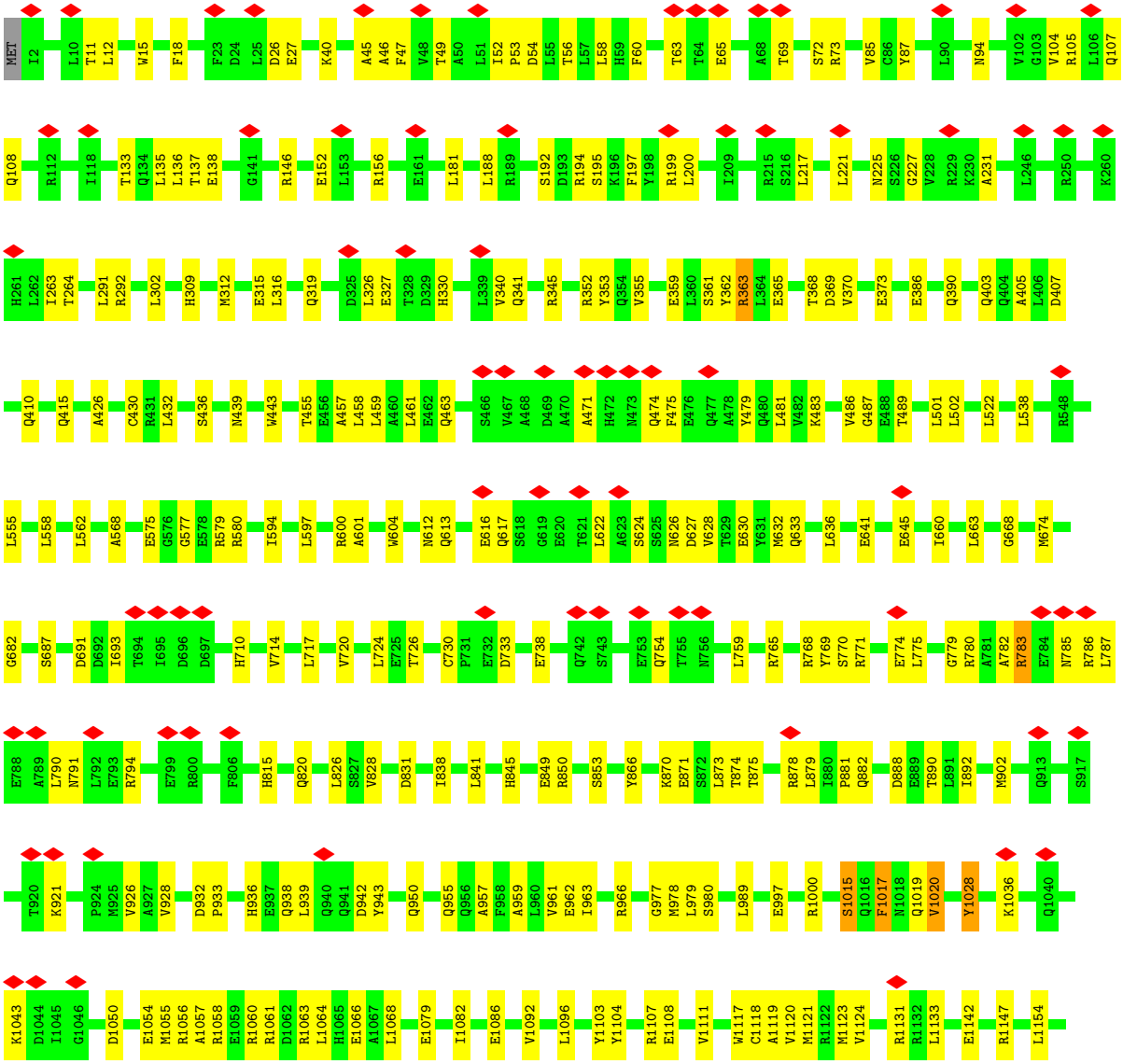
Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
11	G	1	42	11	21	2	6	1	1	0
			Total	C	H	N	O	P	S	
11	H	1	42	11	21	2	6	1	1	0

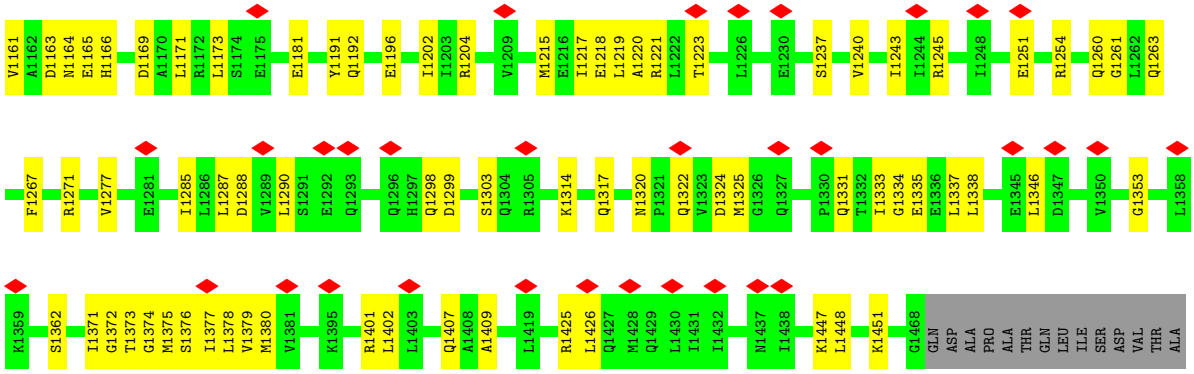
3 Residue-property plots (i)

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

- Molecule 1: Chromosome partition protein MukB

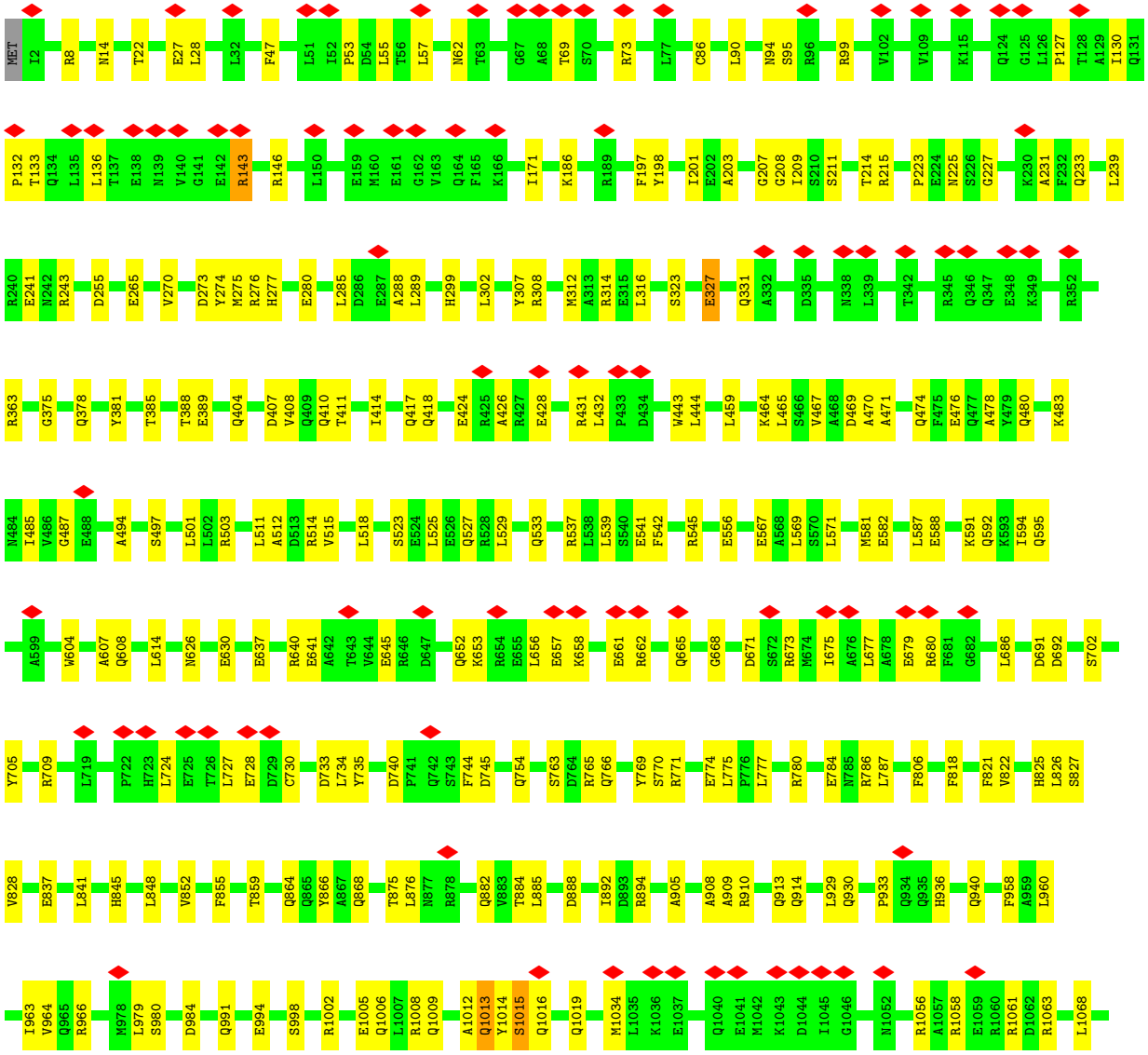
Chain A:

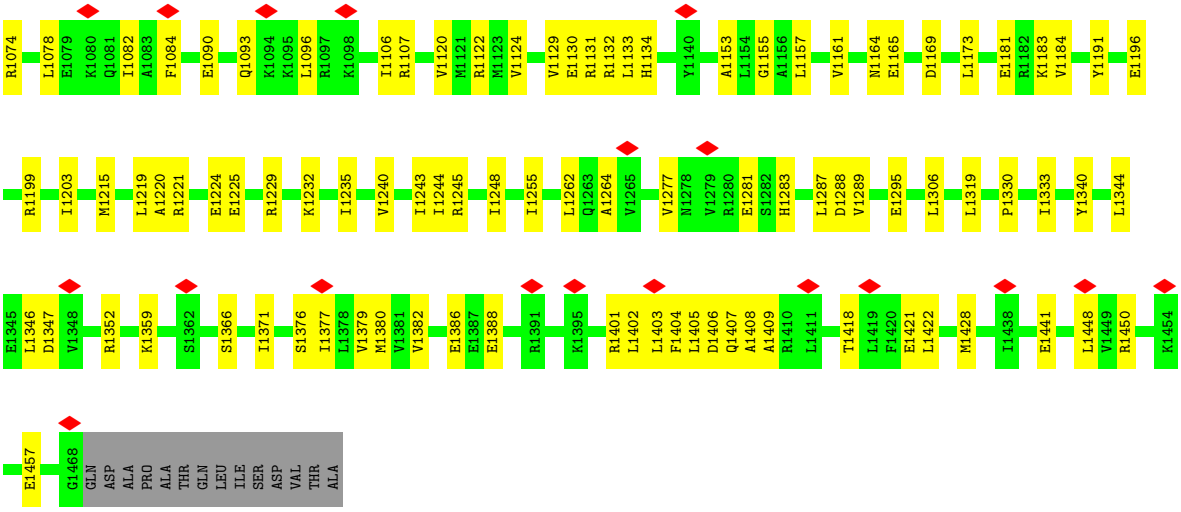




- Molecule 1: Chromosome partition protein MukB

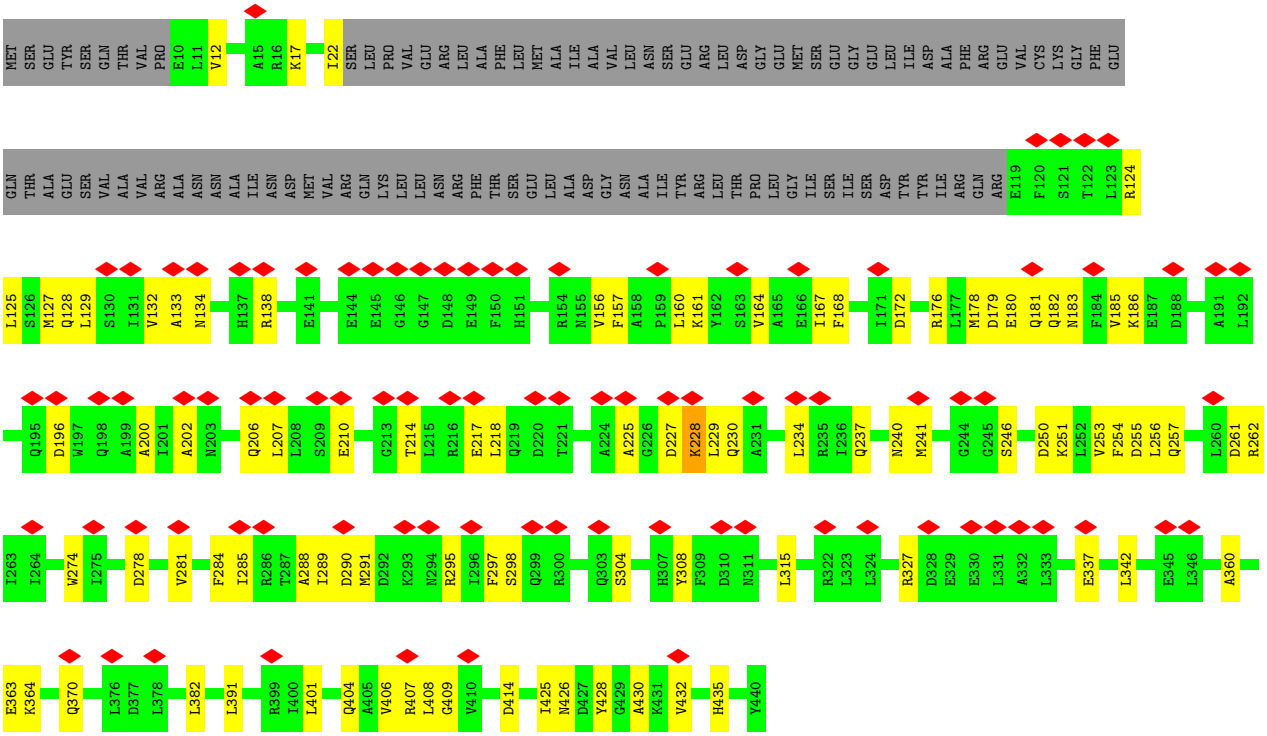
Chain B: 7% 76% 23%





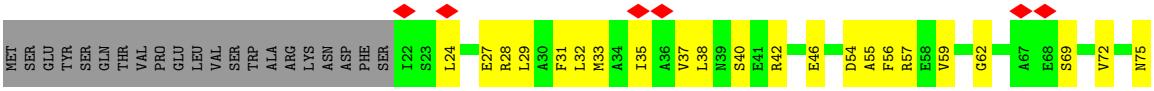
• Molecule 2: Chromosome partition protein MukF

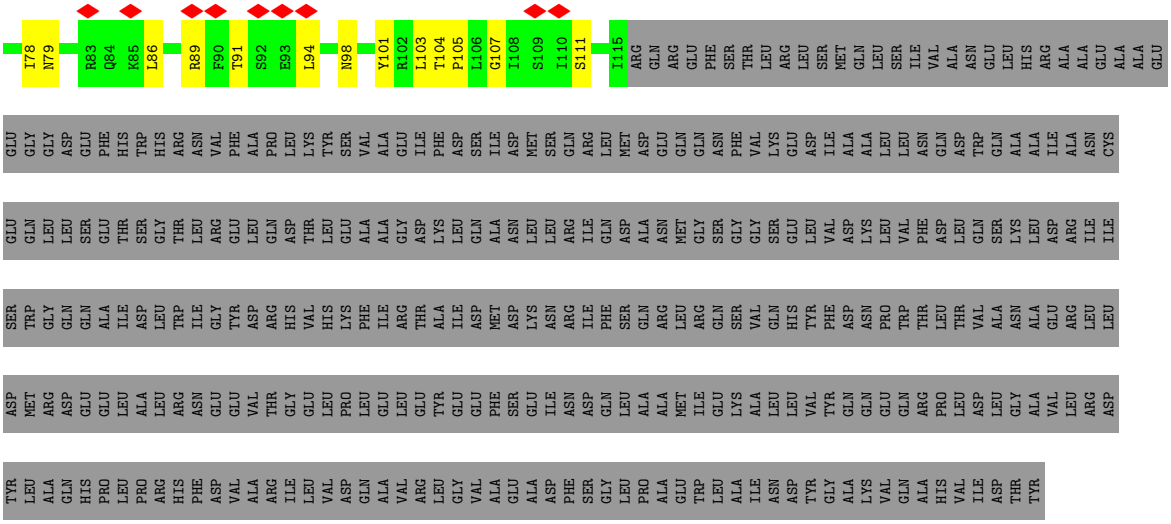
Chain C:



• Molecule 2: Chromosome partition protein MukF

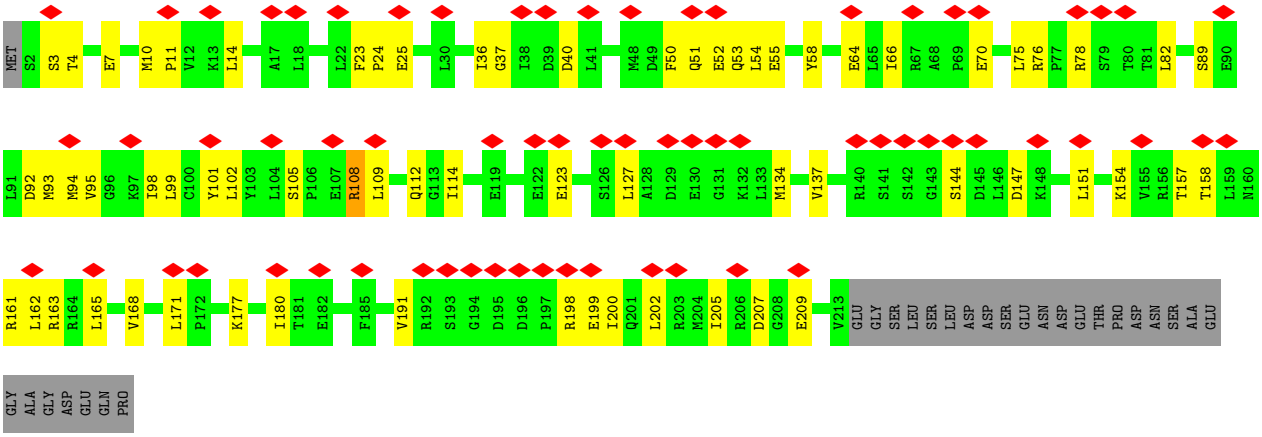
Chain D:





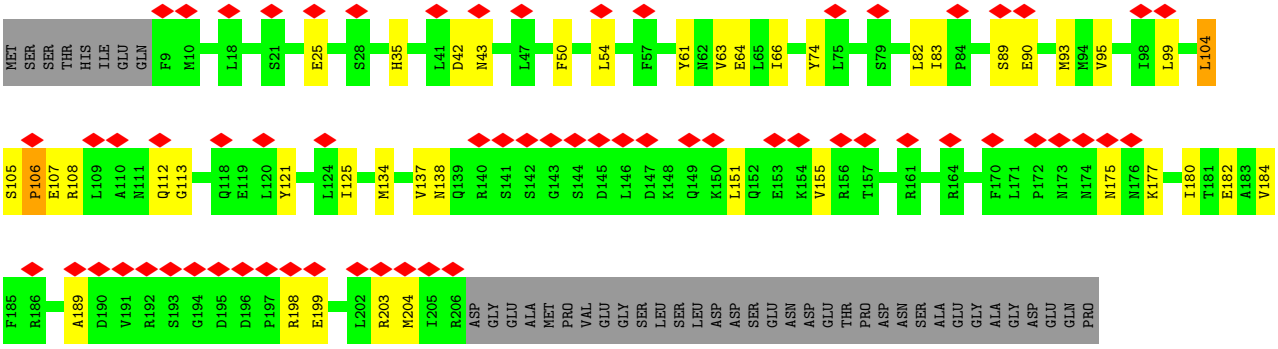
- Molecule 3: Chromosome partition protein MukE

Chain E:



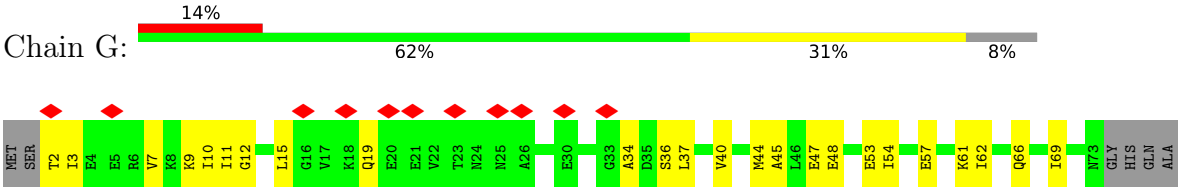
- Molecule 3: Chromosome partition protein MukE

Chain F:



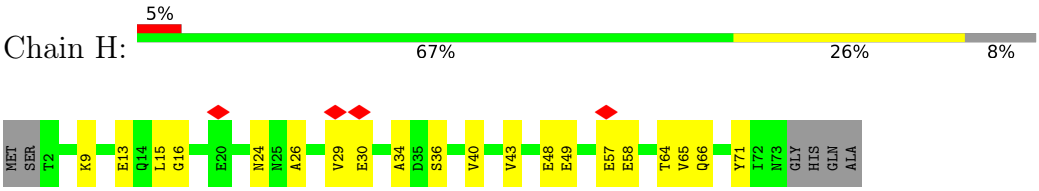
- Molecule 4: Acyl carrier protein

Chain G:



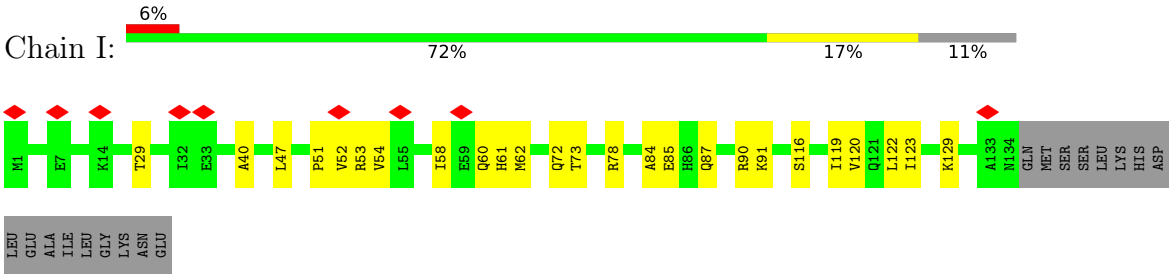
• Molecule 4: Acyl carrier protein

Chain H:



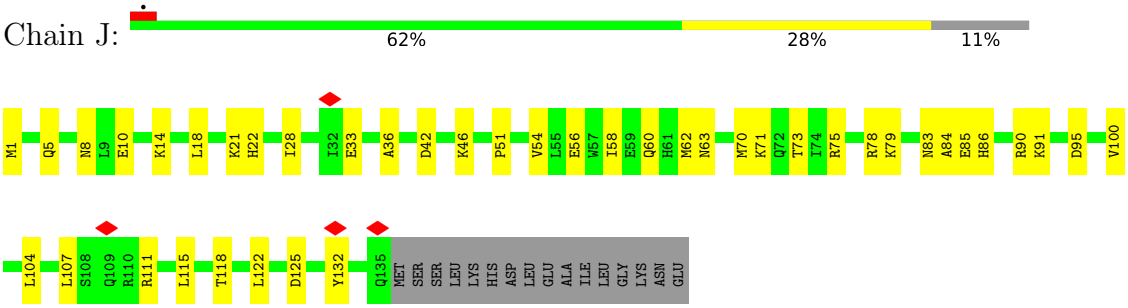
• Molecule 5: Macrodomain Ter protein

Chain I:



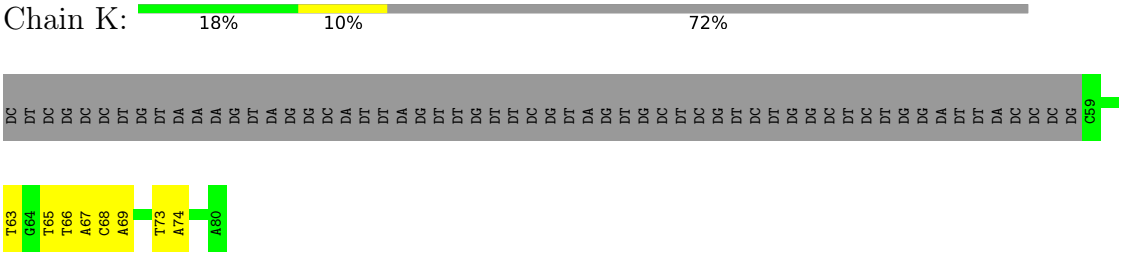
• Molecule 5: Macrodomain Ter protein

Chain J:



• Molecule 6: matS2 DNA 80 b, oligo FBA769

Chain K:

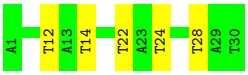


• Molecule 7: matS2 DNA 80 b, oligo FBA770

Chain L:

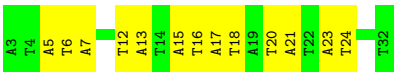
• Molecule 8: DNA 80 b

Chain M:



• Molecule 8: DNA 80 b

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41109	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	462.23843, 462.23843, 462.23843	wwPDB
Map dimensions	318, 318, 318	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45358, 1.45358, 1.45358	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PNS, 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	0.53	15/11999 (0.1%)	0.64	5/16166 (0.0%)
1	B	0.50	11/11999 (0.1%)	0.67	14/16166 (0.1%)
2	C	0.25	0/2753	0.51	0/3727
2	D	0.25	0/741	0.51	0/1000
3	E	0.30	0/1753	0.57	0/2361
3	F	0.27	0/1648	0.62	2/2218 (0.1%)
4	G	0.25	0/565	0.47	0/765
4	H	0.25	0/565	0.44	0/765
5	I	0.26	0/1160	0.54	0/1560
5	J	0.45	2/1169 (0.2%)	0.64	0/1572
6	K	0.52	0/498	0.90	0/766
7	L	0.52	0/509	0.91	0/784
8	M	0.55	0/689	1.04	0/1061
8	N	0.51	0/689	0.98	0/1061
All	All	0.46	28/36737 (0.1%)	0.66	21/49972 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	ARG	CZ-NH1	-7.98	1.22	1.33
1	B	308	ARG	CZ-NH1	-7.79	1.23	1.33
1	A	352	ARG	CZ-NH1	-7.77	1.23	1.33
1	A	345	ARG	CZ-NH1	-7.75	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	ARG	CZ-NH2	-7.50	1.23	1.33
1	A	345	ARG	CZ-NH2	-7.26	1.23	1.33
1	A	352	ARG	CZ-NH2	-7.19	1.23	1.33
1	B	308	ARG	CZ-NH2	-7.17	1.23	1.33
1	A	1020	VAL	CB-CG2	-5.80	1.40	1.52
1	B	381	TYR	CD2-CE2	-5.59	1.30	1.39
1	B	307	TYR	CD2-CE2	-5.59	1.30	1.39
1	A	362	TYR	CD1-CE1	-5.59	1.30	1.39
5	J	132	TYR	CD2-CE2	-5.54	1.31	1.39
1	B	307	TYR	CD1-CE1	-5.53	1.31	1.39
1	B	1014	TYR	CD2-CE2	-5.49	1.31	1.39
5	J	132	TYR	CD1-CE1	-5.49	1.31	1.39
1	B	381	TYR	CD1-CE1	-5.48	1.31	1.39
1	B	1014	TYR	CD1-CE1	-5.48	1.31	1.39
1	A	362	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	361	SER	CB-OG	-5.33	1.35	1.42
1	B	1015	SER	CB-OG	-5.21	1.35	1.42
1	B	375	GLY	N-CA	-5.18	1.38	1.46
1	B	1090	GLU	CB-CG	-5.11	1.42	1.52
1	A	1036	LYS	CE-NZ	-5.10	1.36	1.49
1	A	1015	SER	CB-OG	-5.07	1.35	1.42
1	A	1043	LYS	CE-NZ	-5.07	1.36	1.49
1	A	370	VAL	CB-CG1	-5.03	1.42	1.52
1	A	355	VAL	CB-CG2	-5.01	1.42	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1056	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	362	TYR	CB-CG-CD2	8.19	125.91	121.00
3	F	106	PRO	CA-N-CD	-7.84	100.52	111.50
1	B	307	TYR	CB-CG-CD1	7.64	125.58	121.00
3	F	104	LEU	CA-CB-CG	7.55	132.66	115.30
1	B	363	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	1028	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	B	1084	PHE	CB-CG-CD2	7.10	125.77	120.80
1	B	381	TYR	CB-CG-CD2	7.05	125.23	121.00
1	A	1017	PHE	CB-CG-CD2	6.24	125.17	120.80
1	A	353	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	345	ARG	CD-NE-CZ	5.82	131.75	123.60
1	B	1063	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	314	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	308	ARG	CD-NE-CZ	5.25	130.94	123.60
1	B	1058	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	378	GLN	CA-CB-CG	5.17	124.77	113.40
1	B	1074	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	1013	GLN	CA-CB-CG	5.05	124.51	113.40
1	B	1061	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	381	TYR	CD1-CG-CD2	-5.02	112.37	117.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	TYR	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	11840	11712	11708	252	0
1	B	11840	11713	11707	251	0
2	C	2704	2626	2623	73	0
2	D	733	736	735	26	0
3	E	1722	1719	1718	61	0
3	F	1619	1627	1626	37	0
4	G	562	543	542	20	0
4	H	562	543	542	13	0
5	I	1135	1137	1136	24	0
5	J	1144	1144	1144	32	0
6	K	445	249	250	8	0
7	L	454	248	249	3	0
8	M	615	346	346	5	0
8	N	615	346	346	8	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	31	12	12	3	0
10	B	31	12	12	0	0
11	G	21	21	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	21	21	21	0	0
All	All	36096	34755	34738	726	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 10.

All (726) 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:D:54:ASP:OD1	2:D:57:ARG:NH2	2.00	0.94
5:J:56:GLU:O	5:J:60:GLN:NE2	2.04	0.91
1:A:316:LEU:HD12	1:A:1082:ILE:HD12	1.56	0.88
2:C:262:ARG:NH2	2:D:42:ARG:O	2.07	0.88
5:J:84:ALA:O	5:J:90:ARG:NH1	2.08	0.87
3:E:64:GLU:OE2	3:E:78:ARG:NE	2.07	0.87
4:G:57:GLU:O	4:G:61:LYS:NZ	2.09	0.85
1:A:624:SER:OG	1:A:626:ASN:OD1	1.94	0.85
1:B:591:LYS:O	1:B:595:GLN:NE2	2.10	0.84
2:C:202:ALA:O	2:C:206:GLN:NE2	2.11	0.83
1:A:292:ARG:NH1	1:A:1103:TYR:OH	2.13	0.82
1:B:514:ARG:HE	1:B:518:LEU:HD11	1.43	0.81
1:A:94:ASN:ND2	1:A:181:LEU:O	2.13	0.81
1:A:1245:ARG:NH2	1:A:1288:ASP:OD1	2.14	0.81
1:A:1251:GLU:OE1	1:A:1254:ARG:NH1	2.13	0.81
1:B:255:ASP:OD2	1:B:1199:ARG:NH2	2.14	0.81
1:A:1019:GLN:OE1	1:B:1019:GLN:NE2	2.14	0.80
1:A:720:VAL:O	1:A:724:LEU:N	2.15	0.80
2:C:240:ASN:OD1	2:C:246:SER:OG	2.00	0.79
3:E:92:ASP:OD2	3:E:161:ARG:NH1	2.15	0.79
4:G:66:GLN:NE2	4:G:69:ILE:HD11	1.97	0.79
1:B:469:ASP:OD1	1:B:470:ALA:N	2.16	0.78
1:A:687:SER:O	1:A:691:ASP:N	2.17	0.78
1:B:223:PRO:O	1:B:1340:TYR:OH	2.02	0.78
1:A:771:ARG:NH1	1:B:728:GLU:O	2.18	0.77
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.18	0.77
1:A:461:LEU:HD22	1:A:943:TYR:CE1	2.19	0.77
1:B:8:ARG:NH2	1:B:27:GLU:OE2	2.18	0.77
1:A:73:ARG:NH2	8:M:14:DT:OP1	2.19	0.75
2:C:178:MET:HE3	2:C:218:LEU:HD11	1.67	0.75
1:B:503:ARG:O	1:B:503:ARG:NH1	2.20	0.74
1:A:1015:SER:O	1:A:1019:GLN:NE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:NE2	1:A:1054:GLU:OE2	2.20	0.74
1:A:1142:GLU:N	1:A:1142:GLU:OE1	2.21	0.74
2:C:133:ALA:HB2	2:C:228:LYS:HZ3	1.53	0.74
3:E:123:GLU:OE2	3:E:127:LEU:HD13	1.87	0.74
1:A:200:LEU:HD12	1:A:1378:LEU:HD22	1.69	0.74
1:A:315:GLU:OE1	1:A:319:GLN:NE2	2.20	0.74
2:C:225:ALA:HB1	2:C:228:LYS:HE3	1.70	0.73
1:B:607:ALA:O	1:B:825:HIS:NE2	2.22	0.73
5:I:116:SER:O	5:I:120:VAL:HG23	1.88	0.73
5:I:84:ALA:O	5:I:90:ARG:NH1	2.22	0.72
1:B:273:ASP:OD1	1:B:274:TYR:N	2.22	0.72
3:E:198:ARG:O	3:E:202:LEU:HD13	1.89	0.72
1:A:292:ARG:NH1	4:G:44:MET:SD	2.63	0.71
1:A:152:GLU:OE1	1:A:152:GLU:N	2.22	0.71
1:B:1005:GLU:OE1	1:B:1008:ARG:NH2	2.24	0.71
1:B:677:LEU:HD23	1:B:680:ARG:HH22	1.56	0.70
1:A:1104:TYR:O	1:A:1108:GLU:OE1	2.09	0.70
3:E:98:ILE:HG23	3:E:123:GLU:OE1	1.90	0.70
1:A:575:GLU:OE1	1:A:579:ARG:NH2	2.25	0.70
1:B:511:LEU:HD11	1:B:908:ALA:CB	2.21	0.70
1:A:1451:LYS:NZ	2:C:406:VAL:O	2.20	0.69
3:E:51:GLN:O	3:E:55:GLU:OE1	2.10	0.69
2:C:160:LEU:O	2:C:164:VAL:HG22	1.92	0.69
1:B:626:ASN:O	1:B:630:GLU:OE1	2.10	0.69
1:B:662:ARG:NH1	1:B:671:ASP:OD1	2.26	0.69
1:B:1196:GLU:N	1:B:1196:GLU:OE1	2.25	0.69
3:E:25:GLU:OE2	3:F:82:LEU:HD21	1.93	0.69
1:B:594:ILE:HD12	1:B:845:HIS:CE1	2.28	0.69
1:A:302:LEU:HD22	1:A:1096:LEU:CD1	2.23	0.68
1:A:630:GLU:OE1	1:A:633:GLN:NE2	2.26	0.68
1:A:54:ASP:O	1:A:58:LEU:HD23	1.93	0.68
3:F:63:VAL:HG21	3:F:83:ILE:HD13	1.74	0.68
1:A:765:ARG:NH1	1:B:745:ASP:OD1	2.27	0.68
1:A:45:ALA:HB1	1:A:60:PHE:CE1	2.28	0.68
1:A:1362:SER:O	1:B:62:ASN:ND2	2.27	0.68
10:A:1502:ATP:O3'	1:B:1352:ARG:NH1	2.26	0.68
1:A:771:ARG:NH2	1:B:730:CYS:O	2.27	0.68
1:A:724:LEU:HD11	1:B:769:TYR:CD1	2.28	0.67
1:B:709:ARG:HB3	1:B:777:LEU:HD23	1.76	0.67
1:B:653:LYS:O	1:B:657:GLU:OE1	2.12	0.67
1:A:878:ARG:NH1	1:B:882:GLN:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:158:THR:O	3:E:162:LEU:HD23	1.94	0.67
2:C:327:ARG:NH2	8:N:7:DA:OP1	2.26	0.67
1:B:316:LEU:HD21	1:B:1078:LEU:CB	2.25	0.66
1:B:514:ARG:NE	1:B:518:LEU:HD11	2.11	0.66
3:E:134:MET:HE2	3:E:147:ASP:HB3	1.78	0.66
1:B:22:THR:OG1	1:B:133:THR:OG1	2.12	0.66
1:B:426:ALA:HB3	1:B:963:ILE:HD11	1.78	0.66
1:B:1240:VAL:O	1:B:1244:ILE:HD12	1.95	0.66
3:F:42:ASP:OD1	3:F:43:ASN:N	2.27	0.66
1:A:890:THR:HB	1:A:892:ILE:HG23	1.78	0.66
2:C:22:ILE:O	2:D:24:LEU:N	2.29	0.66
2:D:35:ILE:HG22	2:D:103:LEU:HD21	1.76	0.66
1:A:133:THR:O	1:A:137:THR:OG1	2.10	0.65
1:A:938:GLN:NE2	1:A:942:ASP:OD2	2.29	0.65
1:B:1450:ARG:NH1	1:B:1457:GLU:OE1	2.29	0.65
1:A:849:GLU:OE1	1:A:850:ARG:NH2	2.30	0.65
1:A:600:ARG:NH2	1:A:831:ASP:OD2	2.30	0.65
1:A:1331:GLN:O	1:A:1335:GLU:OE1	2.15	0.65
1:A:1163:ASP:OD1	1:A:1164:ASN:N	2.29	0.65
1:B:55:LEU:HD22	8:M:22:DT:H5”	1.79	0.65
1:B:73:ARG:NH2	8:N:16:DT:OP1	2.29	0.65
1:A:326:LEU:O	1:A:330:HIS:ND1	2.26	0.64
3:E:10:MET:SD	3:E:14:LEU:HD22	2.38	0.64
1:A:1124:VAL:HG21	1:A:1133:LEU:HD12	1.78	0.64
3:E:7:GLU:N	3:E:7:GLU:OE1	2.31	0.64
1:A:636:LEU:HD21	1:A:815:HIS:CE1	2.32	0.64
1:B:99:ARG:NH1	1:B:127:PRO:O	2.31	0.64
1:B:241:GLU:OE2	1:B:1229:ARG:NH2	2.31	0.64
2:C:414:ASP:OD1	2:C:435:HIS:ND1	2.30	0.64
1:A:959:ALA:O	1:A:963:ILE:HD12	1.96	0.64
1:B:556:GLU:OE1	1:B:882:GLN:NE2	2.30	0.64
2:C:227:ASP:OD1	2:C:228:LYS:N	2.31	0.64
3:E:98:ILE:HD12	3:E:123:GLU:OE1	1.98	0.64
1:A:107:GLN:NE2	1:A:108:GLN:O	2.31	0.63
1:A:828:VAL:HG12	1:A:828:VAL:O	1.97	0.63
1:A:997:GLU:OE1	1:A:1000:ARG:NH2	2.30	0.63
1:A:775:LEU:O	1:A:780:ARG:NH1	2.30	0.63
1:A:626:ASN:OD1	1:A:627:ASP:N	2.30	0.63
3:F:189:ALA:HB2	3:F:204:MET:HG3	1.81	0.63
1:A:597:LEU:O	1:A:601:ALA:N	2.31	0.63
1:B:675:ILE:O	1:B:679:GLU:OE1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:LEU:HD21	1:B:705:TYR:CD2	2.34	0.63
1:B:1220:ALA:O	1:B:1224:GLU:OE1	2.16	0.63
3:E:144:SER:OG	3:E:147:ASP:OD1	2.17	0.62
1:B:641:GLU:O	1:B:645:GLU:OE1	2.18	0.62
3:F:104:LEU:HG	3:F:106:PRO:CD	2.30	0.62
1:B:1441:GLU:N	1:B:1441:GLU:OE1	2.32	0.62
2:C:178:MET:CE	2:C:218:LEU:HD11	2.30	0.62
1:A:693:ILE:HG22	1:A:779:GLY:N	2.15	0.62
3:F:137:VAL:HG23	3:F:138:ASN:H	1.64	0.62
1:A:663:LEU:HD11	1:A:790:LEU:HD13	1.82	0.61
1:B:285:LEU:O	1:B:289:LEU:HD23	1.99	0.61
3:E:137:VAL:HG13	3:E:154:LYS:HD3	1.82	0.61
1:A:188:LEU:HD23	1:A:194:ARG:HA	1.82	0.61
3:E:98:ILE:O	3:E:102:LEU:HD23	2.01	0.61
1:A:1192:GLN:NE2	1:A:1196:GLU:OE2	2.34	0.61
3:E:70:GLU:N	3:E:70:GLU:OE1	2.32	0.61
5:J:21:LYS:NZ	7:L:14:DT:OP1	2.23	0.61
1:B:691:ASP:OD1	1:B:692:ASP:N	2.34	0.61
1:B:709:ARG:CB	1:B:777:LEU:HD23	2.31	0.61
2:C:281:VAL:HG22	3:E:109:LEU:HD21	1.83	0.61
1:B:197:PHE:O	1:B:201:ILE:HD12	2.01	0.61
2:C:382:LEU:HD21	2:C:401:LEU:HD22	1.82	0.61
1:B:47:PHE:CE1	1:B:90:LEU:HD11	2.36	0.61
1:A:594:ILE:HD12	1:A:845:HIS:CE1	2.36	0.61
5:I:72:GLN:NE2	6:K:74:DA:OP2	2.34	0.60
1:A:754:GLN:HG3	1:B:724:LEU:HD23	1.82	0.60
3:F:50:PHE:O	3:F:54:LEU:HD23	2.01	0.60
1:B:1221:ARG:O	1:B:1225:GLU:OE1	2.19	0.60
1:B:424:GLU:O	1:B:428:GLU:OE1	2.19	0.60
1:B:1295:GLU:OE1	1:B:1295:GLU:N	2.32	0.60
1:A:977:GLY:O	1:A:980:SER:OG	2.16	0.60
1:B:14:ASN:ND2	1:B:86:CYS:SG	2.74	0.60
1:B:661:GLU:OE1	1:B:662:ARG:NH2	2.34	0.60
1:A:1322:GLN:N	1:A:1322:GLN:OE1	2.33	0.60
1:A:231:ALA:HB1	1:A:1240:VAL:HG22	1.84	0.60
1:A:315:GLU:O	1:A:319:GLN:NE2	2.35	0.60
1:A:1299:ASP:O	1:A:1303:SER:OG	2.19	0.59
1:A:594:ILE:HG23	1:A:838:ILE:HG23	1.82	0.59
1:A:1401:ARG:NH2	1:A:1426:LEU:O	2.35	0.59
5:I:60:GLN:HG3	5:I:61:HIS:ND1	2.17	0.59
2:C:297:PHE:HE1	3:E:191:VAL:HG23	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:47:LEU:HD21	5:I:54:VAL:HA	1.83	0.59
1:A:1107:ARG:NH1	4:G:47:GLU:OE2	2.34	0.59
1:B:1248:ILE:HG23	1:B:1344:LEU:HD21	1.83	0.59
3:E:50:PHE:O	3:E:54:LEU:HD23	2.03	0.59
4:H:24:ASN:O	4:H:66:GLN:N	2.36	0.58
1:B:276:ARG:O	1:B:280:GLU:OE1	2.20	0.58
1:B:1289:VAL:HG21	1:B:1319:LEU:HD22	1.84	0.58
1:B:316:LEU:HD21	1:B:1078:LEU:HB2	1.85	0.58
1:B:316:LEU:HD21	1:B:1078:LEU:HB3	1.85	0.58
2:C:179:ASP:HA	2:C:182:GLN:HG2	1.85	0.58
1:A:403:GLN:N	1:B:407:ASP:OD2	2.36	0.58
1:A:1181:GLU:OE1	1:A:1181:GLU:N	2.34	0.58
1:B:1181:GLU:OE1	1:B:1181:GLU:N	2.34	0.58
5:I:47:LEU:HD11	5:I:53:ARG:HB2	1.84	0.58
1:A:459:LEU:HD23	1:A:463:GLN:OE1	2.04	0.58
1:A:1277:VAL:HG22	1:A:1346:LEU:CD2	2.33	0.58
1:A:1056:ARG:O	1:A:1060:ARG:NE	2.34	0.58
1:B:426:ALA:CB	1:B:963:ILE:HD11	2.34	0.57
2:C:133:ALA:HB2	2:C:228:LYS:NZ	2.19	0.57
1:B:1132:ARG:NH1	1:B:1191:TYR:OH	2.38	0.57
3:E:36:ILE:HG23	3:E:40:ASP:OD2	2.03	0.57
2:C:290:ASP:OD1	2:C:291:MET:N	2.36	0.57
3:F:180:ILE:HG23	3:F:184:VAL:HG21	1.86	0.57
1:A:1117:TRP:HB3	1:A:1121:MET:HE1	1.85	0.57
1:A:1324:ASP:OD1	1:A:1325:MET:N	2.38	0.57
1:B:22:THR:HG1	1:B:133:THR:HG1	1.51	0.57
1:B:497:SER:O	1:B:501:LEU:HD13	2.04	0.57
5:J:14:LYS:O	5:J:18:LEU:HD23	2.05	0.57
1:A:263:ILE:HD11	1:A:1191:TYR:CE1	2.39	0.57
1:A:1333:ILE:O	1:A:1337:LEU:HD23	2.05	0.57
1:B:47:PHE:HE1	1:B:90:LEU:HD11	1.69	0.57
1:A:738:GLU:O	1:B:765:ARG:NH1	2.34	0.56
2:C:285:ILE:HD13	2:C:289:ILE:HD12	1.87	0.56
5:I:122:LEU:O	5:I:122:LEU:HD23	2.05	0.56
1:B:991:GLN:NE2	1:B:994:GLU:OE1	2.37	0.56
1:A:1271:ARG:NH2	1:A:1353:GLY:O	2.39	0.56
1:B:209:ILE:HG23	1:B:214:THR:HG21	1.88	0.56
1:B:1130:GLU:N	1:B:1130:GLU:OE1	2.39	0.56
1:B:186:LYS:NZ	1:B:1388:GLU:OE2	2.38	0.56
1:A:312:MET:HB3	1:A:1082:ILE:HD11	1.88	0.56
5:J:10:GLU:OE2	5:J:78:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:107:GLU:OE2	3:F:113:GLY:N	2.36	0.56
1:B:302:LEU:HD13	1:B:1093:GLN:CG	2.36	0.56
3:F:182:GLU:OE1	3:F:182:GLU:N	2.37	0.56
1:B:1281:GLU:N	1:B:1281:GLU:OE1	2.37	0.56
1:A:668:GLY:O	1:A:783:ARG:NH2	2.39	0.56
1:B:404:GLN:O	1:B:408:VAL:HG23	2.05	0.56
2:C:382:LEU:CD2	2:C:401:LEU:HD22	2.36	0.56
3:F:106:PRO:HD2	3:F:107:GLU:H	1.71	0.56
1:B:774:GLU:OE1	1:B:774:GLU:N	2.37	0.55
5:I:58:ILE:HG23	5:I:62:MET:HE2	1.87	0.55
1:A:769:TYR:OH	1:B:727:LEU:O	2.23	0.55
1:A:1117:TRP:O	1:A:1120:VAL:HG22	2.05	0.55
1:A:15:TRP:CZ3	1:A:46:ALA:HB2	2.42	0.55
1:B:385:THR:O	1:B:389:GLU:OE1	2.25	0.55
1:A:69:THR:OG1	1:B:215:ARG:NH2	2.36	0.55
5:J:71:LYS:O	5:J:75:ARG:NH1	2.39	0.55
1:B:73:ARG:NH1	8:N:15:DA:O3'	2.38	0.55
1:B:525:LEU:HD11	1:B:892:ILE:HD12	1.88	0.55
1:B:821:PHE:O	1:B:825:HIS:HB2	2.06	0.55
1:A:415:GLN:NE2	1:B:958:PHE:CZ	2.75	0.55
1:A:1164:ASN:OD1	1:A:1165:GLU:N	2.39	0.55
1:B:494:ALA:HB1	1:B:929:LEU:HD22	1.89	0.55
3:E:66:ILE:HD13	3:E:76:ARG:NH2	2.22	0.55
4:H:36:SER:O	4:H:40:VAL:HG23	2.07	0.55
1:A:200:LEU:HD12	1:A:1378:LEU:CD2	2.35	0.54
1:A:939:LEU:HG	1:A:943:TYR:CZ	2.42	0.54
1:B:828:VAL:HG12	1:B:828:VAL:O	2.07	0.54
1:B:1203:ILE:O	1:B:1203:ILE:HG22	2.06	0.54
1:A:481:LEU:HD21	1:A:921:LYS:HE3	1.89	0.54
2:D:91:THR:HG21	3:E:112:GLN:HB3	1.88	0.54
1:B:587:LEU:HD13	1:B:848:LEU:HD22	1.88	0.54
2:C:230:GLN:O	2:C:234:LEU:HD23	2.07	0.54
8:N:5:DA:H2'	8:N:6:DT:H71	1.90	0.54
1:A:316:LEU:HD13	1:A:1079:GLU:HG3	1.89	0.54
5:J:62:MET:SD	5:J:63:ASN:O	2.65	0.54
2:C:181:GLN:O	2:C:181:GLN:NE2	2.40	0.54
1:B:302:LEU:HD13	1:B:1093:GLN:HG2	1.90	0.54
1:B:1377:ILE:HD13	1:B:1380:MET:CE	2.37	0.54
3:F:121:TYR:CZ	3:F:125:ILE:HD11	2.43	0.54
1:A:461:LEU:HD13	1:A:943:TYR:CD1	2.42	0.54
1:B:1009:GLN:O	1:B:1013:GLN:OE1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1232:LYS:O	1:B:1235:ILE:HG22	2.08	0.54
1:A:365:GLU:O	1:A:368:THR:OG1	2.22	0.54
1:B:1418:THR:O	1:B:1422:LEU:HD23	2.08	0.54
2:C:404:GLN:OE1	2:C:407:ARG:NH2	2.36	0.54
3:E:52:GLU:OE1	3:E:52:GLU:N	2.30	0.54
3:E:99:LEU:HD22	3:E:180:ILE:CD1	2.38	0.54
5:I:91:LYS:HB3	5:J:95:ASP:OD1	2.08	0.54
3:F:151:LEU:O	3:F:155:VAL:HG23	2.08	0.53
1:A:1277:VAL:HG22	1:A:1346:LEU:HD23	1.91	0.53
3:E:99:LEU:HD22	3:E:180:ILE:HD11	1.90	0.53
3:F:198:ARG:HD2	3:F:198:ARG:N	2.24	0.53
1:B:1262:LEU:HD23	1:B:1264:ALA:H	1.72	0.53
2:C:180:GLU:OE2	2:D:104:THR:OG1	2.14	0.53
2:C:315:LEU:H	3:E:93:MET:CE	2.21	0.53
2:D:46:GLU:N	2:D:46:GLU:OE1	2.42	0.53
1:A:682:GLY:O	1:A:714:VAL:HG13	2.08	0.53
1:A:1409:ALA:HB1	1:B:1409:ALA:HB1	1.90	0.53
1:B:288:ALA:HB2	1:B:1106:ILE:HG22	1.90	0.53
1:A:40:LYS:NZ	10:A:1502:ATP:O3G	2.35	0.53
1:A:359:GLU:OE2	1:A:363:ARG:NH1	2.36	0.53
5:J:115:LEU:N	6:K:67:DA:OP1	2.31	0.53
1:A:52:ILE:O	1:A:58:LEU:HD21	2.08	0.53
1:A:759:LEU:HB2	1:B:724:LEU:HD21	1.90	0.53
1:A:1118:CYS:HA	1:A:1121:MET:HE2	1.90	0.53
2:C:133:ALA:CB	2:C:228:LYS:HZ3	2.20	0.53
1:A:871:GLU:O	1:A:875:THR:HG23	2.09	0.53
1:A:1218:GLU:OE1	1:A:1221:ARG:NH2	2.42	0.53
3:F:105:SER:HB3	3:F:198:ARG:NH2	2.23	0.53
1:B:273:ASP:OD2	1:B:1183:LYS:NZ	2.31	0.53
2:C:124:ARG:O	2:C:128:GLN:OE1	2.27	0.53
1:A:613:GLN:O	1:A:617:GLN:N	2.40	0.52
1:B:57:LEU:HD23	1:B:198:TYR:HB2	1.92	0.52
1:B:525:LEU:CD1	1:B:892:ILE:HD12	2.39	0.52
3:E:82:LEU:HD11	3:F:25:GLU:OE1	2.08	0.52
1:B:444:LEU:HA	1:B:960:LEU:HD13	1.91	0.52
1:B:910:ARG:NH1	1:B:914:GLN:OE1	2.42	0.52
5:I:122:LEU:HD22	5:J:122:LEU:HB3	1.90	0.52
1:A:632:MET:SD	1:B:826:LEU:HD13	2.49	0.52
1:B:444:LEU:HD22	1:B:964:VAL:HG21	1.90	0.52
5:J:28:ILE:O	5:J:63:ASN:N	2.41	0.52
1:A:1261:GLY:O	1:A:1425:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:O	1:B:431:ARG:NH1	2.43	0.52
1:B:494:ALA:CB	1:B:929:LEU:HD22	2.40	0.52
3:F:134:MET:O	3:F:138:ASN:N	2.42	0.52
1:A:1050:ASP:O	1:A:1054:GLU:N	2.35	0.52
1:A:1060:ARG:O	1:A:1063:ARG:HG3	2.09	0.52
2:C:370:GLN:HB2	2:C:408:LEU:HD23	1.90	0.52
1:A:302:LEU:HD22	1:A:1096:LEU:HD12	1.90	0.52
1:A:1055:MET:SD	1:A:1056:ARG:NH1	2.82	0.52
1:B:1245:ARG:NH2	1:B:1288:ASP:OD1	2.41	0.52
3:F:121:TYR:CE2	3:F:125:ILE:HD11	2.45	0.52
1:A:612:ASN:O	1:A:616:GLU:N	2.38	0.52
1:B:775:LEU:HG	1:B:786:ARG:HD3	1.92	0.51
3:F:105:SER:N	3:F:106:PRO:HD3	2.24	0.51
1:B:273:ASP:O	1:B:277:HIS:ND1	2.37	0.51
3:E:154:LYS:O	3:E:158:THR:HG23	2.11	0.51
1:B:47:PHE:CD2	1:B:1404:PHE:HZ	2.28	0.51
1:A:1154:LEU:HD11	1:A:1171:LEU:HD21	1.93	0.51
4:G:57:GLU:OE1	4:G:57:GLU:N	2.44	0.51
1:B:1386:GLU:OE2	1:B:1401:ARG:NE	2.43	0.51
1:B:1405:LEU:HD21	1:B:1408:ALA:HA	1.91	0.51
2:C:196:ASP:HB2	2:C:200:ALA:HB2	1.91	0.51
4:G:53:GLU:O	4:G:54:ILE:HD13	2.10	0.51
1:A:188:LEU:HD12	1:A:188:LEU:N	2.25	0.51
1:A:486:VAL:CG2	1:A:501:LEU:HD21	2.41	0.51
2:D:98:ASN:CG	3:E:171:LEU:HD13	2.31	0.51
2:D:38:LEU:O	2:D:42:ARG:N	2.44	0.51
1:B:1347:ASP:OD2	1:B:1359:LYS:NZ	2.43	0.51
5:I:60:GLN:HG3	5:I:61:HIS:CE1	2.46	0.51
1:A:730:CYS:O	1:B:771:ARG:NH2	2.43	0.51
1:B:1402:LEU:O	1:B:1403:LEU:HD12	2.11	0.51
1:A:459:LEU:HD11	1:B:471:ALA:N	2.27	0.50
1:A:622:LEU:HD12	1:A:628:VAL:HA	1.93	0.50
2:C:426:ASN:OD1	2:C:430:ALA:HB3	2.12	0.50
5:I:29:THR:HG21	5:I:40:ALA:HB3	1.92	0.50
1:B:1283:HIS:O	1:B:1287:LEU:HD23	2.12	0.50
2:C:251:LYS:O	2:C:255:ASP:N	2.42	0.50
2:D:69:SER:OG	2:D:72:VAL:HG12	2.10	0.50
3:F:63:VAL:HG21	3:F:83:ILE:CD1	2.41	0.50
3:F:89:SER:O	3:F:93:MET:SD	2.70	0.50
1:A:405:ALA:O	1:B:418:GLN:NE2	2.43	0.50
1:A:430:CYS:SG	1:A:432:LEU:HD12	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1240:VAL:O	1:B:1243:ILE:HG22	2.11	0.50
3:E:76:ARG:NH1	3:E:207:ASP:O	2.44	0.50
1:A:1217:ILE:HD11	1:B:806:PHE:CE2	2.47	0.50
1:A:1451:LYS:NZ	2:C:409:GLY:O	2.45	0.50
2:C:12:VAL:HG11	2:D:62:GLY:HA3	1.93	0.50
1:A:1220:ALA:O	1:A:1223:THR:OG1	2.26	0.50
1:B:476:GLU:O	1:B:480:GLN:OE1	2.30	0.50
1:B:542:PHE:CE2	1:B:876:LEU:HD21	2.46	0.50
3:F:106:PRO:HD2	3:F:107:GLU:N	2.27	0.50
1:A:65:GLU:OE2	1:B:211:SER:N	2.44	0.50
1:A:826:LEU:HD21	1:B:827:SER:HA	1.94	0.50
1:A:54:ASP:OD1	1:A:56:THR:OG1	2.24	0.50
1:A:455:THR:HG22	1:A:950:GLN:OE1	2.11	0.50
1:B:1161:VAL:HG12	1:B:1161:VAL:O	2.11	0.50
1:B:57:LEU:HD23	1:B:198:TYR:CB	2.42	0.50
1:A:1124:VAL:CG2	1:A:1133:LEU:HD12	2.42	0.49
2:C:297:PHE:CE1	3:E:191:VAL:HG23	2.46	0.49
8:N:23:DA:C8	8:N:24:DT:H72	2.47	0.49
1:A:717:LEU:HD21	1:A:738:GLU:HB2	1.93	0.49
1:B:884:THR:O	1:B:888:ASP:N	2.39	0.49
4:G:2:THR:OG1	4:G:3:ILE:N	2.43	0.49
1:B:607:ALA:HB1	1:B:825:HIS:CE1	2.47	0.49
1:A:15:TRP:N	1:A:18:PHE:O	2.42	0.49
2:D:56:PHE:HA	2:D:59:VAL:HG22	1.93	0.49
2:C:124:ARG:O	2:C:127:MET:HG2	2.12	0.49
10:A:1502:ATP:O1G	1:B:1366:SER:OG	2.30	0.49
2:C:183:ASN:HA	2:C:186:LYS:HE2	1.93	0.49
1:A:604:TRP:NE1	1:A:831:ASP:O	2.41	0.49
3:E:52:GLU:OE2	3:E:53:GLN:NE2	2.45	0.49
3:E:102:LEU:HD13	3:E:108:ARG:HE	1.78	0.49
5:J:22:HIS:HB2	5:J:28:ILE:HD13	1.94	0.49
1:A:457:ALA:O	1:A:461:LEU:HG	2.12	0.49
1:B:55:LEU:O	1:B:55:LEU:HD23	2.12	0.49
1:B:822:VAL:HB	1:B:826:LEU:HD11	1.94	0.49
1:A:410:GLN:HA	1:A:979:LEU:HD22	1.95	0.49
1:A:1056:ARG:C	1:A:1060:ARG:HE	2.15	0.49
1:A:1068:LEU:C	1:A:1068:LEU:HD23	2.33	0.49
3:E:134:MET:HE1	3:E:137:VAL:HG11	1.94	0.49
3:F:137:VAL:HG23	3:F:138:ASN:N	2.26	0.49
4:G:62:ILE:HG22	4:G:62:ILE:O	2.12	0.49
2:C:179:ASP:O	2:C:182:GLN:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:391:LEU:HD13	2:C:428:TYR:CD2	2.47	0.48
1:A:87:TYR:CG	1:A:136:LEU:HD23	2.48	0.48
1:B:464:LYS:HA	1:B:467:VAL:HG22	1.94	0.48
1:A:461:LEU:HD22	1:A:943:TYR:HE1	1.75	0.48
1:B:94:ASN:OD1	1:B:95:SER:N	2.46	0.48
1:B:1012:ALA:O	1:B:1016:GLN:OE1	2.32	0.48
1:B:537:ARG:O	1:B:541:GLU:OE1	2.32	0.48
1:B:1164:ASN:OD1	1:B:1165:GLU:N	2.47	0.48
2:C:125:LEU:O	2:C:129:LEU:HD23	2.14	0.48
3:E:37:GLY:O	3:E:40:ASP:OD1	2.30	0.48
1:B:930:GLN:OE1	1:B:930:GLN:N	2.47	0.48
1:B:1153:ALA:O	1:B:1157:LEU:HD13	2.13	0.48
4:G:11:ILE:HG23	4:G:12:GLY:N	2.29	0.48
1:B:515:VAL:HG22	1:B:905:ALA:HB1	1.94	0.48
2:D:31:PHE:HE1	2:D:55:ALA:HB3	1.77	0.48
1:B:542:PHE:CD2	1:B:876:LEU:HD21	2.49	0.48
2:C:285:ILE:CD1	2:C:289:ILE:HD12	2.43	0.48
4:G:66:GLN:HE22	4:G:69:ILE:HD11	1.75	0.48
1:A:785:ASN:OD1	1:A:786:ARG:NH1	2.47	0.48
3:E:10:MET:SD	3:E:11:PRO:HD2	2.54	0.48
3:E:161:ARG:O	3:E:165:LEU:HD23	2.14	0.48
1:A:217:LEU:HG	1:A:221:LEU:HD12	1.95	0.48
1:A:461:LEU:O	1:A:943:TYR:CE2	2.66	0.48
2:D:104:THR:OG1	2:D:105:PRO:HD2	2.14	0.48
3:E:101:TYR:O	3:E:105:SER:N	2.47	0.48
4:H:58:GLU:OE1	4:H:71:TYR:OH	2.22	0.48
1:B:299:HIS:HA	1:B:1096:LEU:HD11	1.96	0.48
1:A:769:TYR:O	1:B:734:LEU:N	2.46	0.47
1:A:962:GLU:OE1	1:A:966:ARG:NH2	2.47	0.47
1:B:483:LYS:O	1:B:487:GLY:N	2.47	0.47
2:C:134:ASN:OD1	2:C:138:ARG:NH1	2.47	0.47
2:C:281:VAL:HG22	3:E:109:LEU:CD2	2.42	0.47
1:A:849:GLU:OE2	1:A:853:SER:OG	2.33	0.47
1:A:1285:ILE:HD11	1:A:1320:ASN:OD1	2.14	0.47
1:A:1334:GLY:O	1:A:1338:LEU:HD23	2.13	0.47
1:B:1122:ARG:HD3	4:H:16:GLY:O	2.15	0.47
3:F:104:LEU:HG	3:F:106:PRO:HD2	1.95	0.47
1:A:458:LEU:HD22	1:B:467:VAL:HG11	1.97	0.47
1:A:1245:ARG:CG	1:A:1287:LEU:HD21	2.44	0.47
1:B:233:GLN:HG2	2:D:94:LEU:HD13	1.95	0.47
2:C:214:THR:O	2:C:217:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:O	1:A:487:GLY:N	2.43	0.47
1:A:502:LEU:CD1	1:A:926:VAL:HG21	2.45	0.47
1:A:768:ARG:NE	1:B:733:ASP:OD1	2.47	0.47
1:A:1374:GLY:O	1:A:1378:LEU:HG	2.15	0.47
1:B:511:LEU:HD12	1:B:512:ALA:N	2.30	0.47
1:B:1012:ALA:O	1:B:1015:SER:OG	2.11	0.47
3:E:202:LEU:HA	3:E:205:ILE:HG22	1.96	0.47
5:I:51:PRO:HA	5:I:54:VAL:HG12	1.97	0.47
1:A:199:ARG:NH1	8:M:12:DT:OP1	2.42	0.47
1:B:243:ARG:NH2	1:B:1306:LEU:O	2.47	0.47
4:H:9:LYS:HZ1	4:H:49:GLU:CD	2.18	0.47
1:A:939:LEU:HD21	1:A:943:TYR:CE2	2.50	0.47
1:B:733:ASP:OD2	1:B:735:TYR:OH	2.22	0.47
1:B:1402:LEU:C	1:B:1403:LEU:HD12	2.35	0.47
1:A:636:LEU:HD21	1:A:815:HIS:HE1	1.79	0.47
1:A:1260:GLN:O	1:A:1263:GLN:NE2	2.48	0.46
1:B:1107:ARG:NE	4:H:48:GLU:OE1	2.48	0.46
3:F:175:ASN:OD1	3:F:177:LYS:HE3	2.15	0.46
1:A:555:LEU:HD11	1:A:558:LEU:HD22	1.97	0.46
1:A:782:ALA:C	1:A:783:ARG:HD3	2.36	0.46
1:B:511:LEU:HD11	1:B:908:ALA:HB3	1.95	0.46
2:D:32:LEU:HD21	2:D:111:SER:HB2	1.97	0.46
5:J:107:LEU:HD11	5:J:111:ARG:HE	1.79	0.46
1:A:1169:ASP:O	1:A:1173:LEU:HG	2.15	0.46
1:A:1314:LYS:O	1:A:1317:GLN:HG2	2.16	0.46
1:B:143:ARG:O	1:B:143:ARG:HD3	2.16	0.46
3:E:76:ARG:NE	3:E:209:GLU:OE1	2.48	0.46
5:I:122:LEU:HD23	5:I:122:LEU:C	2.36	0.46
1:A:522:LEU:HB2	1:A:902:MET:HE3	1.97	0.46
1:A:791:ASN:OD1	1:A:794:ARG:NH1	2.48	0.46
1:B:146:ARG:NH1	2:C:337:GLU:OE1	2.48	0.46
1:B:69:THR:HG23	1:B:69:THR:O	2.16	0.46
2:D:104:THR:HG23	2:D:107:GLY:H	1.81	0.46
5:J:54:VAL:O	5:J:58:ILE:HG12	2.15	0.46
1:B:1155:GLY:N	5:J:8:ASN:ND2	2.64	0.46
5:J:14:LYS:HG2	5:J:70:MET:HE3	1.97	0.46
1:A:72:SER:OG	1:A:73:ARG:N	2.48	0.46
1:B:288:ALA:HB2	1:B:1106:ILE:CG2	2.45	0.46
1:A:577:GLY:O	1:A:580:ARG:HG2	2.16	0.46
2:C:284:PHE:O	2:C:288:ALA:N	2.38	0.46
5:I:47:LEU:HD12	5:I:47:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ILE:HD11	1:A:197:PHE:CD2	2.51	0.46
1:B:143:ARG:NH2	2:C:342:LEU:O	2.48	0.46
1:B:821:PHE:CE2	1:B:825:HIS:CD2	3.04	0.46
5:I:122:LEU:CD2	5:J:122:LEU:HB3	2.46	0.46
1:A:820:GLN:O	1:A:820:GLN:NE2	2.46	0.45
1:A:1164:ASN:OD1	1:A:1166:HIS:N	2.49	0.45
1:A:63:THR:HG21	1:A:1407:GLN:HG3	1.98	0.45
1:A:302:LEU:HD21	1:A:1092:VAL:HG12	1.97	0.45
1:A:369:ASP:O	1:A:373:GLU:OE1	2.34	0.45
1:A:955:GLN:HA	1:B:459:LEU:HD21	1.98	0.45
1:A:1277:VAL:HG22	1:A:1346:LEU:HD21	1.97	0.45
1:B:478:ALA:HB1	1:B:929:LEU:HD21	1.98	0.45
2:C:168:PHE:CE2	2:C:256:LEU:HD12	2.52	0.45
1:B:702:SER:O	1:B:709:ARG:NH1	2.47	0.45
2:C:207:LEU:O	2:C:210:GLU:HG2	2.17	0.45
1:B:588:GLU:O	1:B:592:GLN:OE1	2.35	0.45
5:J:42:ASP:O	5:J:46:LYS:HG3	2.16	0.45
1:A:326:LEU:HB3	1:A:1068:LEU:HD12	1.98	0.45
1:A:828:VAL:O	1:A:828:VAL:CG1	2.63	0.45
1:A:888:ASP:HB3	1:A:890:THR:HG23	1.99	0.45
2:D:29:LEU:O	2:D:33:MET:HG2	2.17	0.45
3:E:171:LEU:HD12	3:E:177:LYS:HB2	1.97	0.45
1:A:641:GLU:O	1:A:645:GLU:HG2	2.17	0.45
1:A:1147:ARG:NH1	5:I:85:GLU:OE2	2.50	0.45
1:B:410:GLN:O	1:B:411:THR:OG1	2.32	0.45
2:C:128:GLN:O	2:C:132:VAL:HG23	2.17	0.45
3:E:66:ILE:HD12	3:E:76:ARG:HB2	1.99	0.45
3:F:95:VAL:O	3:F:99:LEU:CD1	2.65	0.45
1:B:132:PRO:O	1:B:136:LEU:HD13	2.16	0.45
1:B:784:GLU:O	1:B:787:LEU:HG	2.17	0.45
5:J:118:THR:O	5:J:122:LEU:HD13	2.16	0.45
1:A:724:LEU:HD23	1:B:754:GLN:HG3	1.97	0.45
1:B:545:ARG:NH1	1:B:875:THR:OG1	2.48	0.45
3:F:64:GLU:O	3:F:66:ILE:HD12	2.16	0.45
3:E:95:VAL:O	3:E:99:LEU:HG	2.17	0.45
5:J:79:LYS:NZ	5:J:83:ASN:OD1	2.43	0.45
1:A:1237:SER:OG	1:A:1290:LEU:O	2.35	0.44
1:B:208:GLY:HA2	1:B:1371:ILE:HA	1.99	0.44
1:B:225:ASN:OD1	1:B:227:GLY:N	2.46	0.44
3:E:134:MET:SD	3:E:151:LEU:HB2	2.57	0.44
1:A:1376:SER:O	1:A:1379:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:O	1:B:388:THR:OG1	2.24	0.44
1:B:594:ILE:HD11	1:B:841:LEU:HB3	1.98	0.44
1:B:1006:GLN:O	1:B:1009:GLN:NE2	2.47	0.44
4:G:9:LYS:HA	4:G:19:GLN:OE1	2.17	0.44
5:I:119:ILE:HG12	5:J:104:LEU:HD21	1.98	0.44
1:A:87:TYR:CB	1:A:136:LEU:HD23	2.48	0.44
1:A:138:GLU:OE2	1:A:146:ARG:NE	2.44	0.44
1:A:1202:ILE:O	1:A:1202:ILE:HG22	2.17	0.44
1:B:763:SER:HB3	1:B:766:GLN:OE1	2.17	0.44
2:C:228:LYS:HD2	2:C:229:LEU:N	2.32	0.44
2:C:274:TRP:CD1	2:C:278:ASP:OD2	2.70	0.44
1:A:47:PHE:CZ	1:A:1402:LEU:HD22	2.52	0.44
1:A:594:ILE:HD11	1:A:841:LEU:HB3	1.99	0.44
1:B:665:GLN:NE2	1:B:671:ASP:OD2	2.51	0.44
1:A:726:THR:O	1:A:726:THR:HG22	2.18	0.44
1:B:469:ASP:OD1	1:B:469:ASP:C	2.56	0.44
1:B:587:LEU:HD12	1:B:845:HIS:CD2	2.52	0.44
1:B:1277:VAL:HG12	1:B:1346:LEU:HD13	2.00	0.44
4:G:7:VAL:O	4:G:11:ILE:HG22	2.17	0.44
1:A:263:ILE:HG23	1:A:264:THR:N	2.33	0.44
1:A:1108:GLU:HA	1:A:1111:VAL:HG22	1.99	0.44
1:B:231:ALA:HB1	1:B:1240:VAL:HG22	1.98	0.44
1:B:1376:SER:O	1:B:1379:VAL:HG22	2.18	0.44
1:A:309:HIS:NE2	1:A:1086:GLU:HB2	2.33	0.44
1:A:978:MET:HE1	1:A:989:LEU:HB2	2.00	0.44
1:A:1120:VAL:O	1:A:1124:VAL:HG12	2.18	0.44
1:A:1161:VAL:HG22	1:A:1161:VAL:O	2.17	0.44
1:A:1245:ARG:HG3	1:A:1287:LEU:HD21	2.00	0.44
1:B:465:LEU:HD21	1:B:940:GLN:OE1	2.18	0.44
1:B:855:PHE:O	1:B:859:THR:HG23	2.18	0.44
2:D:91:THR:CG2	3:E:114:ILE:HD12	2.48	0.44
3:E:137:VAL:HG21	3:E:151:LEU:HD13	2.00	0.44
1:A:312:MET:HA	1:A:315:GLU:HG3	2.00	0.44
1:B:99:ARG:NH2	1:B:130:ILE:O	2.43	0.44
1:B:143:ARG:NH1	2:C:342:LEU:O	2.51	0.44
1:B:485:ILE:HG21	1:B:501:LEU:HD23	1.99	0.44
1:B:1009:GLN:O	1:B:1012:ALA:HB3	2.18	0.44
1:A:459:LEU:CD1	1:B:470:ALA:HB3	2.48	0.43
1:A:604:TRP:HA	1:A:828:VAL:HG11	2.00	0.43
1:B:302:LEU:HD13	1:B:1093:GLN:HG3	2.00	0.43
1:A:327:GLU:HA	1:A:1068:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:LEU:HD11	1:B:769:TYR:CG	2.53	0.43
1:A:770:SER:OG	1:B:733:ASP:OD1	2.34	0.43
1:B:233:GLN:CG	2:D:94:LEU:HD13	2.48	0.43
3:F:105:SER:N	3:F:106:PRO:CD	2.81	0.43
5:I:78:ARG:NH1	7:L:5:DG:OP2	2.49	0.43
5:J:85:GLU:OE1	5:J:86:HIS:CE1	2.71	0.43
3:E:199:GLU:OE2	3:E:200:ILE:CD1	2.67	0.43
1:A:1103:TYR:OH	4:G:44:MET:SD	2.76	0.43
1:B:940:GLN:O	1:B:940:GLN:NE2	2.52	0.43
3:E:101:TYR:CE2	3:E:127:LEU:HD21	2.53	0.43
1:A:782:ALA:O	1:A:783:ARG:C	2.56	0.43
1:A:1371:ILE:O	1:A:1375:MET:HG2	2.19	0.43
1:B:203:ALA:O	1:B:207:GLY:N	2.51	0.43
1:B:933:PRO:O	1:B:936:HIS:HB3	2.18	0.43
4:G:36:SER:O	4:G:40:VAL:HG23	2.18	0.43
5:I:52:VAL:HG13	5:I:53:ARG:HG2	2.00	0.43
5:J:51:PRO:HA	5:J:54:VAL:HG23	2.00	0.43
1:A:53:PRO:HB3	1:A:104:VAL:HG11	2.00	0.43
1:A:192:SER:O	1:A:195:SER:OG	2.29	0.43
1:A:774:GLU:OE1	1:A:774:GLU:N	2.52	0.43
1:A:890:THR:CB	1:A:892:ILE:HG23	2.45	0.43
1:B:414:ILE:HA	1:B:417:GLN:OE1	2.19	0.43
3:F:90:GLU:HA	3:F:93:MET:HE2	2.00	0.43
2:C:281:VAL:CG2	3:E:109:LEU:HD21	2.47	0.43
8:N:17:DA:C8	8:N:18:DT:H72	2.54	0.43
1:B:512:ALA:O	1:B:515:VAL:HG23	2.19	0.43
2:D:37:VAL:O	2:D:40:SER:OG	2.27	0.43
3:F:61:TYR:HA	3:F:82:LEU:HD22	2.01	0.43
1:B:239:LEU:O	1:B:239:LEU:HD23	2.18	0.43
1:B:1418:THR:O	1:B:1421:GLU:HG2	2.19	0.43
2:C:156:VAL:HG12	2:C:156:VAL:O	2.19	0.43
1:A:26:ASP:OD1	1:A:27:GLU:N	2.52	0.43
1:A:432:LEU:HD11	1:A:443:TRP:CD1	2.53	0.43
1:A:479:TYR:OH	1:A:489:THR:O	2.25	0.43
1:A:486:VAL:HG23	1:A:501:LEU:HD21	2.01	0.43
1:A:1119:ALA:HB1	1:A:1123:MET:HE1	2.01	0.43
1:B:637:GLU:O	1:B:640:ARG:HG3	2.19	0.43
1:B:882:GLN:HB3	1:B:885:LEU:HD12	2.01	0.43
2:C:179:ASP:O	2:C:182:GLN:CG	2.67	0.43
3:E:23:PHE:N	3:E:24:PRO:HD2	2.34	0.43
1:A:386:GLU:O	1:A:390:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:LYS:C	1:A:1448:LEU:HD12	2.39	0.42
1:B:27:GLU:C	1:B:28:LEU:HD22	2.40	0.42
1:B:614:LEU:HD21	1:B:818:PHE:CD1	2.54	0.42
1:A:340:VAL:HG12	1:A:1054:GLU:HG2	2.01	0.42
1:B:478:ALA:CB	1:B:929:LEU:HD21	2.48	0.42
1:A:870:LYS:O	1:A:874:THR:HG23	2.19	0.42
1:A:1017:PHE:O	1:A:1020:VAL:HG22	2.20	0.42
1:B:209:ILE:HG23	1:B:214:THR:CG2	2.48	0.42
1:B:837:GLU:O	1:B:841:LEU:HD13	2.20	0.42
2:C:230:GLN:NE2	2:C:261:ASP:OD1	2.52	0.42
2:C:363:GLU:CD	2:C:364:LYS:HD3	2.39	0.42
5:J:100:VAL:O	5:J:104:LEU:HD23	2.19	0.42
1:A:291:LEU:CD2	1:A:1103:TYR:HB2	2.48	0.42
1:A:316:LEU:HD12	1:A:1082:ILE:CD1	2.37	0.42
1:A:1057:ALA:O	1:A:1061:ARG:HG2	2.19	0.42
1:B:1129:VAL:HA	1:B:1133:LEU:HB3	2.00	0.42
2:D:75:ASN:HA	2:D:78:ILE:HG12	2.01	0.42
4:G:15:LEU:HD22	4:G:34:ALA:HB2	2.01	0.42
4:H:9:LYS:O	4:H:13:GLU:OE1	2.37	0.42
5:J:5:GLN:NE2	6:K:63:DT:OP1	2.43	0.42
8:N:12:DT:H2"	8:N:13:DA:C8	2.54	0.42
1:A:54:ASP:OD1	1:A:56:THR:N	2.52	0.42
1:A:407:ASP:OD1	1:B:966:ARG:NH1	2.52	0.42
1:A:568:ALA:HB3	1:A:866:TYR:HE2	1.84	0.42
1:B:545:ARG:NH1	1:B:875:THR:HG21	2.34	0.42
1:A:978:MET:HE1	1:A:989:LEU:N	2.34	0.42
1:A:1063:ARG:HA	1:A:1066:GLU:HG3	2.00	0.42
1:B:652:GLN:O	1:B:656:LEU:HD23	2.19	0.42
1:B:979:LEU:O	1:B:980:SER:OG	2.33	0.42
1:B:1120:VAL:HG13	1:B:1184:VAL:HG21	2.01	0.42
2:C:308:TYR:CD1	3:E:94:MET:CE	3.03	0.42
4:H:64:THR:HG22	4:H:65:VAL:N	2.34	0.42
1:B:273:ASP:OD1	1:B:273:ASP:C	2.57	0.42
1:B:323:SER:HA	1:B:1068:LEU:HD11	2.02	0.42
4:H:15:LEU:HD13	4:H:34:ALA:HB2	2.02	0.42
5:J:14:LYS:HG2	5:J:70:MET:CE	2.50	0.42
1:A:522:LEU:HB3	1:A:902:MET:HE1	2.00	0.42
1:B:485:ILE:HG21	1:B:501:LEU:CD2	2.50	0.42
1:B:567:GLU:O	1:B:571:LEU:HD13	2.19	0.42
1:B:1403:LEU:HD13	1:B:1428:MET:SD	2.60	0.42
2:C:182:GLN:O	2:C:185:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ILE:HG13	2:D:79:ASN:N	2.35	0.42
3:E:58:TYR:CD2	3:E:75:LEU:HD11	2.55	0.42
1:A:45:ALA:O	1:A:49:THR:HG22	2.20	0.42
1:A:710:HIS:O	1:A:710:HIS:CG	2.73	0.42
1:B:529:LEU:O	1:B:533:GLN:OE1	2.38	0.42
1:B:892:ILE:HG22	1:B:894:ARG:NH2	2.35	0.42
1:A:881:PRO:O	1:A:882:GLN:HG3	2.20	0.42
1:A:1267:PHE:CD1	1:A:1372:GLY:HA3	2.55	0.42
2:C:360:ALA:O	2:C:363:GLU:HG3	2.20	0.42
2:D:27:GLU:HG2	2:D:28:ARG:N	2.34	0.42
3:F:95:VAL:O	3:F:99:LEU:HD13	2.20	0.42
5:J:33:GLU:HG2	5:J:36:ALA:HB3	2.02	0.42
1:A:302:LEU:HD22	1:A:1096:LEU:HD11	2.00	0.41
1:B:1215:MET:O	1:B:1219:LEU:HD13	2.21	0.41
1:B:1248:ILE:CG2	1:B:1344:LEU:HD21	2.50	0.41
1:B:1289:VAL:HG21	1:B:1319:LEU:CD2	2.48	0.41
2:C:253:VAL:O	2:C:257:GLN:HG2	2.20	0.41
3:E:134:MET:CE	3:E:147:ASP:O	2.68	0.41
4:G:37:LEU:N	11:G:101:PNS:O26	2.41	0.41
1:A:622:LEU:HD13	1:A:627:ASP:OD2	2.20	0.41
1:B:1255:ILE:HG21	1:B:1277:VAL:HG11	2.02	0.41
2:C:250:ASP:O	2:C:254:PHE:N	2.53	0.41
5:I:129:LYS:NZ	5:J:125:ASP:OD2	2.47	0.41
1:A:932:ASP:OD1	1:A:933:PRO:HD2	2.20	0.41
1:A:1061:ARG:HA	1:A:1064:LEU:HD12	2.02	0.41
1:B:864:GLN:O	1:B:868:GLN:OE1	2.38	0.41
3:F:199:GLU:O	3:F:203:ARG:HG2	2.20	0.41
1:A:225:ASN:OD1	1:A:227:GLY:N	2.46	0.41
1:A:674:MET:SD	1:A:710:HIS:HB2	2.60	0.41
1:A:957:ALA:O	1:A:961:VAL:HG23	2.21	0.41
1:B:171:ILE:HG22	8:M:24:DT:P	2.61	0.41
1:B:327:GLU:HG3	1:B:1068:LEU:HD21	2.03	0.41
1:B:1448:LEU:N	1:B:1448:LEU:HD12	2.35	0.41
2:C:241:MET:O	2:C:241:MET:HG3	2.20	0.41
3:E:3:SER:O	3:E:4:THR:OG1	2.30	0.41
4:G:10:ILE:HD11	4:G:45:ALA:HB1	2.02	0.41
5:J:1:MET:CE	6:K:63:DT:H4'	2.49	0.41
5:J:91:LYS:NZ	6:K:66:DT:OP2	2.45	0.41
1:A:11:THR:C	1:A:12:LEU:HD12	2.40	0.41
1:A:562:LEU:HD13	1:A:873:LEU:HB2	2.02	0.41
1:A:1107:ARG:NE	4:G:48:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:MET:HB3	1:B:1082:ILE:HD11	2.02	0.41
2:C:237:GLN:HB2	2:C:253:VAL:HG11	2.01	0.41
3:E:94:MET:O	3:E:98:ILE:HG12	2.20	0.41
4:G:7:VAL:HA	4:G:10:ILE:HG22	2.02	0.41
5:I:87:GLN:OE1	5:I:90:ARG:NH2	2.54	0.41
5:J:73:THR:HG22	7:L:13:DG:H2'	2.03	0.41
1:A:1215:MET:O	1:A:1219:LEU:HD13	2.20	0.41
1:B:581:MET:SD	1:B:582:GLU:N	2.94	0.41
1:B:1406:ASP:OD1	1:B:1407:GLN:N	2.52	0.41
3:E:157:THR:HG23	8:M:28:DT:OP2	2.21	0.41
5:J:58:ILE:HA	5:J:62:MET:HB2	2.02	0.41
1:A:555:LEU:HD11	1:A:558:LEU:CD2	2.50	0.41
1:A:1373:THR:O	1:A:1377:ILE:HG12	2.21	0.41
1:B:909:ALA:O	1:B:913:GLN:OE1	2.38	0.41
2:C:132:VAL:HG23	2:C:167:ILE:HG21	2.03	0.41
2:D:86:LEU:O	2:D:104:THR:HG22	2.21	0.41
3:E:157:THR:O	3:E:161:ARG:HG3	2.20	0.41
6:K:65:DT:H2'	6:K:66:DT:H72	2.01	0.41
1:A:85:VAL:HG13	1:A:105:ARG:HD3	2.02	0.41
1:A:1240:VAL:O	1:A:1243:ILE:HG22	2.21	0.41
1:B:668:GLY:N	1:B:780:ARG:HD3	2.35	0.41
2:C:327:ARG:HB3	3:F:93:MET:HE3	2.03	0.41
1:A:309:HIS:NE2	1:A:1082:ILE:HG23	2.35	0.41
1:A:471:ALA:N	1:A:474:GLN:OE1	2.54	0.41
1:A:660:ILE:HA	1:A:663:LEU:HD12	2.02	0.41
1:B:275:MET:HE2	1:B:1134:HIS:HA	2.02	0.41
1:B:480:GLN:HA	1:B:483:LYS:HZ3	1.86	0.41
1:B:1124:VAL:HG22	1:B:1124:VAL:O	2.21	0.41
1:B:1255:ILE:HG21	1:B:1277:VAL:CG1	2.51	0.41
2:D:89:ARG:NH1	2:D:101:TYR:OH	2.42	0.41
4:H:57:GLU:HG2	4:H:58:GLU:N	2.35	0.41
1:A:475:PHE:N	1:A:928:VAL:HG21	2.36	0.41
1:B:270:VAL:O	1:B:273:ASP:OD1	2.39	0.41
1:B:432:LEU:HD13	1:B:443:TRP:CD2	2.56	0.41
1:B:569:LEU:HD12	1:B:866:TYR:CB	2.51	0.41
2:C:160:LEU:HD12	2:C:164:VAL:HG11	2.02	0.41
2:C:425:ILE:HD13	2:C:432:VAL:CG2	2.50	0.41
3:E:89:SER:O	3:E:92:ASP:HB2	2.21	0.41
3:F:64:GLU:HB3	3:F:66:ILE:HD11	2.02	0.41
3:F:104:LEU:HD11	3:F:198:ARG:NE	2.36	0.41
1:A:135:LEU:O	1:A:156:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:SER:O	1:A:1380:MET:HG2	2.21	0.40
1:B:53:PRO:HG2	1:B:171:ILE:HD12	2.02	0.40
1:B:604:TRP:O	1:B:608:GLN:HG2	2.22	0.40
1:B:1169:ASP:O	1:B:1173:LEU:HG	2.21	0.40
1:B:1379:VAL:HA	1:B:1382:VAL:HG12	2.03	0.40
2:C:157:PHE:O	2:C:161:LYS:HB3	2.21	0.40
2:C:172:ASP:O	2:C:176:ARG:HG3	2.21	0.40
3:F:108:ARG:O	3:F:112:GLN:NE2	2.49	0.40
1:A:426:ALA:HB2	1:A:963:ILE:CD1	2.51	0.40
1:A:459:LEU:HD21	1:B:474:GLN:OE1	2.22	0.40
1:A:663:LEU:HD13	1:A:787:LEU:HD13	2.03	0.40
1:A:733:ASP:OD1	1:B:770:SER:OG	2.30	0.40
1:B:539:LEU:HD11	1:B:884:THR:HG22	2.03	0.40
4:H:40:VAL:O	4:H:43:VAL:HG12	2.21	0.40
1:A:436:SER:HG	1:A:439:ASN:CG	2.22	0.40
1:A:538:LEU:HD22	1:A:879:LEU:HD13	2.03	0.40
1:A:1055:MET:O	1:A:1058:ARG:HG2	2.21	0.40
1:A:1121:MET:HA	1:A:1124:VAL:HG12	2.02	0.40
1:B:265:GLU:HB3	1:B:1157:LEU:HD12	2.03	0.40
1:B:984:ASP:OD1	1:B:984:ASP:N	2.53	0.40
3:E:52:GLU:HA	3:E:55:GLU:OE1	2.22	0.40
4:G:10:ILE:HG23	4:G:11:ILE:N	2.37	0.40
4:H:26:ALA:O	4:H:65:VAL:HG23	2.21	0.40
5:I:73:THR:OG1	6:K:73:DT:OP2	2.39	0.40
8:N:20:DT:H2"	8:N:21:DA:C8	2.56	0.40
1:A:933:PRO:O	1:A:936:HIS:HB3	2.20	0.40
1:B:740:ASP:O	1:B:744:PHE:N	2.54	0.40
1:B:1330:PRO:HA	1:B:1333:ILE:HG22	2.03	0.40
3:F:35:HIS:ND1	3:F:74:TYR:HB3	2.36	0.40
6:K:68:DC:H2'	6:K:69:DA:C8	2.57	0.40
1:B:523:SER:O	1:B:527:GLN:OE1	2.40	0.40
1:B:848:LEU:O	1:B:852:VAL:HG23	2.21	0.40
1:B:998:SER:O	1:B:1002:ARG:HG2	2.22	0.40
2:C:295:ARG:HG2	2:C:298:SER:HB3	2.03	0.40
2:C:304:SER:O	2:C:308:TYR:N	2.55	0.40
3:E:163:ARG:HA	3:E:168:VAL:HG13	2.04	0.40
4:H:29:VAL:HG13	4:H:30:GLU:N	2.36	0.40
5:I:120:VAL:O	5:I:123:ILE:HG22	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	1465/1482 (99%)	1417 (97%)	48 (3%)	0	100	100
1	B	1465/1482 (99%)	1412 (96%)	53 (4%)	0	100	100
2	C	331/440 (75%)	315 (95%)	16 (5%)	0	100	100
2	D	92/440 (21%)	89 (97%)	3 (3%)	0	100	100
3	E	210/240 (88%)	207 (99%)	3 (1%)	0	100	100
3	F	196/240 (82%)	186 (95%)	10 (5%)	0	100	100
4	G	70/78 (90%)	69 (99%)	1 (1%)	0	100	100
4	H	70/78 (90%)	66 (94%)	4 (6%)	0	100	100
5	I	132/151 (87%)	129 (98%)	3 (2%)	0	100	100
5	J	133/151 (88%)	130 (98%)	3 (2%)	0	100	100
All	All	4164/4782 (87%)	4020 (96%)	144 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1269/1281 (99%)	1266 (100%)	3 (0%)	93	96
1	B	1269/1281 (99%)	1262 (99%)	7 (1%)	86	92
2	C	286/376 (76%)	284 (99%)	2 (1%)	84	90
2	D	79/376 (21%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	189/212 (89%)	188 (100%)	1 (0%)	88	93
3	F	177/212 (84%)	177 (100%)	0	100	100
4	G	63/67 (94%)	63 (100%)	0	100	100
4	H	63/67 (94%)	63 (100%)	0	100	100
5	I	121/136 (89%)	121 (100%)	0	100	100
5	J	122/136 (90%)	122 (100%)	0	100	100
All	All	3638/4144 (88%)	3625 (100%)	13 (0%)	91	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	783	ARG
1	A	1131	ARG
1	A	1204	ARG
1	B	143	ARG
1	B	327	GLU
1	B	331	GLN
1	B	658	LYS
1	B	673	ARG
1	B	1034	MET
1	B	1131	ARG
2	C	17	LYS
2	C	228	LYS
3	E	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	A	410	GLN
1	A	723	HIS
1	A	815	HIS
1	A	1006	GLN
1	A	1009	GLN
1	A	1019	GLN
1	A	1065	HIS
1	B	62	ASN
1	B	595	GLN
1	B	1019	GLN

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Mol	Chain	Res	Type
1	B	1166	HIS
2	C	182	GLN
2	C	206	GLN
2	C	230	GLN
5	I	61	HIS
5	J	60	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
10	ATP	A	1502	9	26,33,33	0.63	0	31,52,52	1.07	1 (3%)
11	PNS	H	101	4	13,20,21	0.19	0	18,26,29	0.44	0
10	ATP	B	1502	9	26,33,33	0.63	0	31,52,52	1.07	3 (9%)
11	PNS	G	101	4	13,20,21	0.18	0	18,26,29	0.34	0

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
10	ATP	A	1502	9	-	1/18/38/38	0/3/3/3
11	PNS	H	101	4	-	3/24/26/27	-
10	ATP	B	1502	9	-	2/18/38/38	0/3/3/3
11	PNS	G	101	4	-	2/24/26/27	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	1502	ATP	C5-C6-N6	2.29	123.83	120.35
10	A	1502	ATP	C5-C6-N6	2.27	123.80	120.35
10	B	1502	ATP	O3'-C3'-C2'	-2.04	105.23	111.82
10	B	1502	ATP	PB-O3B-PG	2.02	139.77	132.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	101	PNS	C37-C38-C39-N41
10	A	1502	ATP	PB-O3B-PG-O1G
11	H	101	PNS	C37-C38-C39-O40
10	B	1502	ATP	PA-O3A-PB-O2B
11	G	101	PNS	O33-C32-C34-O35
11	H	101	PNS	O33-C32-C34-O35
11	G	101	PNS	C43-C42-N41-C39
10	B	1502	ATP	PA-O3A-PB-O1B

There are no ring outliers.

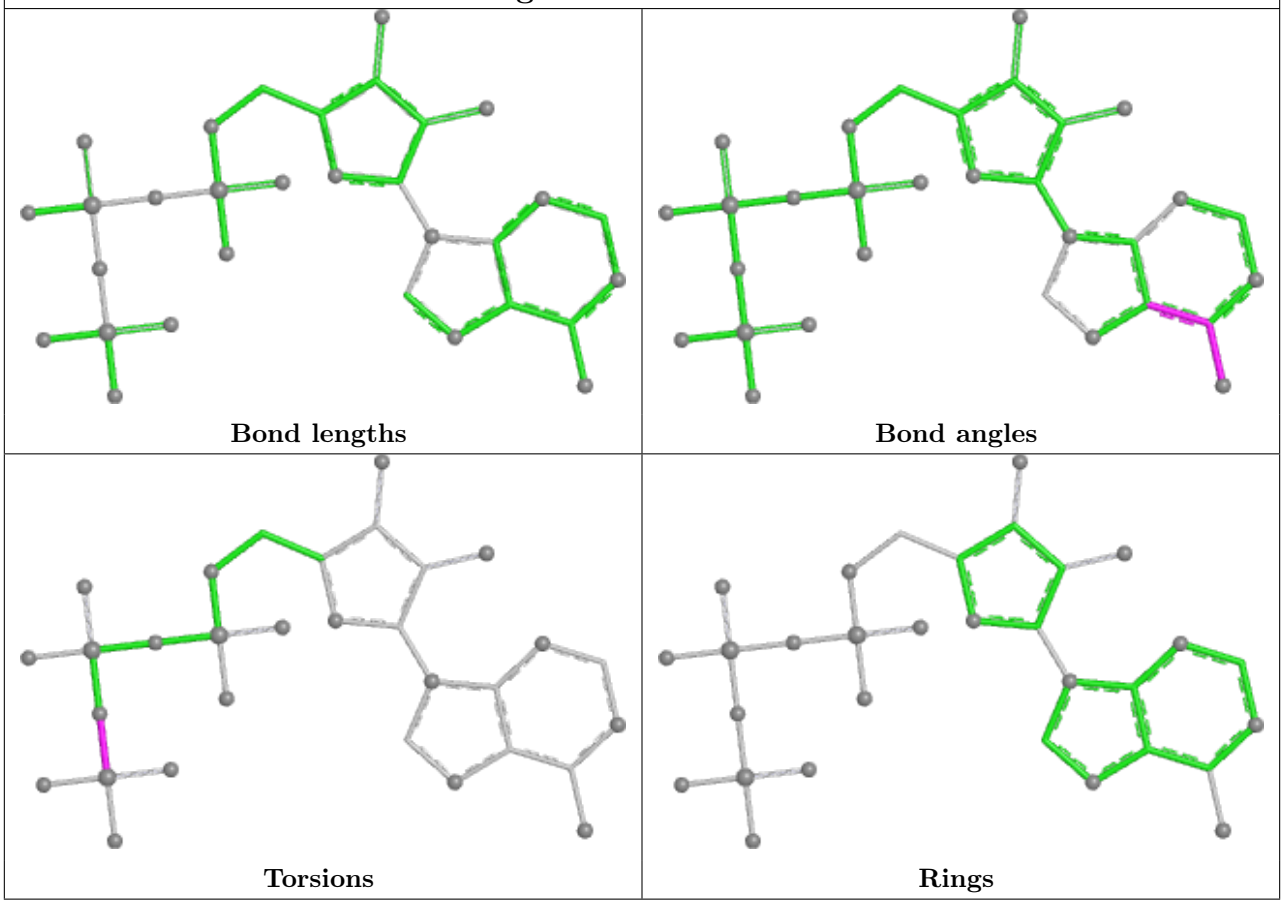
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1502	ATP	3	0
11	G	101	PNS	1	0

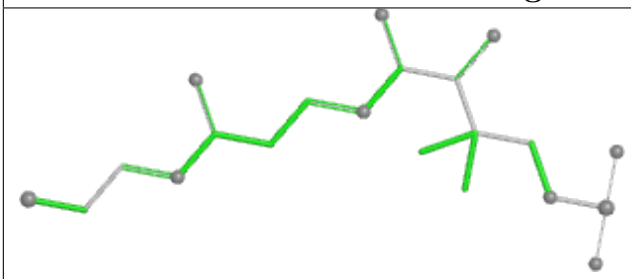
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

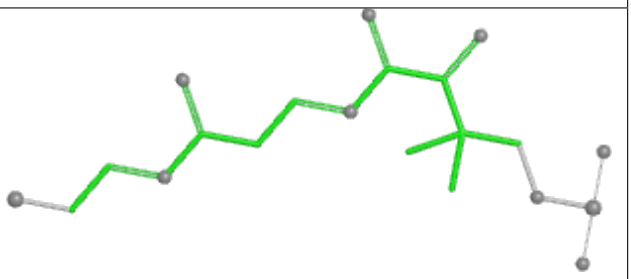
Ligand ATP A 1502



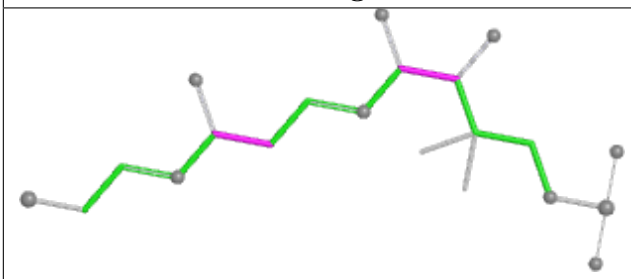
Ligand PNS H 101



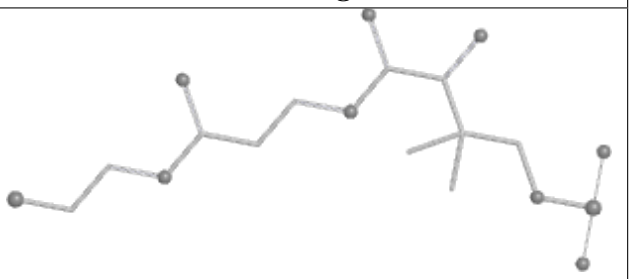
Bond lengths



Bond angles

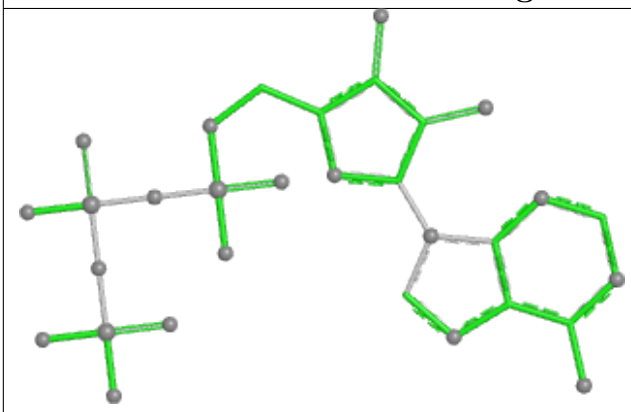


Torsions

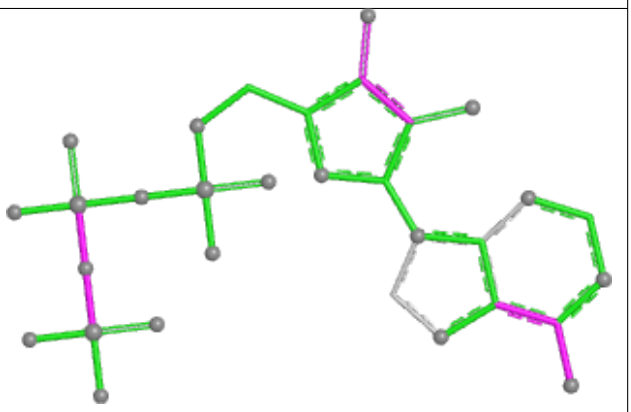


Rings

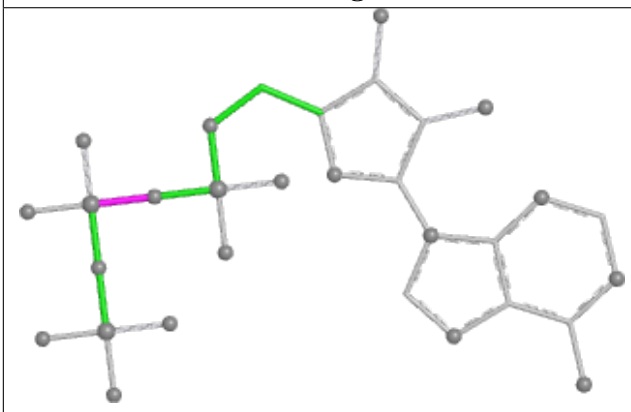
Ligand ATP B 1502



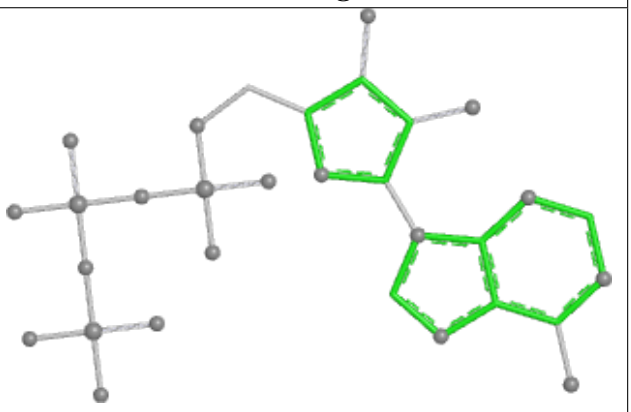
Bond lengths



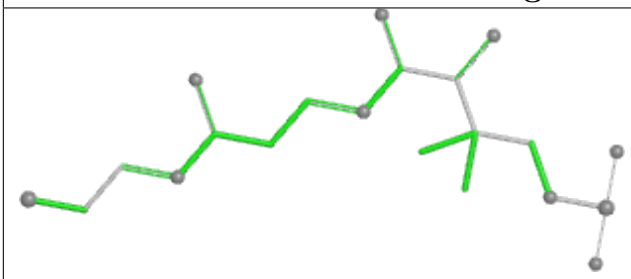
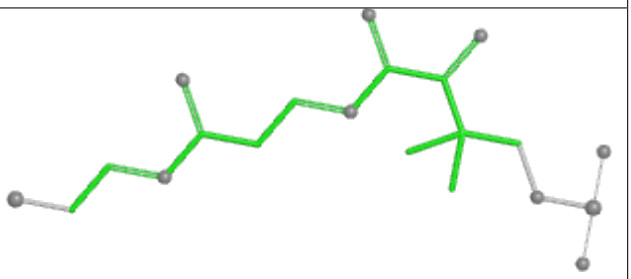
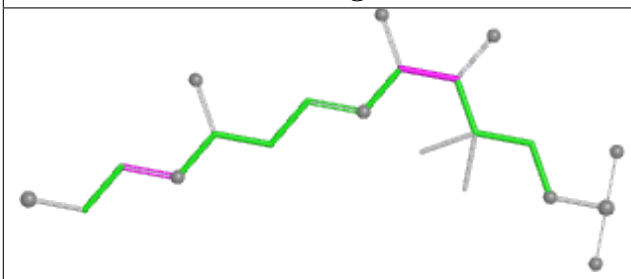
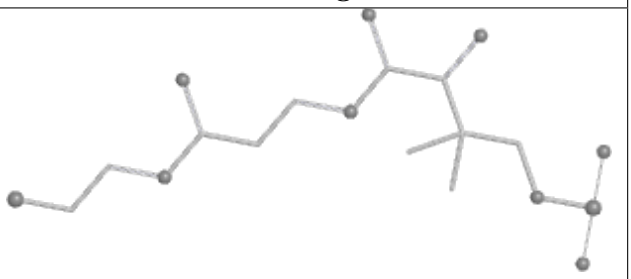
Bond angles



Torsions



Rings

Ligand PNS G 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

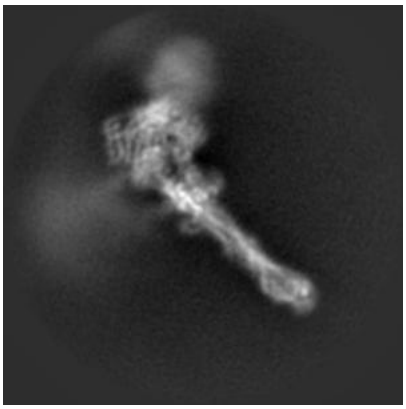
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12659. These allow visual inspection of the internal detail of the map and identification of artifacts.

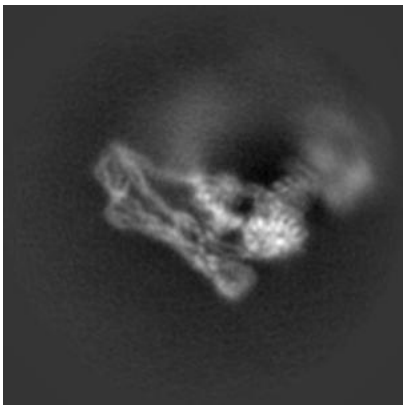
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

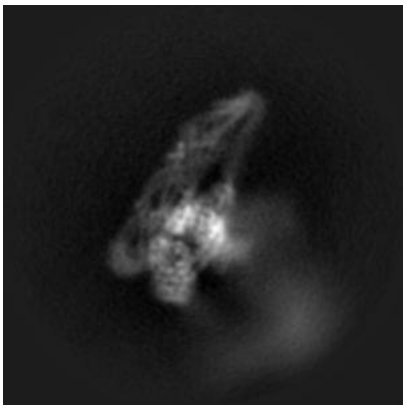
6.1.1 Primary map



X

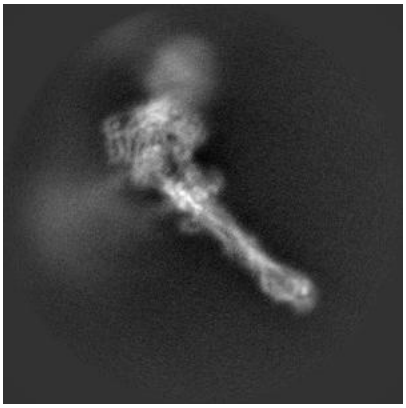


Y

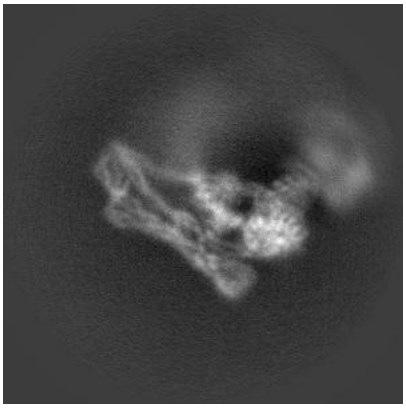


Z

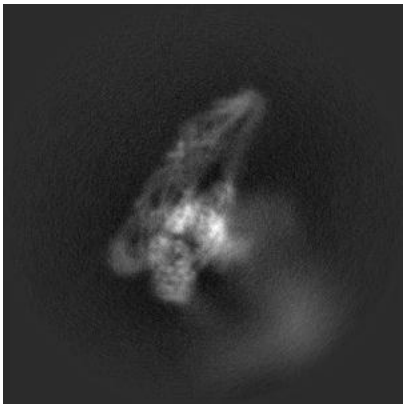
6.1.2 Raw map



X



Y

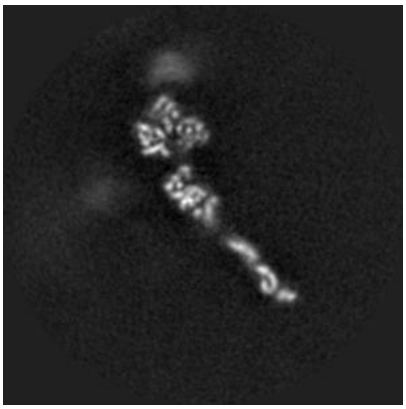


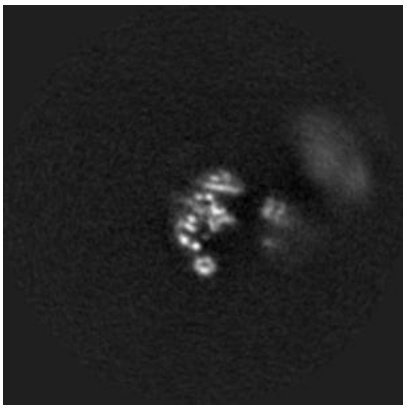
Z

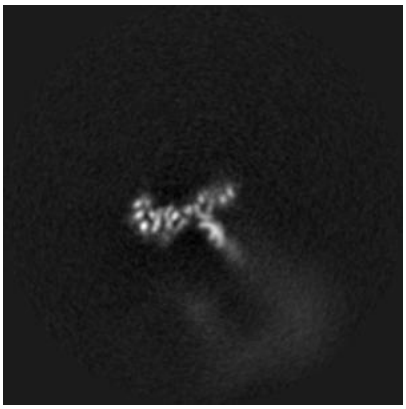
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

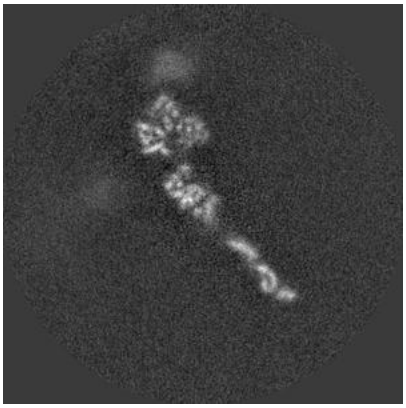
6.2.1 Primary map

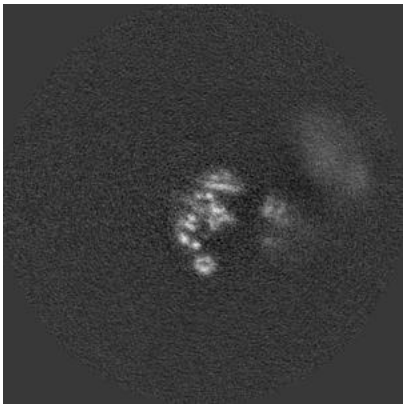

X Index: 159

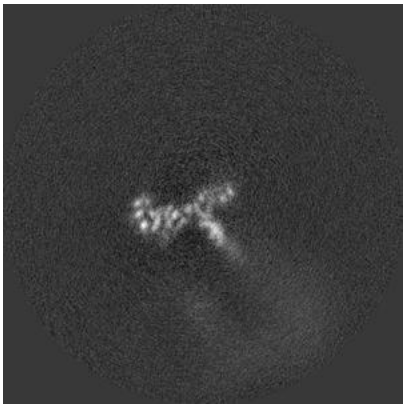

Y Index: 159


Z Index: 159

6.2.2 Raw map


X Index: 159

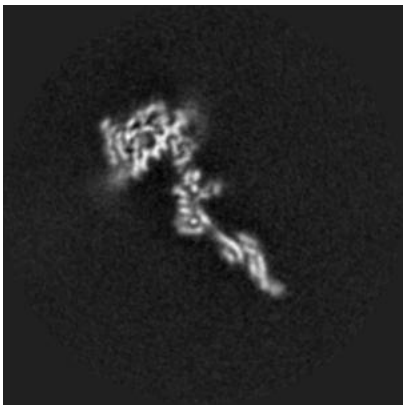

Y Index: 159

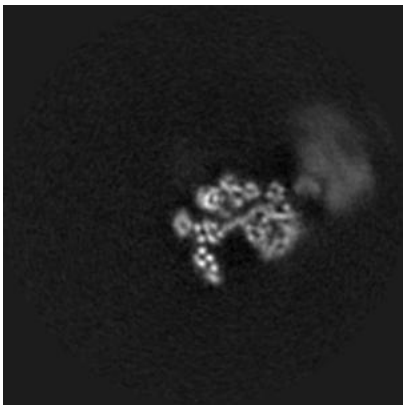

Z Index: 159

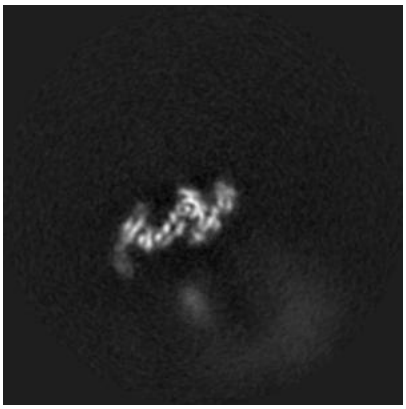
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

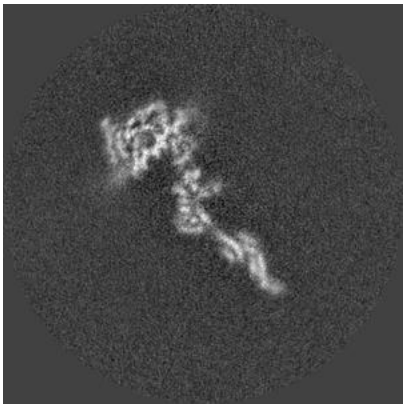
6.3.1 Primary map

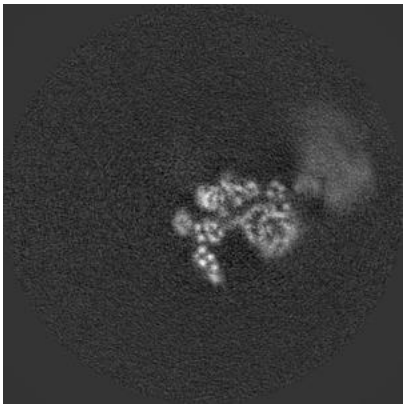

X Index: 141

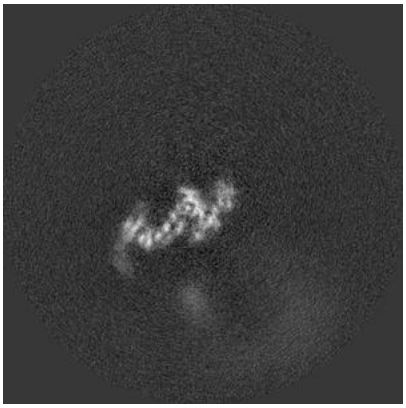

Y Index: 144


Z Index: 169

6.3.2 Raw map


X Index: 141


Y Index: 143


Z Index: 169

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

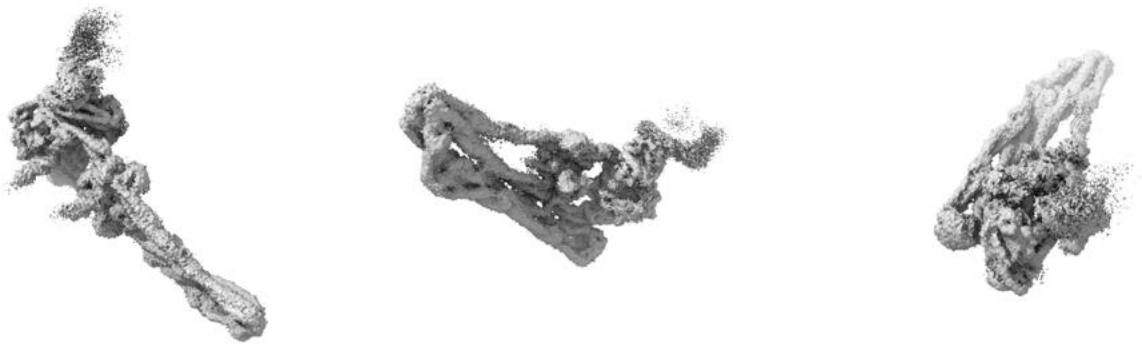
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

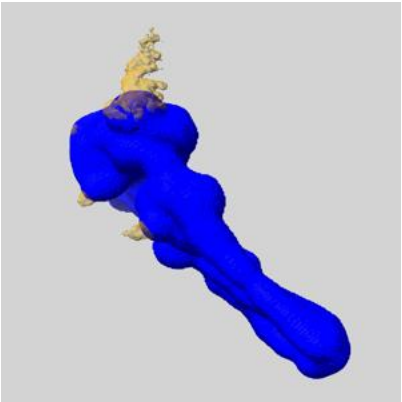
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

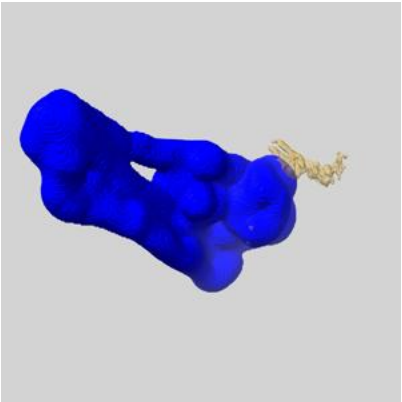
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

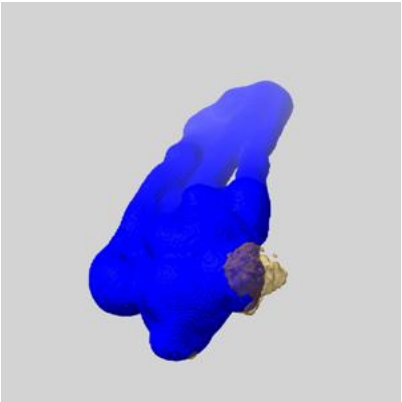
6.5.1 emd_12659_msk_1.map (i)



X



Y

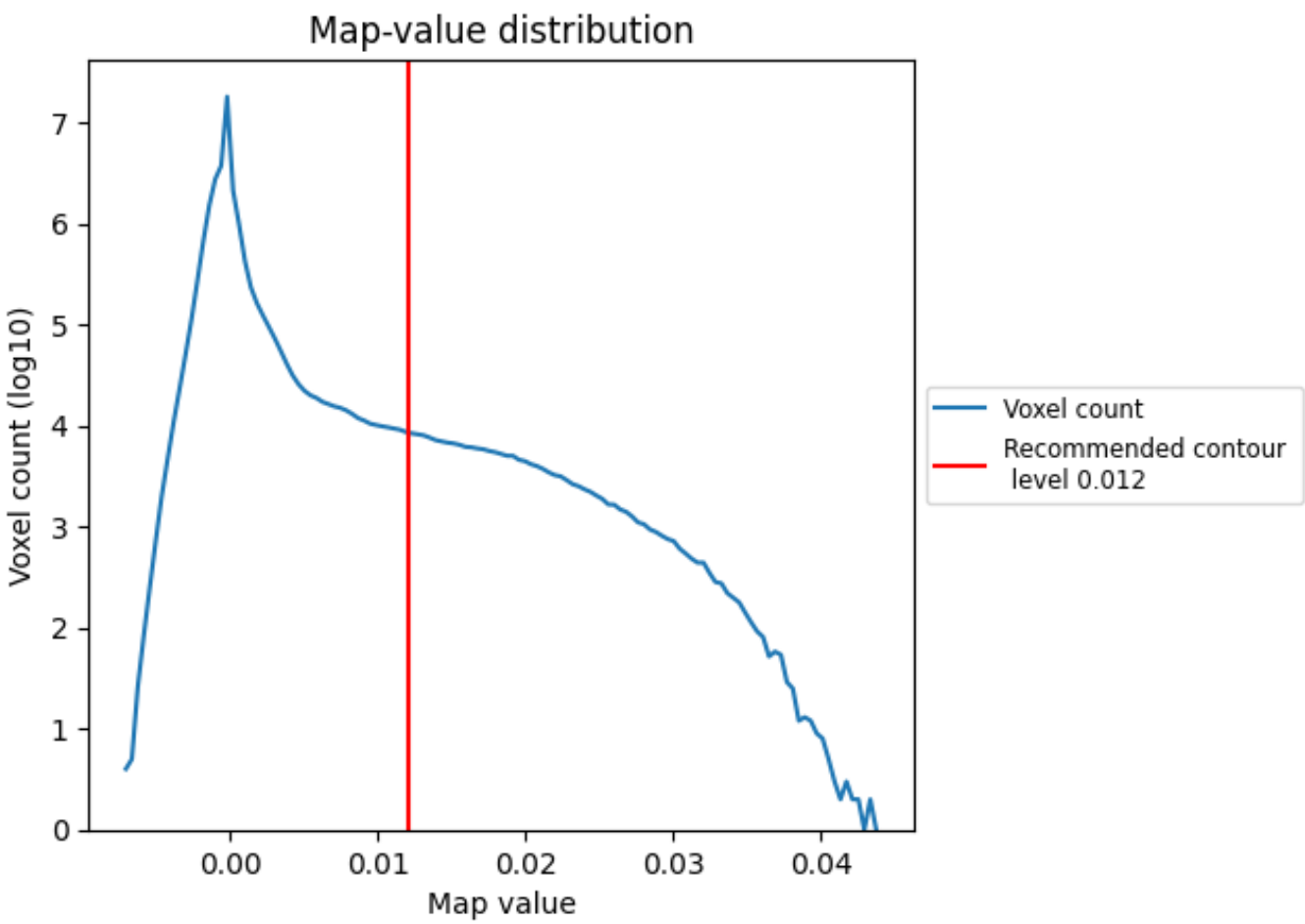


Z

7 Map analysis (i)

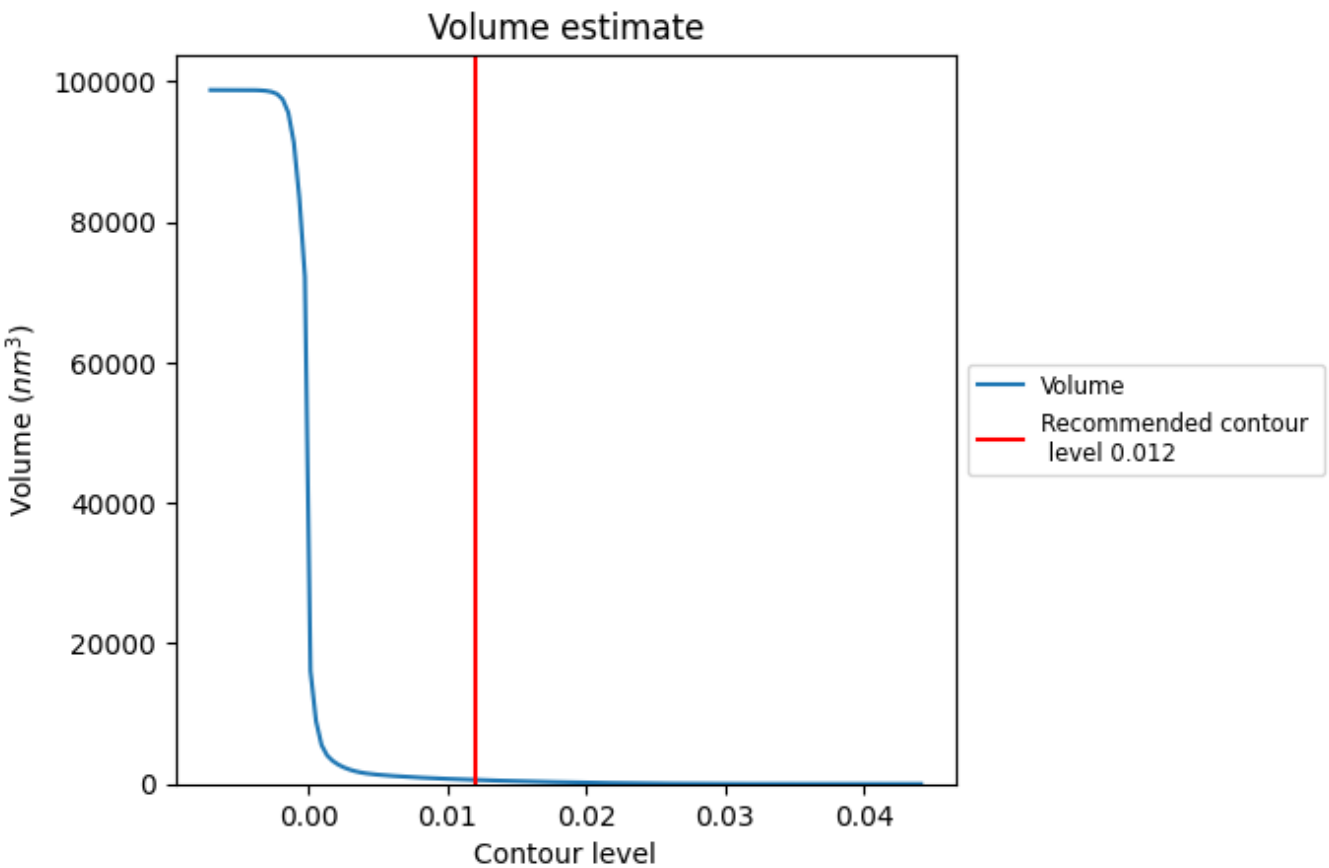
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

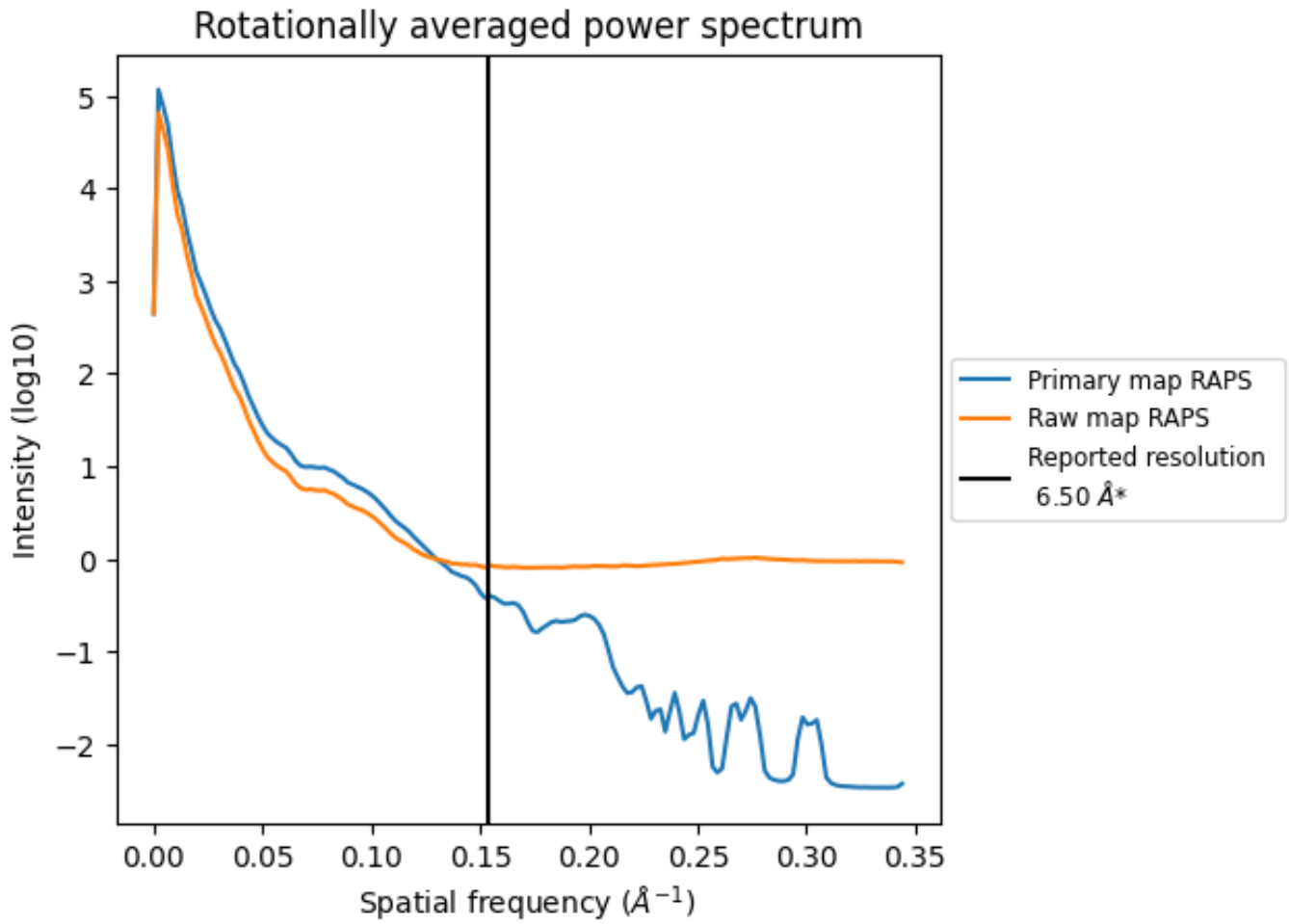
7.2 Volume estimate (i)



The volume at the recommended contour level is 581 nm^3; this corresponds to an approximate mass of 525 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)

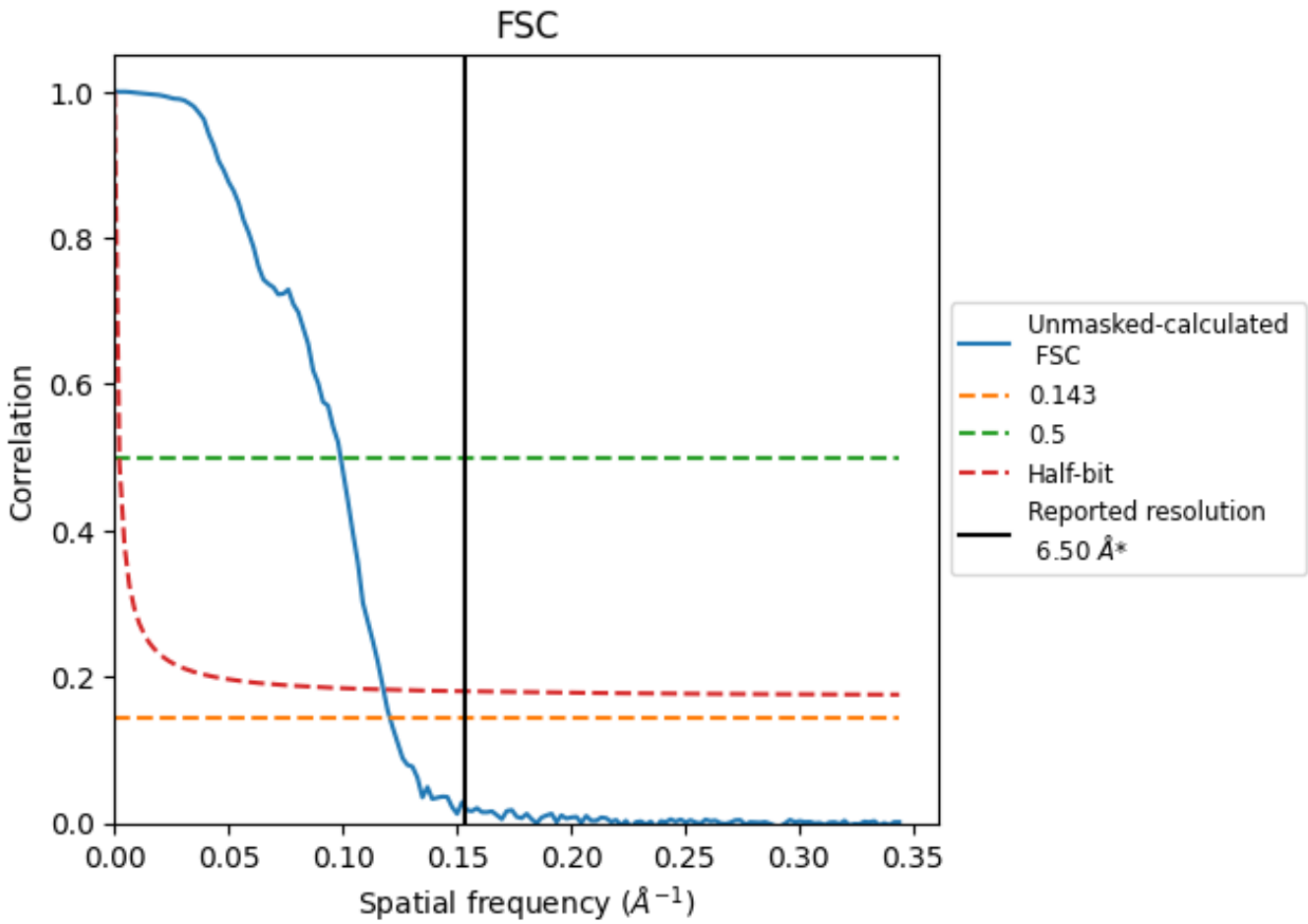


*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

8.2 Resolution estimates (i)

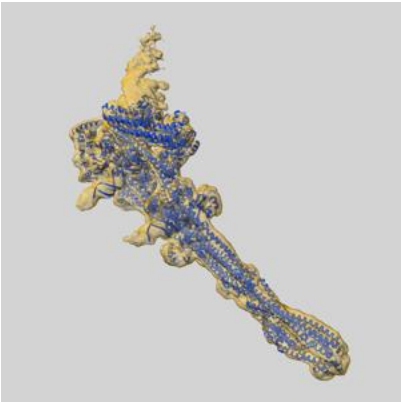
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.28	10.09	8.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.28 differs from the reported value 6.5 by more than 10 %

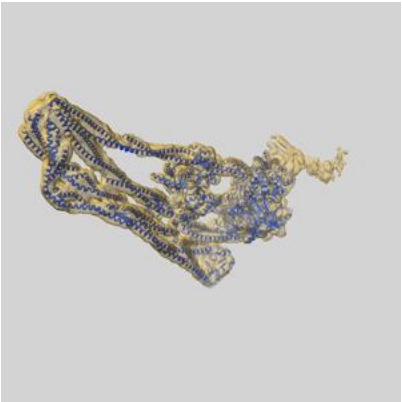
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12659 and PDB model 7NYZ. Per-residue inclusion information can be found in section 3 on page 7.

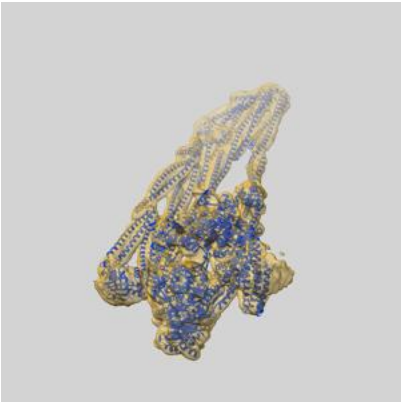
9.1 Map-model overlay (i)



X



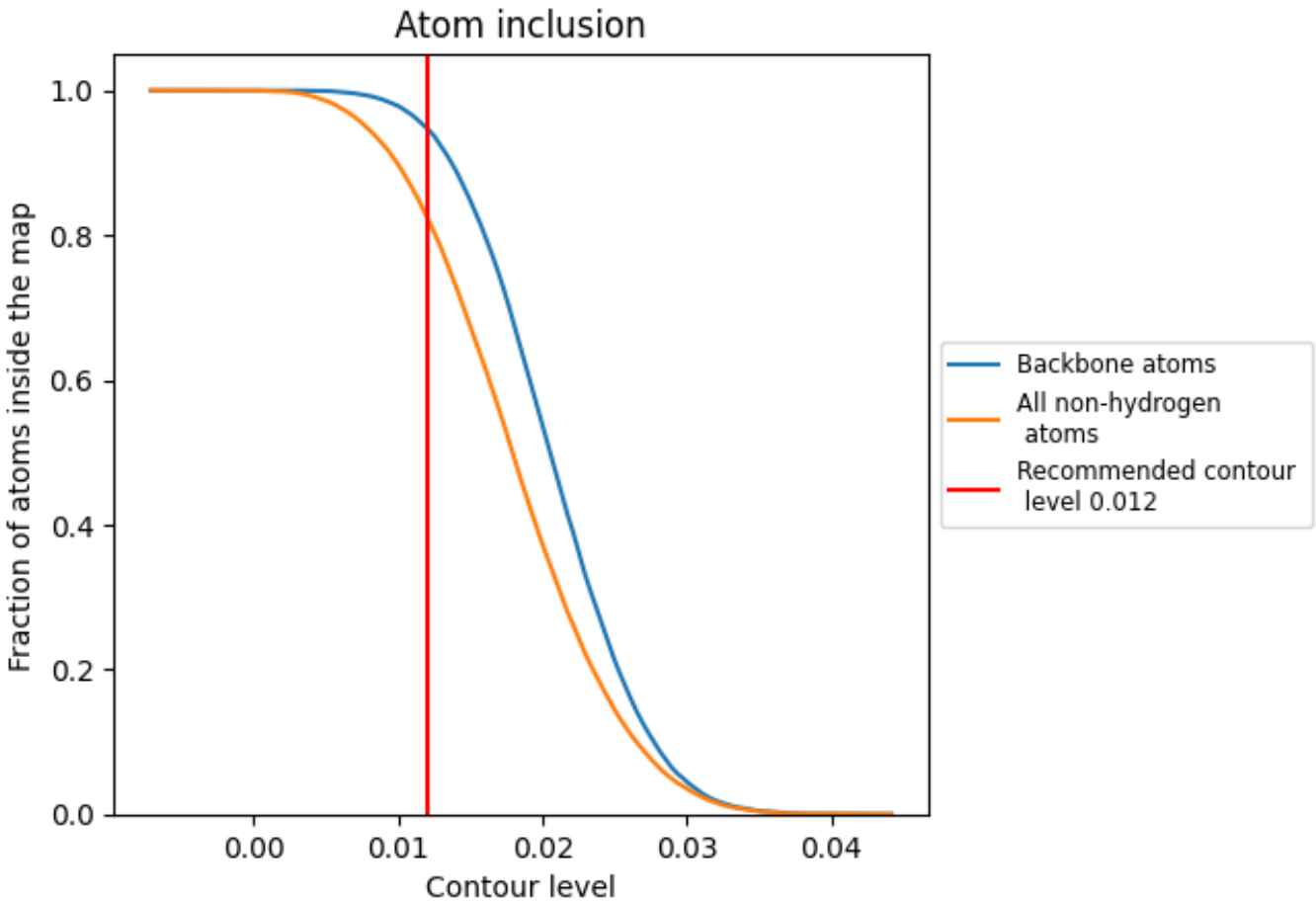
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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, 95% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.