Full wwPDB EM Validation Report ⓘ

Mar 13, 2025 – 02:44 PM JST

PDB ID	:	8YD1
EMDB ID	:	EMD-39162
Title	:	CryoEM structure of M. tuberculosis ClpC1P1P2 complex bound to bortezomib, conformation 1
Authors	:	Zhou, B.; Zhao, H.; Gao, Y.; Chen, X.; Zhang, T.; He, J.; Xiong, X.
Deposited on	:	2024-02-19
Resolution	:	2.81 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:

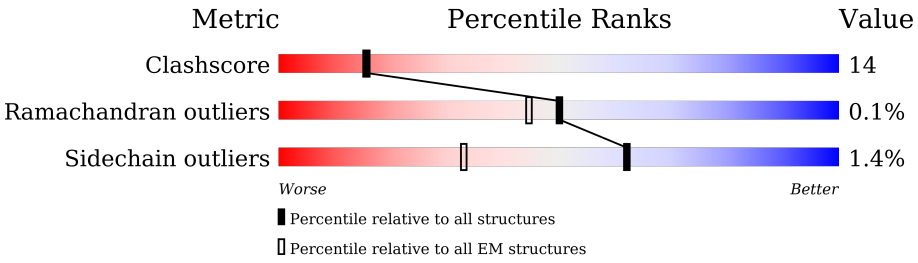
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.81 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	657	5% 68% 18% 13%
1	B	657	68% 18% 14%
1	C	657	70% 17% 13%
1	D	657	8% 66% 16% 17%
1	E	657	32% 8% 59%
1	F	657	9% 50% 18% 31%
2	G	181	69% 30%
2	H	181	69% 30%

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Mol	Chain	Length	Quality of chain
2	I	181	69% 31%
2	J	181	73% 26%
2	K	181	68% 31%
2	L	181	69% 30%
2	M	181	67% 31%
3	N	178	77% 22%
3	O	178	79% 20%
3	P	178	79% 20%
3	Q	178	80% 19%
3	R	178	77% 22%
3	S	178	76% 24%
3	T	178	79% 20%
4	a	24	17% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	901	-	-	X	-
6	ATP	A	902	-	-	X	-
6	ATP	A	904	-	-	X	-
6	ATP	B	903	-	-	X	-
6	ATP	C	901	-	-	X	-
6	ATP	C	904	-	-	X	-
6	ATP	D	903	-	-	X	-
7	ADP	D	901	-	-	X	-
7	ADP	F	901	-	-	X	-
8	BO2	G	301	-	-	X	-
8	BO2	H	301	-	-	X	-
8	BO2	I	301	-	-	X	-
8	BO2	J	301	-	-	X	-
8	BO2	K	301	-	-	X	-
8	BO2	L	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BO2	O	201	-	-	X	-
8	BO2	P	201	-	-	X	-
8	BO2	Q	201	-	-	X	-
8	BO2	R	201	-	-	X	-
8	BO2	S	201	-	-	X	-
8	BO2	T	201	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 43488 atoms, of which 48 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-dependent Clp protease ATP-binding subunit ClpC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	573	Total	C	N	O	S	0	0
			4496	2833	805	848	10		
1	B	564	Total	C	N	O	S	0	0
			4414	2784	791	829	10		
1	C	570	Total	C	N	O	S	0	0
			4478	2825	801	841	11		
1	D	544	Total	C	N	O	S	0	0
			4267	2690	768	798	11		
1	E	268	Total	C	N	O	S	0	0
			2083	1310	375	394	4		
1	F	456	Total	C	N	O	S	0	0
			3602	2280	646	666	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ALA	GLU	engineered mutation	UNP P9WPC9
A	444	SER	PHE	engineered mutation	UNP P9WPC9
A	626	ALA	GLU	engineered mutation	UNP P9WPC9
B	288	ALA	GLU	engineered mutation	UNP P9WPC9
B	444	SER	PHE	engineered mutation	UNP P9WPC9
B	626	ALA	GLU	engineered mutation	UNP P9WPC9
C	288	ALA	GLU	engineered mutation	UNP P9WPC9
C	444	SER	PHE	engineered mutation	UNP P9WPC9
C	626	ALA	GLU	engineered mutation	UNP P9WPC9
D	288	ALA	GLU	engineered mutation	UNP P9WPC9
D	444	SER	PHE	engineered mutation	UNP P9WPC9
D	626	ALA	GLU	engineered mutation	UNP P9WPC9
E	288	ALA	GLU	engineered mutation	UNP P9WPC9
E	444	SER	PHE	engineered mutation	UNP P9WPC9
E	626	ALA	GLU	engineered mutation	UNP P9WPC9
F	288	ALA	GLU	engineered mutation	UNP P9WPC9
F	444	SER	PHE	engineered mutation	UNP P9WPC9
F	626	ALA	GLU	engineered mutation	UNP P9WPC9

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	H	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	I	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	J	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	K	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	L	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	M	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	O	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	P	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	Q	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	R	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	S	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	T	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		

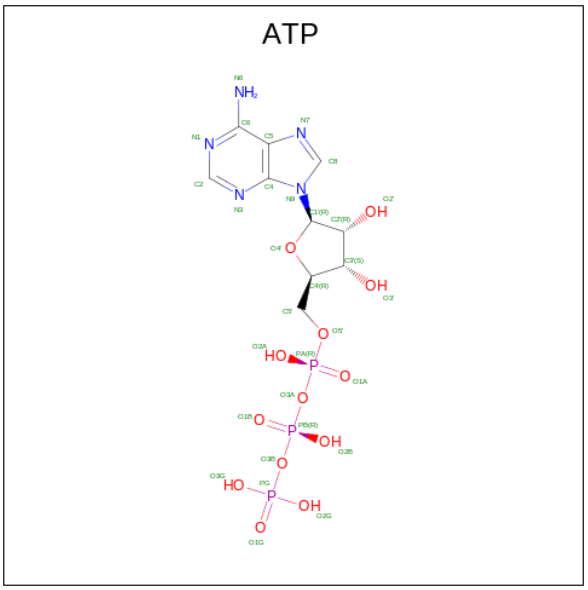
- Molecule 4 is a protein called Beta-casein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	24	Total	C	N	O	S	0	0
			181	119	29	31	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

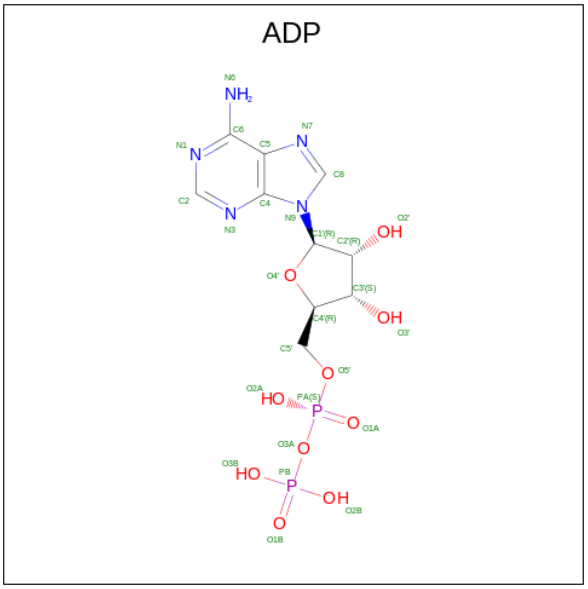
Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Mg 2 2	0
5	B	2	Total Mg 2 2	0
5	C	2	Total Mg 2 2	0
5	D	1	Total Mg 1 1	0

- Molecule 6 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).



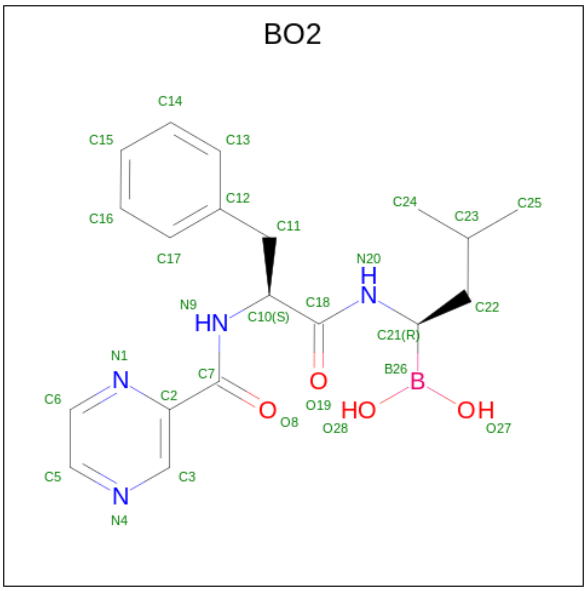
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O P 31 10 5 13 3	0
6	A	1	Total C H N O P 43 10 12 5 13 3	0
6	B	1	Total C N O P 31 10 5 13 3	0
6	B	1	Total C N O P 31 10 5 13 3	0
6	C	1	Total C N O P 31 10 5 13 3	0
6	C	1	Total C N O P 31 10 5 13 3	0
6	D	1	Total C H N O P 43 10 12 5 13 3	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	D	1	Total C H N O P 39 10 12 5 10 2	0
7	E	1	Total C N O P 27 10 5 10 2	0
7	F	1	Total C H N O P 39 10 12 5 10 2	0

- Molecule 8 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: $C_{19}H_{25}BN_4O_4$) (labeled as "Ligand of Interest" by depositor).



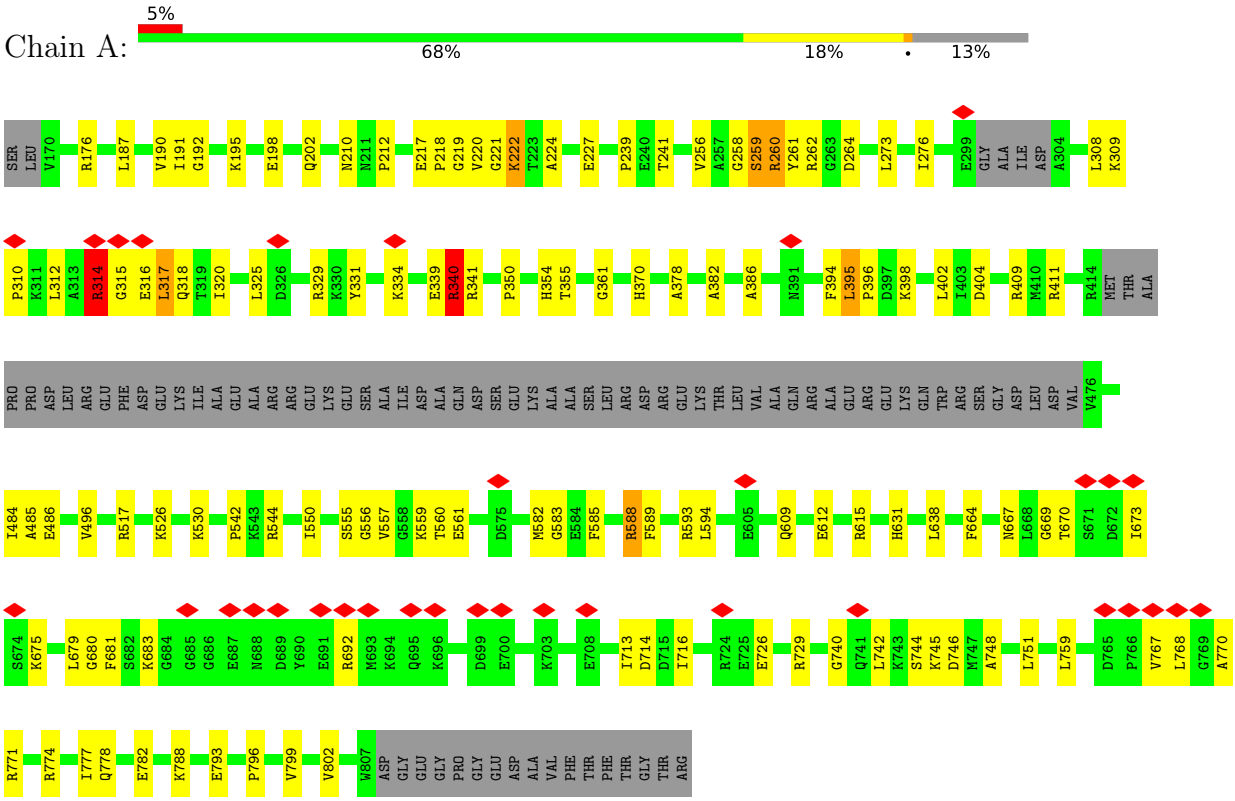
Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	H	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	I	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	J	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	K	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	L	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	M	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	N	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	O	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	P	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	Q	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	R	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	S	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	T	1	Total	B	C	N	O	0
			28	1	19	4	4	

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.

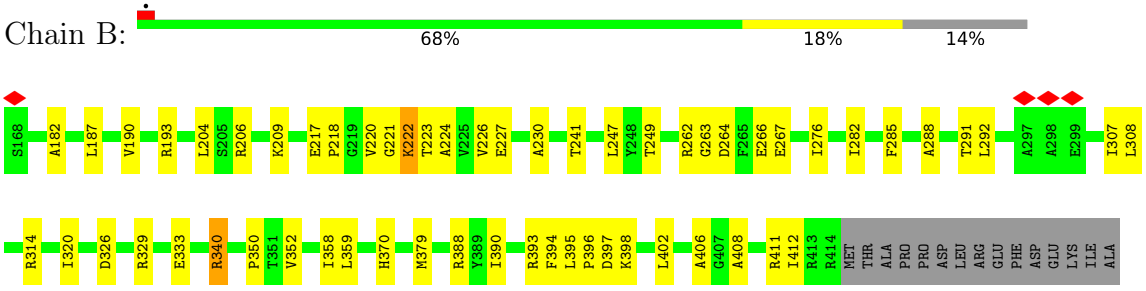
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

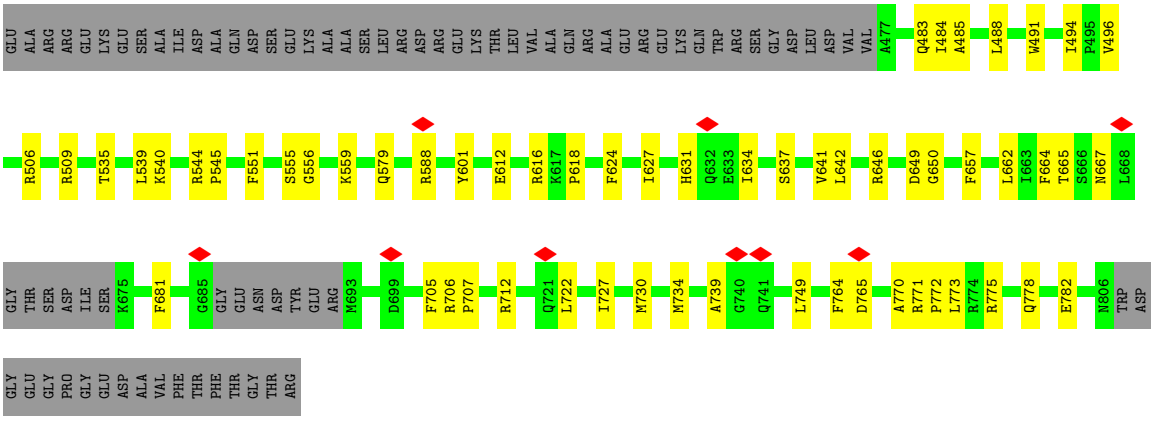
Chain A:



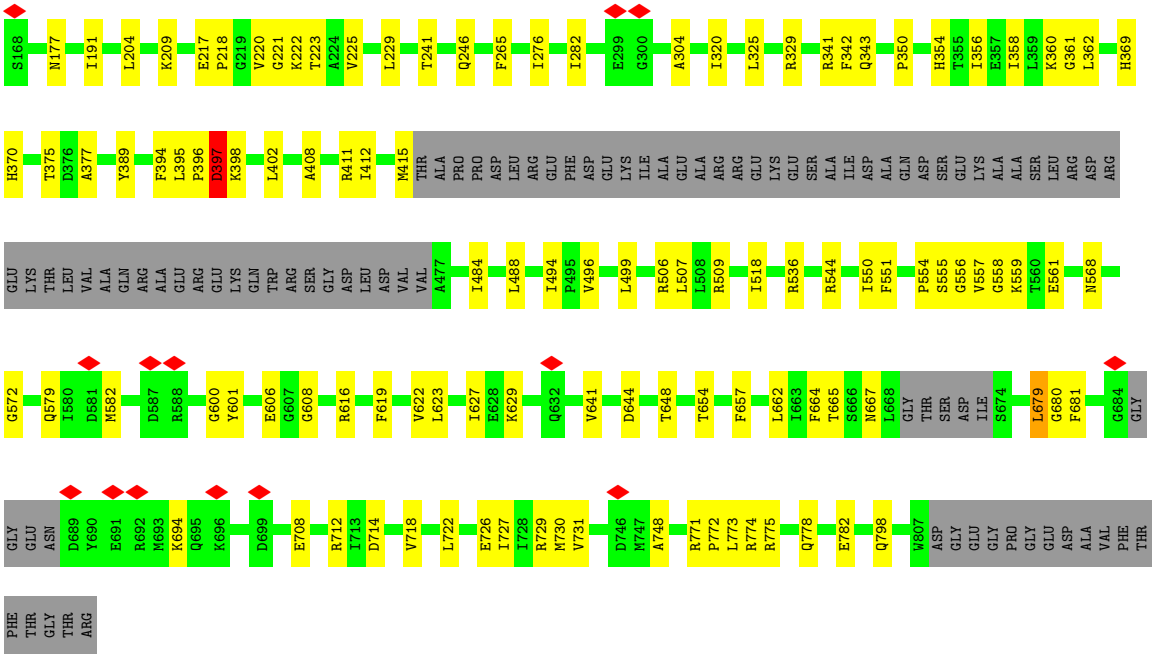
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

Chain B:

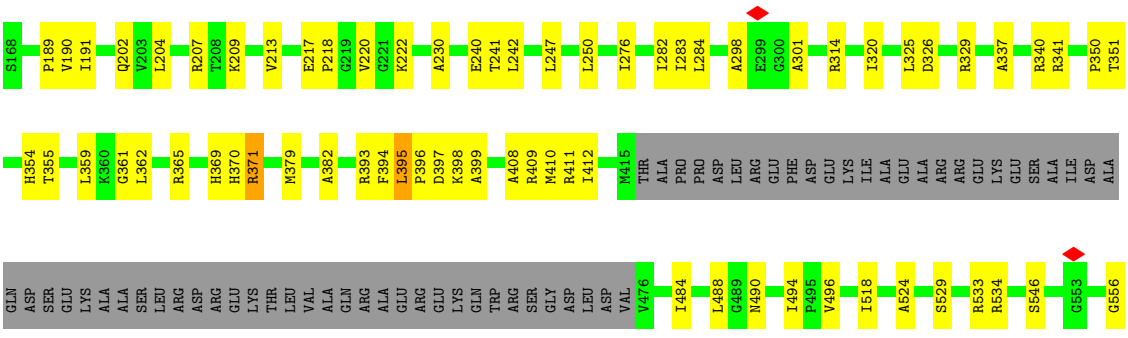


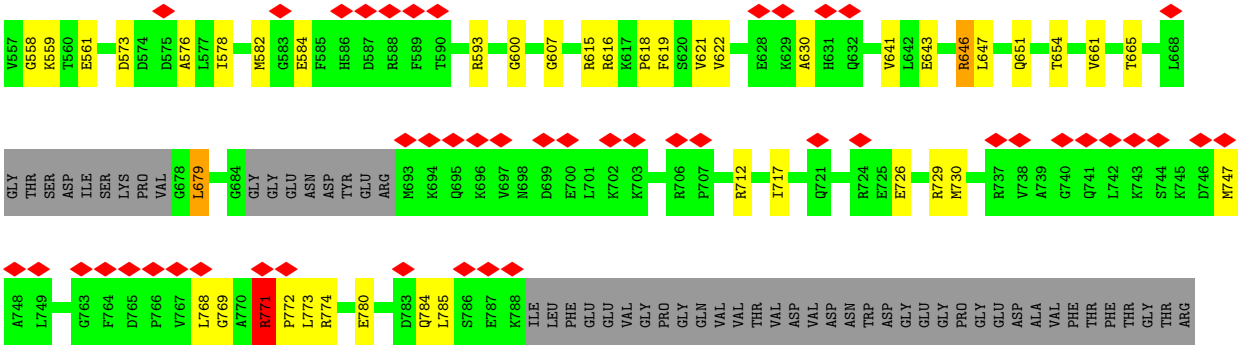


• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1



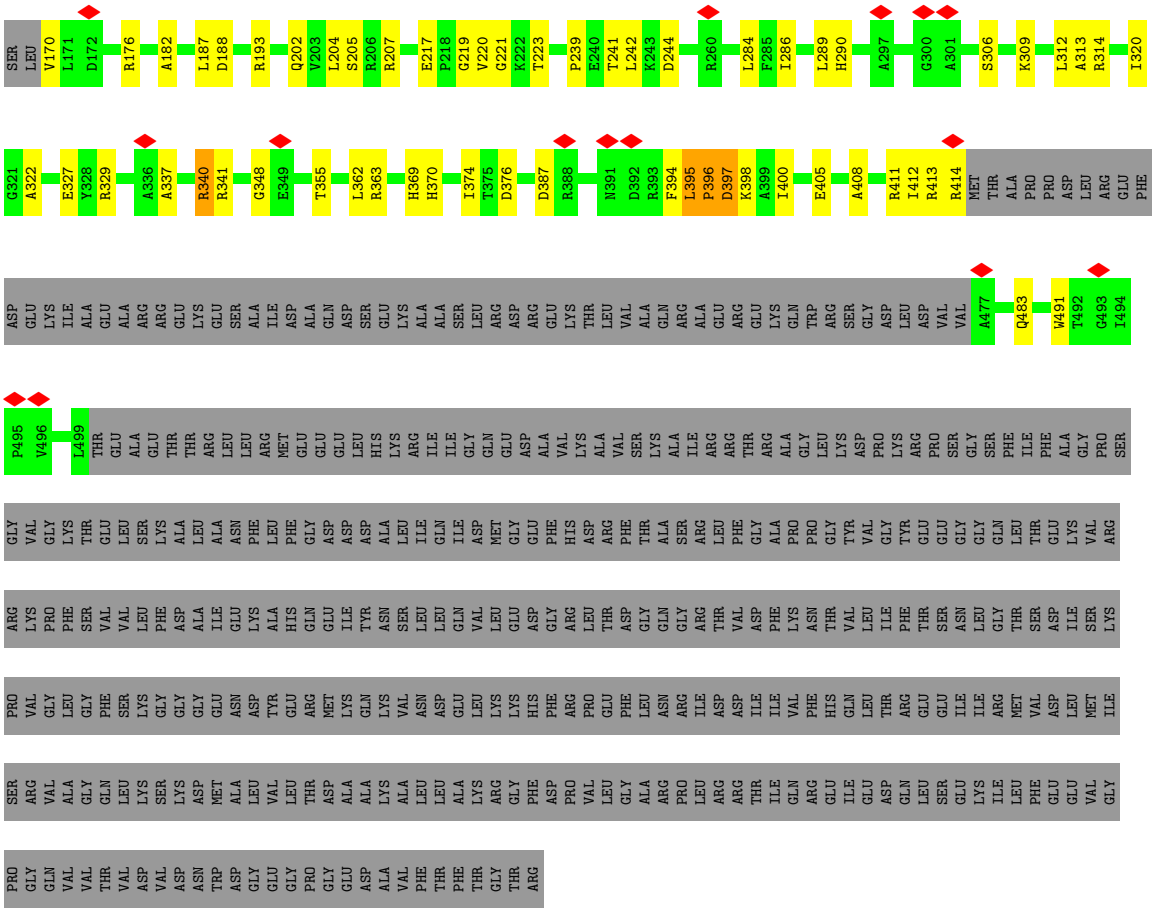
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1





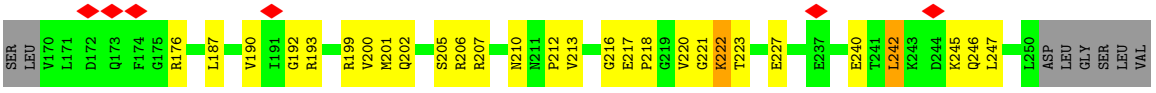
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

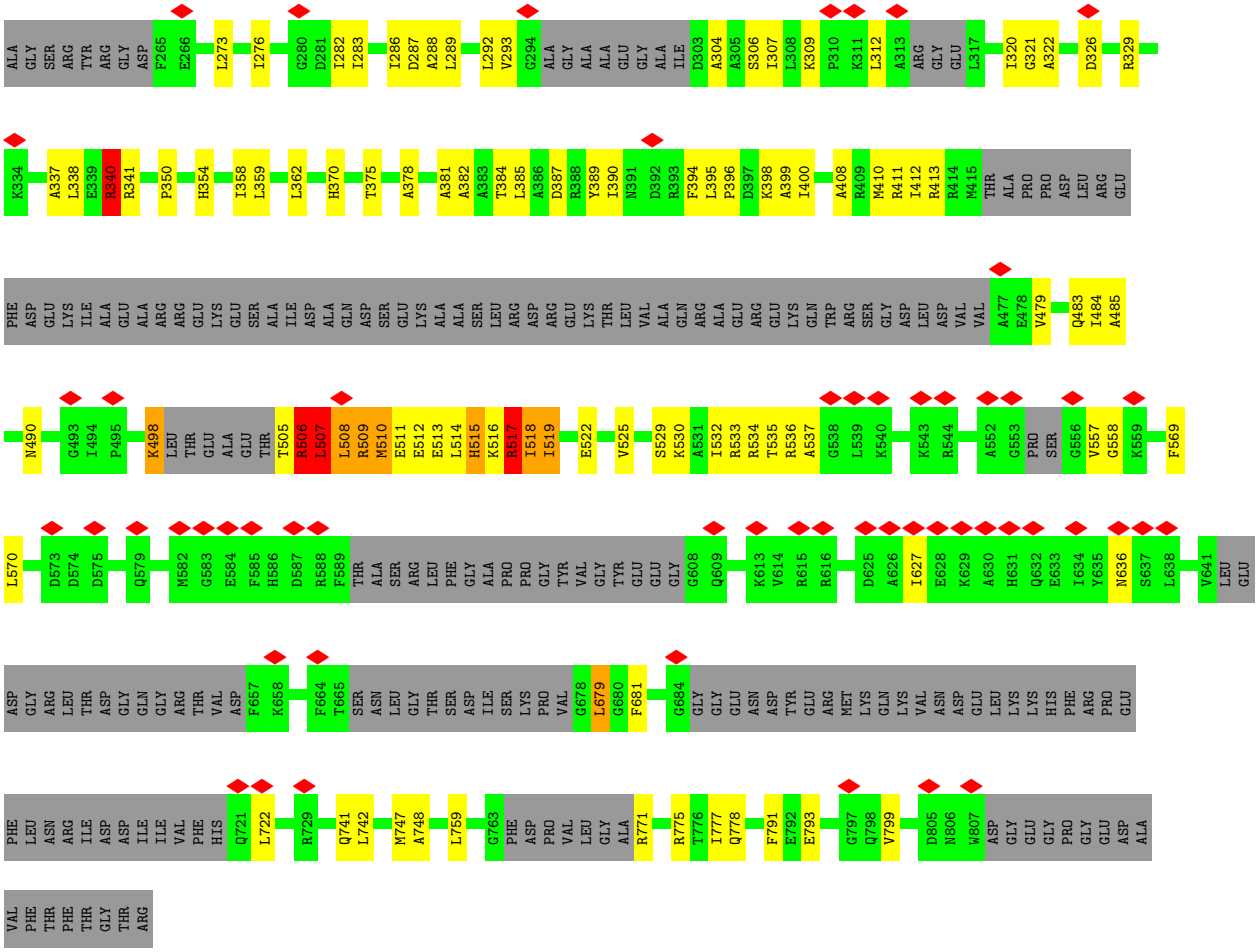
Chain E:



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

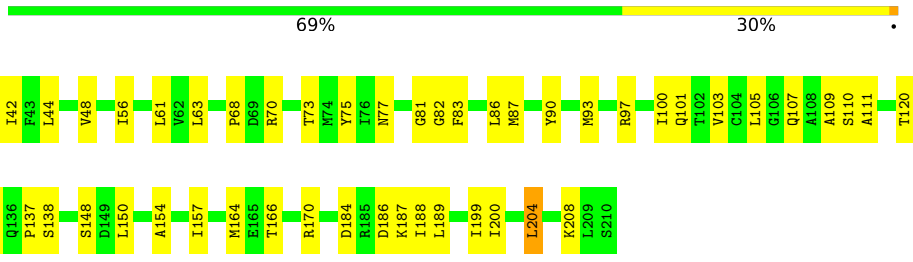
Chain F:





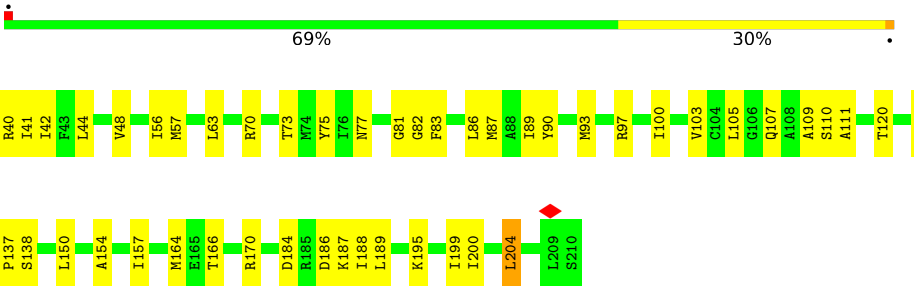
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain G:



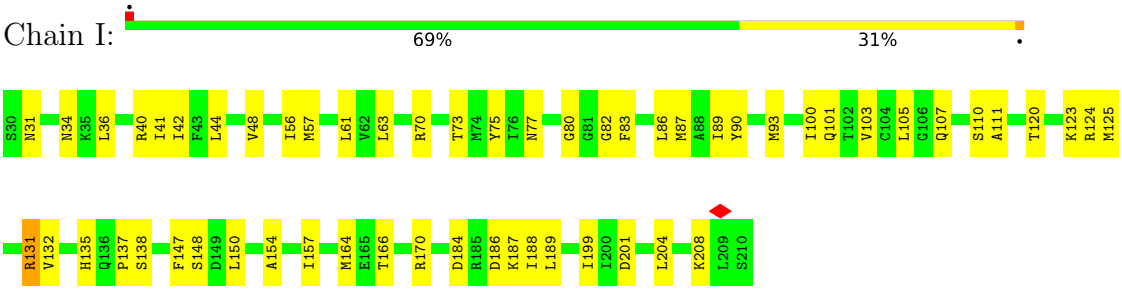
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain H:



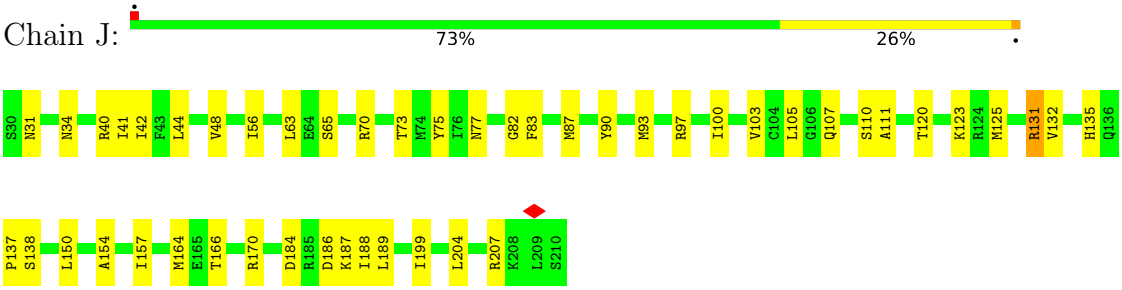
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain I:



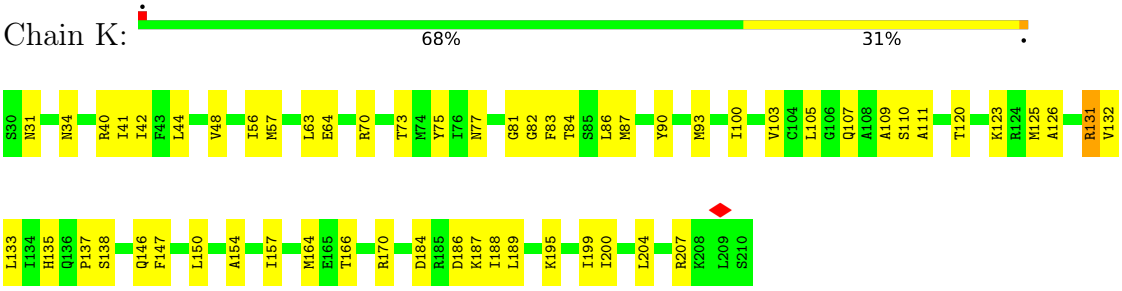
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain J:



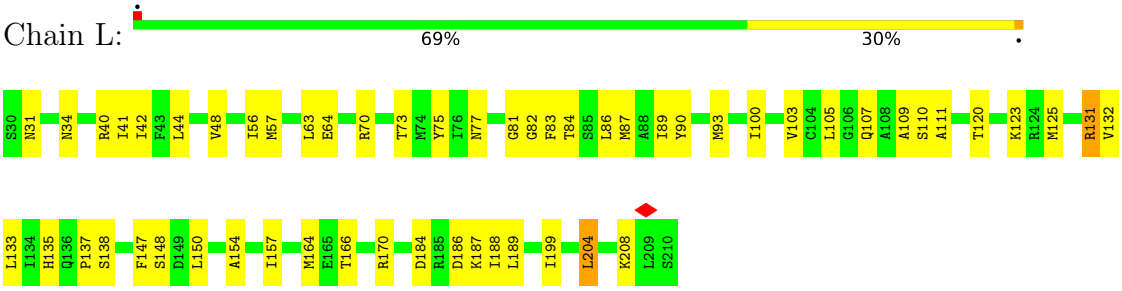
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain K:



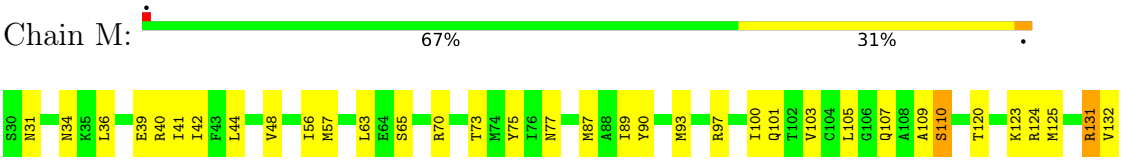
• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

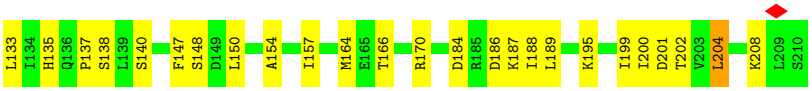
Chain L:



• Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

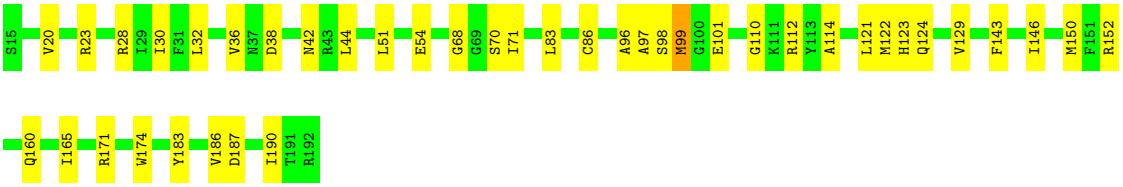
Chain M:





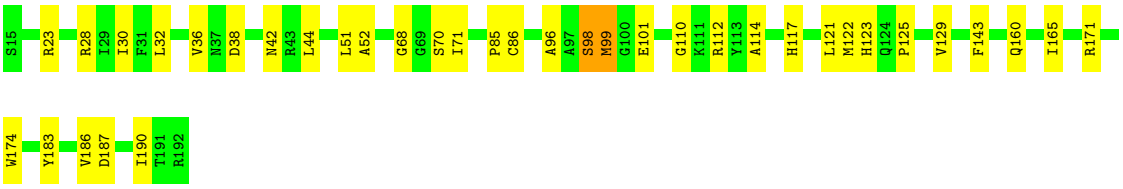
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain N:



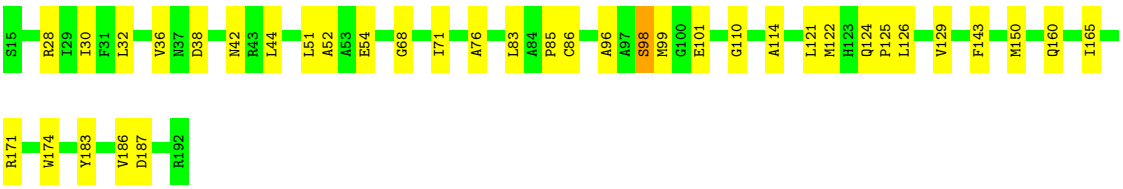
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain O:



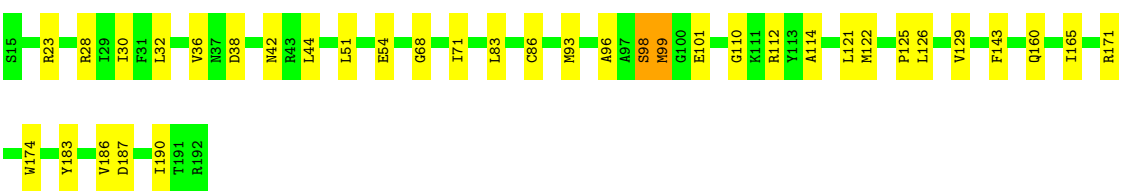
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain P:



• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain Q:



• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

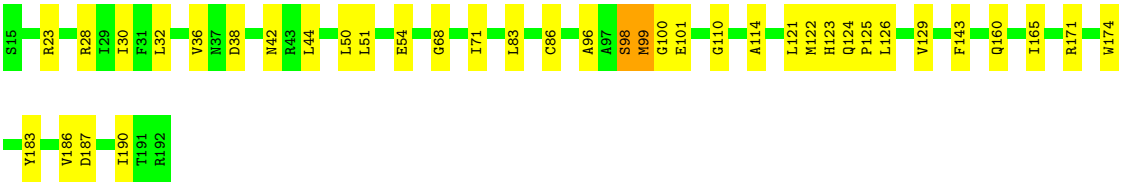
Chain R:

• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain S:

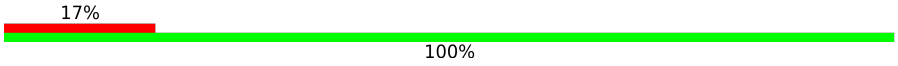
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

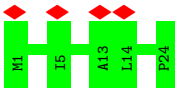
Chain T:



• Molecule 4: Beta-casein

Chain a:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	363.52, 363.52, 363.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	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: ADP, BO2, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/4560	0.56	0/6141
1	B	0.41	0/4474	0.59	0/6022
1	C	0.41	0/4541	0.57	1/6113 (0.0%)
1	D	0.37	1/4324 (0.0%)	0.56	2/5815 (0.0%)
1	E	0.35	0/2109	0.58	1/2846 (0.0%)
1	F	0.32	0/3640	0.58	1/4883 (0.0%)
2	G	0.51	0/1406	0.62	1/1902 (0.1%)
2	H	0.51	0/1406	0.62	1/1902 (0.1%)
2	I	0.51	0/1406	0.62	1/1902 (0.1%)
2	J	0.51	0/1406	0.62	1/1902 (0.1%)
2	K	0.51	0/1406	0.62	1/1902 (0.1%)
2	L	0.51	0/1406	0.62	1/1902 (0.1%)
2	M	0.51	0/1406	0.62	1/1902 (0.1%)
3	N	0.52	0/1379	0.57	0/1864
3	O	0.53	0/1379	0.57	0/1864
3	P	0.52	0/1379	0.57	0/1864
3	Q	0.52	0/1379	0.57	0/1864
3	R	0.52	0/1379	0.57	0/1864
3	S	0.54	0/1379	0.57	0/1864
3	T	0.53	0/1379	0.57	0/1864
4	a	0.34	0/181	0.75	0/245
All	All	0.45	1/43324 (0.0%)	0.58	12/58427 (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	3
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	F	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	VAL	CB-CG2	-5.15	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	679	LEU	CA-CB-CG	6.39	129.99	115.30
1	E	244	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	785	LEU	CA-CB-CG	5.92	128.91	115.30
1	F	679	LEU	CA-CB-CG	5.65	128.30	115.30
1	C	679	LEU	CA-CB-CG	5.62	128.22	115.30
2	G	204	LEU	CA-CB-CG	5.13	127.11	115.30
2	M	204	LEU	CA-CB-CG	5.13	127.10	115.30
2	H	204	LEU	CA-CB-CG	5.12	127.08	115.30
2	J	204	LEU	CA-CB-CG	5.12	127.07	115.30
2	I	204	LEU	CA-CB-CG	5.12	127.06	115.30
2	K	204	LEU	CA-CB-CG	5.12	127.07	115.30
2	L	204	LEU	CA-CB-CG	5.11	127.04	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ARG	Sidechain
1	A	314	ARG	Sidechain
1	A	340	ARG	Sidechain
1	B	340	ARG	Sidechain
1	D	771	ARG	Sidechain
1	F	340	ARG	Sidechain
1	F	506	ARG	Sidechain
1	F	517	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	4496	0	4586	148	0
1	B	4414	0	4525	124	0
1	C	4478	0	4578	117	0
1	D	4267	0	4381	169	0
1	E	2083	0	2138	103	0
1	F	3602	0	3723	159	0
2	G	1389	0	1402	46	0
2	H	1389	0	1402	44	0
2	I	1389	0	1402	44	0
2	J	1389	0	1402	40	0
2	K	1389	0	1402	48	0
2	L	1389	0	1402	45	0
2	M	1389	0	1402	46	0
3	N	1357	0	1348	38	0
3	O	1357	0	1348	33	0
3	P	1357	0	1348	34	0
3	Q	1357	0	1348	35	0
3	R	1357	0	1348	41	0
3	S	1357	0	1348	45	0
3	T	1357	0	1348	38	0
4	a	181	0	208	0	0
5	A	2	0	0	0	0
5	B	2	0	0	2	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	62	12	24	35	0
6	B	62	0	24	34	0
6	C	62	0	24	46	0
6	D	31	12	12	11	0
7	D	27	12	12	41	0
7	E	27	0	12	8	0
7	F	27	12	11	14	0
8	G	28	0	25	13	0
8	H	28	0	25	13	0
8	I	28	0	25	13	0
8	J	28	0	25	12	0
8	K	28	0	25	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	28	0	25	14	0
8	M	28	0	25	7	0
8	N	28	0	25	8	0
8	O	28	0	25	12	0
8	P	28	0	25	12	0
8	Q	28	0	25	12	0
8	R	28	0	25	18	0
8	S	28	0	25	13	0
8	T	28	0	25	11	0
All	All	43440	48	43858	1251	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 14.

All (1251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ARG:HH22	1:E:241:THR:CB	1.23	1.51
1:D:411:ARG:NH2	1:E:241:THR:HB	1.23	1.46
1:E:411:ARG:HD2	1:F:205:SER:CB	1.48	1.41
1:D:730:MET:HE1	7:D:901:ADP:N3	1.23	1.38
1:D:371:ARG:NH2	1:D:411:ARG:HE	1.15	1.36
1:E:411:ARG:CD	1:F:205:SER:HB3	1.52	1.35
1:D:730:MET:CE	7:D:901:ADP:N3	1.90	1.34
1:F:221:GLY:CA	7:F:901:ADP:O1A	1.73	1.34
1:D:411:ARG:HH12	1:E:241:THR:CG2	1.41	1.31
1:C:518:ILE:HD12	6:C:904:ATP:N1	1.49	1.27
1:D:411:ARG:NH1	1:E:241:THR:HG21	1.46	1.27
1:D:774:ARG:NH1	7:D:901:ADP:O3'	1.67	1.26
1:F:370:HIS:CD2	1:F:411:ARG:HH12	1.54	1.26
1:D:412:ILE:HD11	1:E:202:GLN:CA	1.71	1.20
1:D:371:ARG:NH2	1:D:411:ARG:NE	1.89	1.18
1:C:518:ILE:HD12	6:C:904:ATP:C6	1.79	1.17
1:D:518:ILE:HA	7:D:901:ADP:N1	1.59	1.16
1:F:370:HIS:HA	1:F:411:ARG:NH1	1.57	1.16
1:D:371:ARG:CZ	1:D:411:ARG:HE	1.59	1.15
1:F:370:HIS:CG	1:F:411:ARG:HH12	1.64	1.15
6:D:903:ATP:H3'	1:E:314:ARG:NH2	1.65	1.11
1:F:370:HIS:CD2	1:F:411:ARG:NH1	2.19	1.11
1:A:221:GLY:HA2	6:A:904:ATP:O2A	1.50	1.10
1:A:220:VAL:HA	1:A:396:PRO:HG2	1.22	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:ARG:HH22	1:E:241:THR:CG2	1.66	1.08
1:D:518:ILE:HB	7:D:901:ADP:N6	1.68	1.08
1:C:412:ILE:HD11	1:D:202:GLN:HA	1.39	1.05
1:D:561:GLU:CG	7:D:901:ADP:H3'	1.85	1.05
1:D:730:MET:HE2	7:D:901:ADP:H1'	1.35	1.04
3:Q:125:PRO:HA	8:Q:201:BO2:H221	1.40	1.04
1:D:411:ARG:NH1	1:E:241:THR:CG2	2.12	1.03
1:C:518:ILE:CD1	6:C:904:ATP:C6	2.41	1.03
1:F:221:GLY:HA2	7:F:901:ADP:O1A	0.87	1.03
1:D:411:ARG:NH2	1:E:241:THR:CB	1.95	1.02
1:D:412:ILE:CD1	1:E:202:GLN:HA	1.90	1.02
1:C:771:ARG:HE	6:C:904:ATP:H5'1	1.21	1.02
1:C:771:ARG:NH1	6:C:904:ATP:O1G	1.93	1.01
1:D:370:HIS:HA	1:D:411:ARG:HD2	1.42	1.01
1:D:561:GLU:HG3	7:D:901:ADP:H3'	1.40	1.00
1:A:774:ARG:HH11	6:A:902:ATP:H4'	1.24	1.00
1:C:369:HIS:O	1:C:411:ARG:NH1	1.94	0.99
6:D:903:ATP:H3'	1:E:314:ARG:HH22	1.28	0.99
3:T:125:PRO:HA	8:T:201:BO2:H221	1.43	0.97
1:A:222:LYS:N	6:A:904:ATP:O1B	1.97	0.97
1:F:370:HIS:CA	1:F:411:ARG:NH1	2.26	0.97
1:A:222:LYS:HD2	6:A:904:ATP:O1B	1.64	0.97
3:R:71:ILE:HG12	8:R:201:BO2:HN9	1.26	0.97
1:D:412:ILE:HD11	1:E:202:GLN:HA	0.97	0.96
1:D:518:ILE:HB	7:D:901:ADP:HN62	1.22	0.96
1:E:412:ILE:HD11	1:F:202:GLN:HA	1.47	0.96
1:A:218:PRO:HD2	1:A:394:PHE:HE2	1.26	0.96
1:C:350:PRO:HD2	1:C:396:PRO:HD3	1.46	0.96
1:D:371:ARG:HH22	1:D:411:ARG:CZ	1.78	0.95
1:E:411:ARG:CZ	1:F:205:SER:O	2.14	0.95
1:F:395:LEU:HD23	1:F:398:LYS:HE3	1.49	0.95
3:S:98:SER:HB2	3:S:123:HIS:CE1	2.03	0.94
1:A:556:GLY:HA2	6:A:902:ATP:O3A	1.48	0.93
1:D:371:ARG:HH22	1:D:411:ARG:NE	1.57	0.92
3:O:125:PRO:HA	8:O:201:BO2:H221	1.50	0.91
1:F:221:GLY:HA2	7:F:901:ADP:PA	2.10	0.91
1:A:770:ALA:O	1:A:774:ARG:HG3	1.71	0.91
3:R:125:PRO:HA	8:R:201:BO2:H221	1.53	0.91
1:F:370:HIS:HA	1:F:411:ARG:HH11	1.26	0.91
1:D:371:ARG:HH22	1:D:411:ARG:NH2	1.69	0.90
1:A:770:ALA:HB2	6:A:902:ATP:N3	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ALA:CB	6:A:902:ATP:N3	2.35	0.90
1:D:561:GLU:HG2	7:D:901:ADP:O2A	1.70	0.90
1:D:730:MET:CE	7:D:901:ADP:H1'	2.02	0.89
1:E:220:VAL:HA	1:E:396:PRO:HG2	1.53	0.89
1:D:220:VAL:HA	1:D:396:PRO:HG2	1.54	0.89
1:D:412:ILE:CD1	1:E:202:GLN:CA	2.50	0.89
1:A:771:ARG:HE	6:A:902:ATP:C5'	1.86	0.88
1:D:411:ARG:NH2	1:E:241:THR:CG2	2.29	0.88
1:A:355:THR:HG21	1:A:395:LEU:HD22	1.54	0.87
1:F:370:HIS:CG	1:F:411:ARG:NH1	2.40	0.87
1:F:370:HIS:CA	1:F:411:ARG:HH11	1.87	0.86
1:D:411:ARG:HH12	1:E:241:THR:HG21	0.70	0.85
1:A:555:SER:OG	6:A:902:ATP:O2G	1.93	0.85
1:A:774:ARG:NH1	6:A:902:ATP:H4'	1.90	0.85
3:N:98:SER:HB2	3:N:123:HIS:CE1	2.11	0.85
1:D:558:GLY:CA	7:D:901:ADP:N7	2.40	0.85
1:A:218:PRO:HD2	1:A:394:PHE:CE2	2.12	0.84
1:D:730:MET:CE	7:D:901:ADP:C4	2.58	0.84
1:A:202:GLN:HA	1:F:412:ILE:HD11	1.58	0.84
3:O:98:SER:O	3:O:101:GLU:HG3	1.78	0.84
1:D:411:ARG:CZ	1:E:241:THR:CG2	2.55	0.84
1:D:730:MET:HE2	7:D:901:ADP:C1'	2.08	0.84
1:F:370:HIS:CB	1:F:411:ARG:NH1	2.40	0.83
1:F:220:VAL:HA	1:F:396:PRO:HG2	1.58	0.83
1:A:217:GLU:HB3	1:A:394:PHE:CE2	2.14	0.82
1:A:555:SER:OG	6:A:902:ATP:PG	2.38	0.82
1:C:223:THR:HG22	6:C:901:ATP:O2B	1.79	0.82
3:P:150:MET:HE2	8:P:201:BO2:H251	1.59	0.81
1:D:518:ILE:CB	7:D:901:ADP:N6	2.43	0.81
1:B:734:MET:CE	6:B:903:ATP:H1'	2.10	0.81
3:R:71:ILE:HD11	8:R:201:BO2:H23	1.63	0.81
6:C:904:ATP:PG	1:D:712:ARG:NH2	2.54	0.81
1:B:222:LYS:HD2	6:B:904:ATP:PB	2.20	0.81
1:B:559:LYS:HZ2	6:B:903:ATP:PB	2.03	0.81
3:S:98:SER:O	3:S:101:GLU:HG3	1.78	0.81
1:C:408:ALA:O	1:C:412:ILE:HG13	1.80	0.80
1:F:370:HIS:HD2	1:F:411:ARG:NH1	1.79	0.80
2:J:164:MET:HG3	8:J:301:BO2:H251	1.63	0.80
1:D:561:GLU:HG3	7:D:901:ADP:C3'	2.11	0.80
1:A:202:GLN:HG2	1:F:412:ILE:HD12	1.64	0.80
3:P:125:PRO:HA	8:P:201:BO2:H221	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:98:SER:O	3:Q:101:GLU:HG3	1.82	0.79
3:S:150:MET:HE2	8:S:201:BO2:H251	1.65	0.79
1:C:518:ILE:CD1	6:C:904:ATP:N6	2.46	0.79
1:B:358:ILE:HD12	6:B:904:ATP:C6	2.18	0.78
1:A:555:SER:HA	6:A:902:ATP:O2G	1.82	0.78
1:A:308:LEU:HB3	1:A:312:LEU:HG	1.65	0.78
1:A:770:ALA:HB2	6:A:902:ATP:C2	2.19	0.78
2:J:137:PRO:HG3	8:J:301:BO2:H253	1.64	0.77
1:B:730:MET:HE1	6:B:903:ATP:N1	1.99	0.77
1:F:350:PRO:HG3	1:F:396:PRO:HG3	1.66	0.77
2:J:83:PHE:HD1	8:J:301:BO2:H252	1.47	0.77
3:R:98:SER:O	3:R:101:GLU:HG3	1.84	0.77
3:S:98:SER:HB2	3:S:123:HIS:HE1	1.46	0.77
3:R:71:ILE:HG12	8:R:201:BO2:N9	1.99	0.77
3:T:98:SER:O	3:T:101:GLU:HG3	1.85	0.77
1:B:730:MET:HE1	6:B:903:ATP:C2	2.20	0.77
1:D:518:ILE:HG22	7:D:901:ADP:C6	2.20	0.76
1:D:412:ILE:CD1	1:E:202:GLN:CB	2.63	0.76
1:E:412:ILE:CD1	1:F:202:GLN:HA	2.16	0.76
1:F:190:VAL:HA	7:F:901:ADP:N1	1.99	0.76
1:A:220:VAL:CA	1:A:396:PRO:HG2	2.10	0.76
1:F:510:MET:HG2	1:F:570:LEU:HD21	1.68	0.76
3:N:98:SER:O	3:N:101:GLU:HG3	1.85	0.76
1:A:350:PRO:HD2	1:A:396:PRO:HD3	1.68	0.75
1:D:371:ARG:CZ	1:D:411:ARG:NE	2.42	0.75
1:A:555:SER:OG	6:A:902:ATP:O1G	2.03	0.75
1:B:730:MET:CE	6:B:903:ATP:C2	2.70	0.75
1:C:518:ILE:HD11	6:C:904:ATP:N6	2.01	0.75
1:D:371:ARG:HH22	1:D:411:ARG:HH21	1.34	0.75
3:P:98:SER:O	3:P:101:GLU:HG3	1.85	0.74
1:D:730:MET:SD	7:D:901:ADP:N3	2.61	0.74
2:J:82:GLY:H	8:J:301:BO2:H13	1.50	0.74
1:A:350:PRO:CD	1:A:396:PRO:HG3	2.17	0.74
1:C:412:ILE:CD1	1:D:202:GLN:HA	2.16	0.74
1:E:370:HIS:ND1	1:E:411:ARG:NH2	2.34	0.74
1:B:222:LYS:HD2	6:B:904:ATP:O1B	1.88	0.73
1:F:408:ALA:O	1:F:412:ILE:HG13	1.89	0.73
1:D:412:ILE:CD1	1:E:202:GLN:HB2	2.19	0.73
1:B:220:VAL:HA	1:B:396:PRO:HG2	1.70	0.73
1:B:730:MET:HE3	6:B:903:ATP:C4	2.24	0.73
1:A:771:ARG:HE	6:A:902:ATP:H5'1	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:CZ	1:B:544:ARG:NH1	2.52	0.73
3:N:71:ILE:HD11	8:N:201:BO2:H23	1.71	0.73
3:N:98:SER:HB2	3:N:123:HIS:HE1	1.53	0.73
2:H:83:PHE:HD1	8:H:301:BO2:H252	1.55	0.72
2:K:164:MET:HG3	8:K:301:BO2:H251	1.71	0.72
3:R:150:MET:HE2	8:R:201:BO2:H251	1.71	0.72
1:A:218:PRO:CD	1:A:394:PHE:HE2	2.02	0.72
1:D:350:PRO:HD2	1:D:396:PRO:HD3	1.70	0.72
1:D:730:MET:SD	7:D:901:ADP:C2	2.82	0.72
1:D:411:ARG:HH22	1:E:241:THR:CA	2.02	0.72
3:N:150:MET:HE2	8:N:201:BO2:H251	1.71	0.72
2:G:83:PHE:HD1	8:G:301:BO2:H252	1.54	0.71
1:E:411:ARG:HD2	1:F:205:SER:HB3	0.74	0.71
2:G:164:MET:HG3	8:G:301:BO2:H251	1.71	0.71
1:F:217:GLU:HB3	1:F:394:PHE:CE2	2.25	0.71
1:F:370:HIS:HD2	1:F:411:ARG:CZ	2.02	0.71
1:A:221:GLY:CA	6:A:904:ATP:O2A	2.36	0.71
2:G:75:TYR:HB3	2:G:105:LEU:HD11	1.73	0.71
2:G:137:PRO:HG3	8:G:301:BO2:H253	1.73	0.71
1:A:555:SER:CA	6:A:902:ATP:O2G	2.39	0.71
2:K:75:TYR:HB3	2:K:105:LEU:HD11	1.73	0.71
2:K:83:PHE:HD1	8:K:301:BO2:H252	1.54	0.71
2:L:75:TYR:HB3	2:L:105:LEU:HD11	1.73	0.71
1:C:370:HIS:HA	1:C:411:ARG:HD2	1.70	0.71
1:C:568:ASN:OD1	1:C:572:GLY:C	2.28	0.70
2:H:164:MET:HG3	8:H:301:BO2:H251	1.73	0.70
2:L:40:ARG:HD3	2:L:70:ARG:HH11	1.56	0.70
1:F:220:VAL:CA	1:F:396:PRO:HG2	2.22	0.70
2:L:83:PHE:HD1	8:L:301:BO2:H252	1.56	0.70
2:M:75:TYR:HB3	2:M:105:LEU:HD11	1.73	0.70
3:P:71:ILE:HD11	8:P:201:BO2:H23	1.72	0.70
3:S:143:PHE:HE1	8:S:201:BO2:H5	1.55	0.70
2:H:40:ARG:HD3	2:H:70:ARG:HH11	1.56	0.70
2:I:40:ARG:HD3	2:I:70:ARG:HH11	1.56	0.70
2:M:40:ARG:HD3	2:M:70:ARG:HH11	1.56	0.70
1:F:509:ARG:HG2	1:F:536:ARG:HB3	1.72	0.70
3:O:143:PHE:HE1	8:O:201:BO2:H5	1.57	0.70
1:F:370:HIS:CD2	1:F:411:ARG:CZ	2.74	0.70
1:F:511:GLU:HG2	1:F:569:PHE:HZ	1.57	0.70
1:A:774:ARG:NH1	1:B:544:ARG:NH1	2.40	0.69
1:B:559:LYS:NZ	6:B:903:ATP:PB	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:164:MET:HG3	8:L:301:BO2:H251	1.73	0.69
2:G:40:ARG:HD3	2:G:70:ARG:HH11	1.56	0.69
2:H:75:TYR:HB3	2:H:105:LEU:HD11	1.73	0.69
2:I:75:TYR:HB3	2:I:105:LEU:HD11	1.73	0.69
2:K:40:ARG:HD3	2:K:70:ARG:HH11	1.56	0.69
1:C:518:ILE:HD11	6:C:904:ATP:C6	2.25	0.69
1:E:400:ILE:HD13	7:E:901:ADP:H1'	1.74	0.69
1:F:513:GLU:HA	1:F:516:LYS:HG2	1.74	0.69
2:J:40:ARG:HD3	2:J:70:ARG:HH11	1.56	0.69
1:B:730:MET:HE3	6:B:903:ATP:C5	2.27	0.69
2:J:83:PHE:CD1	8:J:301:BO2:H252	2.27	0.69
1:F:513:GLU:HB2	1:F:569:PHE:HE1	1.58	0.69
1:D:730:MET:HE2	7:D:901:ADP:C4	2.28	0.69
1:E:412:ILE:HD11	1:F:202:GLN:CA	2.22	0.69
1:E:408:ALA:O	1:E:411:ARG:HG2	1.93	0.69
2:K:137:PRO:HG3	8:K:301:BO2:H253	1.75	0.69
1:B:667:ASN:ND2	6:B:903:ATP:O1G	2.26	0.68
1:B:734:MET:HE1	6:B:903:ATP:H1'	1.74	0.68
2:J:75:TYR:HB3	2:J:105:LEU:HD11	1.73	0.68
1:D:558:GLY:HA2	7:D:901:ADP:N7	2.05	0.68
2:I:164:MET:HG3	8:I:301:BO2:H251	1.74	0.68
1:B:559:LYS:HZ1	6:B:903:ATP:PG	2.16	0.68
1:D:217:GLU:HB3	1:D:394:PHE:CZ	2.28	0.68
1:D:561:GLU:CG	7:D:901:ADP:C3'	2.66	0.68
1:F:370:HIS:CB	1:F:411:ARG:HH12	2.02	0.68
2:H:137:PRO:HG3	8:H:301:BO2:H253	1.75	0.68
1:A:202:GLN:HA	1:F:412:ILE:CD1	2.23	0.68
1:D:561:GLU:HG2	7:D:901:ADP:H3'	1.75	0.68
1:D:411:ARG:HH22	1:E:241:THR:HG22	1.59	0.67
6:D:903:ATP:O1G	1:E:341:ARG:NH1	2.26	0.67
2:K:82:GLY:H	8:K:301:BO2:H13	1.58	0.67
1:A:557:VAL:N	6:A:902:ATP:O1B	2.27	0.67
3:N:68:GLY:HA3	3:N:98:SER:HB3	1.76	0.67
1:A:771:ARG:HE	6:A:902:ATP:H5'2	1.59	0.67
2:G:82:GLY:H	8:G:301:BO2:H13	1.60	0.67
2:I:83:PHE:HD1	8:I:301:BO2:H252	1.58	0.67
2:L:208:LYS:HB2	2:M:97:ARG:HD2	1.77	0.67
3:P:150:MET:CE	8:P:201:BO2:H251	2.24	0.67
3:T:125:PRO:CA	8:T:201:BO2:H221	2.23	0.67
1:C:627:ILE:HD13	1:C:664:PHE:HB3	1.75	0.67
1:F:362:LEU:HD11	7:F:901:ADP:C2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:137:PRO:HG3	8:L:301:BO2:H253	1.77	0.67
2:M:137:PRO:HA	8:M:301:BO2:H221	1.76	0.67
1:F:221:GLY:N	7:F:901:ADP:O1A	2.28	0.67
1:F:396:PRO:O	1:F:400:ILE:HD12	1.95	0.66
1:F:679:LEU:HB3	2:M:65:SER:HB3	1.77	0.66
1:A:395:LEU:N	1:A:398:LYS:HE2	2.11	0.66
1:D:774:ARG:NH1	7:D:901:ADP:HO3'	1.93	0.66
1:E:408:ALA:HA	1:E:411:ARG:HG2	1.77	0.66
1:F:394:PHE:O	1:F:398:LYS:HG3	1.96	0.66
2:M:131:ARG:HH21	2:M:188:ILE:HG12	1.61	0.66
1:A:555:SER:CB	6:A:902:ATP:O2G	2.44	0.66
1:A:770:ALA:HB1	6:A:902:ATP:N3	2.09	0.66
6:C:901:ATP:O1G	1:D:341:ARG:NH1	2.29	0.66
1:A:273:LEU:HD22	1:A:317:LEU:HD13	1.77	0.65
2:J:131:ARG:HH21	2:J:188:ILE:HG12	1.61	0.65
3:S:71:ILE:HD11	8:S:201:BO2:H23	1.79	0.65
1:D:411:ARG:NH1	1:E:241:THR:HG22	2.11	0.65
3:S:71:ILE:HG12	8:S:201:BO2:C7	2.27	0.65
1:F:382:ALA:HA	1:F:484:ILE:HG21	1.79	0.65
1:D:518:ILE:CA	7:D:901:ADP:N1	2.50	0.65
1:A:771:ARG:HH12	1:B:712:ARG:HG2	1.61	0.65
1:D:679:LEU:HD11	2:I:36:LEU:HG	1.78	0.64
2:H:131:ARG:HH21	2:H:188:ILE:HG12	1.61	0.64
2:I:131:ARG:HH21	2:I:188:ILE:HG12	1.61	0.64
2:K:131:ARG:HH21	2:K:188:ILE:HG12	1.61	0.64
1:A:222:LYS:HD2	6:A:904:ATP:PB	2.36	0.64
1:F:370:HIS:CD2	1:F:411:ARG:HH22	2.16	0.64
1:B:209:LYS:HD3	1:B:340:ARG:HH12	1.62	0.64
1:C:221:GLY:N	6:C:901:ATP:O1B	2.30	0.64
1:D:408:ALA:O	1:D:412:ILE:HG13	1.97	0.64
1:D:411:ARG:NH2	1:E:241:THR:HG22	2.10	0.64
1:F:517:ARG:H	1:F:517:ARG:HD3	1.62	0.64
1:C:771:ARG:HE	6:C:904:ATP:C5'	2.07	0.63
1:B:506:ARG:HG2	1:B:509:ARG:HH21	1.63	0.63
2:I:82:GLY:H	8:I:301:BO2:H13	1.61	0.63
2:L:82:GLY:H	8:L:301:BO2:H13	1.62	0.63
2:L:131:ARG:HH21	2:L:188:ILE:HG12	1.61	0.63
1:B:412:ILE:HG22	1:B:412:ILE:O	1.98	0.63
6:C:904:ATP:O3G	1:D:712:ARG:NH2	2.30	0.63
1:A:260:ARG:HH12	1:B:267:GLU:HB3	1.64	0.63
1:B:408:ALA:HA	1:B:411:ARG:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:HD3	1:D:365:ARG:HE	1.64	0.63
1:D:394:PHE:O	1:D:398:LYS:HG2	1.98	0.63
1:A:221:GLY:HA2	6:A:904:ATP:PA	2.38	0.63
1:C:771:ARG:CZ	6:C:904:ATP:O1G	2.47	0.63
1:D:411:ARG:CZ	1:E:241:THR:HB	2.20	0.63
1:C:748:ALA:HB3	1:C:798:GLN:HE22	1.64	0.63
1:D:412:ILE:HD13	1:E:202:GLN:HB2	1.80	0.63
1:D:558:GLY:HA3	7:D:901:ADP:N7	2.14	0.63
1:F:370:HIS:CD2	1:F:411:ARG:NH2	2.66	0.62
3:Q:125:PRO:CA	8:Q:201:BO2:H221	2.22	0.62
1:E:411:ARG:NE	1:F:205:SER:HB3	2.13	0.62
3:S:143:PHE:CE1	8:S:201:BO2:H5	2.33	0.62
1:B:730:MET:SD	6:B:903:ATP:C2	2.92	0.62
1:F:218:PRO:CD	1:F:394:PHE:HE2	2.12	0.62
3:O:125:PRO:CA	8:O:201:BO2:H221	2.27	0.62
1:D:369:HIS:O	1:D:371:ARG:NH1	2.33	0.62
2:G:131:ARG:HH21	2:G:188:ILE:HG12	1.61	0.62
1:D:768:LEU:HB3	1:D:772:PRO:HG3	1.81	0.62
1:B:206:ARG:NH2	1:B:209:LYS:O	2.32	0.62
1:D:222:LYS:NZ	6:D:903:ATP:O2G	2.32	0.61
6:D:903:ATP:H3'	1:E:314:ARG:HH21	1.62	0.61
1:F:217:GLU:N	1:F:222:LYS:HE3	2.15	0.61
3:P:143:PHE:HE1	8:P:201:BO2:H5	1.63	0.61
3:S:54:GLU:OE2	3:T:23:ARG:NH2	2.30	0.61
3:T:71:ILE:HG12	8:T:201:BO2:C7	2.30	0.61
1:A:224:ALA:HB2	6:A:904:ATP:O2A	1.99	0.61
1:E:220:VAL:HA	1:E:396:PRO:CG	2.29	0.61
1:F:512:GLU:HA	1:F:515:HIS:ND1	2.16	0.61
1:B:730:MET:SD	6:B:903:ATP:N3	2.72	0.61
1:C:518:ILE:HA	6:C:904:ATP:N1	2.14	0.61
1:A:350:PRO:HD2	1:A:396:PRO:CD	2.29	0.61
1:B:217:GLU:HB3	1:B:394:PHE:CE2	2.36	0.61
1:B:223:THR:OG1	5:B:901:MG:MG	1.41	0.61
6:D:903:ATP:C3'	1:E:314:ARG:NH2	2.54	0.61
1:F:518:ILE:HD12	1:F:522:GLU:HG3	1.81	0.61
1:C:221:GLY:HA2	6:C:901:ATP:O1A	2.00	0.61
2:K:83:PHE:CD1	8:K:301:BO2:H252	2.36	0.61
2:I:137:PRO:HG3	8:I:301:BO2:H253	1.82	0.61
1:A:260:ARG:CZ	1:B:264:ASP:HA	2.29	0.61
3:N:23:ARG:NH2	3:T:54:GLU:OE2	2.33	0.61
3:R:69:GLY:O	8:R:201:BO2:H10	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:CB	6:A:904:ATP:O2A	2.50	0.60
1:D:771:ARG:N	1:D:772:PRO:HD2	2.16	0.60
1:A:350:PRO:HD2	1:A:396:PRO:HG3	1.83	0.60
1:C:362:LEU:HD11	6:C:901:ATP:N3	2.15	0.60
1:C:558:GLY:HA2	6:C:904:ATP:O2A	2.00	0.60
1:D:411:ARG:HH11	1:E:205:SER:HB3	1.67	0.60
1:F:337:ALA:HA	1:F:340:ARG:HD2	1.82	0.60
1:A:670:THR:O	1:B:706:ARG:NH2	2.35	0.60
3:N:68:GLY:CA	3:N:98:SER:HB3	2.32	0.60
1:A:411:ARG:HH21	1:B:241:THR:CG2	2.15	0.60
1:A:767:VAL:HG13	1:A:768:LEU:HG	1.83	0.60
3:Q:143:PHE:HE1	8:Q:201:BO2:H5	1.67	0.60
1:C:771:ARG:NE	6:C:904:ATP:H5'1	2.05	0.60
1:B:556:GLY:O	6:B:903:ATP:H8	1.85	0.59
1:C:544:ARG:NH1	1:C:714:ASP:OD1	2.34	0.59
1:C:679:LEU:HD11	2:H:36:LEU:HG	1.84	0.59
2:I:120:THR:HB	2:I:123:LYS:HD3	1.85	0.59
3:Q:71:ILE:HG12	8:Q:201:BO2:C7	2.32	0.59
1:C:358:ILE:HG23	6:C:901:ATP:C2	2.38	0.59
1:E:395:LEU:HA	1:E:398:LYS:HG2	1.83	0.59
2:J:164:MET:CG	8:J:301:BO2:H251	2.32	0.59
1:C:220:VAL:HA	1:C:396:PRO:CG	2.33	0.59
2:G:120:THR:HB	2:G:123:LYS:HD3	1.85	0.59
1:A:350:PRO:HD2	1:A:396:PRO:CG	2.33	0.59
1:A:411:ARG:HH21	1:B:241:THR:HG21	1.68	0.59
1:B:223:THR:HG1	5:B:901:MG:MG	1.11	0.59
1:D:559:LYS:HB2	7:D:901:ADP:O1B	2.02	0.59
1:F:362:LEU:CD1	7:F:901:ADP:C2	2.85	0.59
1:A:315:GLY:HA2	1:A:341:ARG:HH22	1.68	0.59
1:A:774:ARG:NH1	1:B:544:ARG:HH11	2.01	0.59
1:D:411:ARG:NH1	1:E:205:SER:HB3	2.17	0.59
2:G:97:ARG:HD2	2:M:208:LYS:HB2	1.83	0.59
1:F:395:LEU:N	1:F:398:LYS:HE2	2.18	0.59
1:B:772:PRO:HG3	1:B:775:ARG:HH21	1.68	0.59
1:D:529:SER:OG	1:D:533:ARG:NH2	2.36	0.59
2:L:120:THR:HB	2:L:123:LYS:HD3	1.85	0.59
1:A:339:GLU:HG2	1:A:340:ARG:HH12	1.68	0.58
3:T:71:ILE:HG12	8:T:201:BO2:N9	2.18	0.58
1:A:198:GLU:HG2	1:A:202:GLN:NE2	2.18	0.58
1:A:556:GLY:CA	6:A:902:ATP:O1B	2.46	0.58
1:B:559:LYS:NZ	6:B:903:ATP:PG	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:120:THR:HB	2:M:123:LYS:HD3	1.85	0.58
1:A:331:TYR:HA	1:A:334:LYS:HE3	1.85	0.58
1:E:413:ARG:NH1	1:E:483:GLN:OE1	2.35	0.58
2:J:120:THR:HB	2:J:123:LYS:HD3	1.85	0.58
6:C:904:ATP:O1G	1:D:712:ARG:NH2	2.35	0.58
2:H:82:GLY:H	8:H:301:BO2:H13	1.67	0.58
3:Q:96:ALA:O	3:Q:101:GLU:HB3	2.03	0.58
1:F:513:GLU:HB2	1:F:569:PHE:CE1	2.36	0.58
2:G:83:PHE:CD1	8:G:301:BO2:H252	2.35	0.58
2:H:83:PHE:CD1	8:H:301:BO2:H252	2.38	0.58
3:O:96:ALA:O	3:O:101:GLU:HB3	2.03	0.58
1:C:220:VAL:HA	1:C:396:PRO:HG2	1.84	0.58
1:C:350:PRO:HB3	1:C:354:HIS:HD2	1.68	0.58
2:H:120:THR:HB	2:H:123:LYS:HD3	1.85	0.58
2:K:120:THR:HB	2:K:123:LYS:HD3	1.85	0.58
1:A:615:ARG:NH2	1:B:333:GLU:OE1	2.36	0.58
3:S:71:ILE:HG12	8:S:201:BO2:N9	2.19	0.58
1:A:261:TYR:HB2	1:A:264:ASP:OD2	2.04	0.58
1:C:506:ARG:HG2	1:C:509:ARG:HH21	1.69	0.58
1:E:400:ILE:CD1	7:E:901:ADP:H1'	2.34	0.58
3:Q:71:ILE:HG12	8:Q:201:BO2:N9	2.19	0.58
1:F:218:PRO:HD2	1:F:394:PHE:HE2	1.68	0.57
3:O:143:PHE:CE1	8:O:201:BO2:H5	2.39	0.57
1:C:488:LEU:HD23	1:C:496:VAL:HG21	1.85	0.57
1:F:273:LEU:HD23	1:F:276:ILE:HD12	1.86	0.57
1:A:771:ARG:NE	6:A:902:ATP:H5'2	2.19	0.57
1:C:641:VAL:HG13	1:C:657:PHE:HD2	1.68	0.57
1:F:511:GLU:HG2	1:F:569:PHE:CZ	2.38	0.57
1:C:556:GLY:O	6:C:904:ATP:H8	1.88	0.57
2:J:207:ARG:NH1	2:K:64:GLU:OE2	2.35	0.57
3:T:143:PHE:HE1	8:T:201:BO2:H5	1.68	0.57
1:A:544:ARG:HH12	1:A:714:ASP:HB3	1.68	0.57
2:M:157:ILE:HD13	8:M:301:BO2:H6	1.86	0.57
1:C:568:ASN:OD1	1:C:572:GLY:O	2.21	0.57
3:R:98:SER:OG	8:R:201:BO2:H222	2.05	0.57
1:D:217:GLU:HB3	1:D:394:PHE:CE2	2.39	0.57
2:G:150:LEU:HD22	3:N:129:VAL:HG22	1.87	0.57
1:E:219:GLY:N	7:E:901:ADP:O1B	2.37	0.57
3:P:96:ALA:O	3:P:101:GLU:HB3	2.04	0.57
1:A:219:GLY:HA2	1:B:340:ARG:HE	1.70	0.57
3:O:114:ALA:HB2	3:O:186:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HA	1:A:396:PRO:CG	2.15	0.57
1:A:555:SER:HG	6:A:902:ATP:PG	2.23	0.57
3:R:114:ALA:HB2	3:R:186:VAL:HG11	1.87	0.57
1:B:350:PRO:HD2	1:B:396:PRO:HD3	1.86	0.56
1:D:209:LYS:HD3	1:D:340:ARG:HH11	1.69	0.56
1:F:509:ARG:HD3	1:F:537:ALA:HB3	1.87	0.56
1:F:220:VAL:HA	1:F:396:PRO:CG	2.33	0.56
3:P:114:ALA:HB2	3:P:186:VAL:HG11	1.87	0.56
1:B:556:GLY:O	6:B:903:ATP:C8	2.58	0.56
6:B:904:ATP:O1G	1:C:341:ARG:NH1	2.39	0.56
1:E:370:HIS:CG	1:E:411:ARG:HH21	2.24	0.56
1:F:748:ALA:HB3	1:F:799:VAL:HG13	1.86	0.56
3:Q:114:ALA:HB2	3:Q:186:VAL:HG11	1.87	0.56
3:S:114:ALA:HB2	3:S:186:VAL:HG11	1.87	0.56
3:S:150:MET:CE	8:S:201:BO2:H251	2.34	0.56
1:E:217:GLU:HG2	1:E:394:PHE:CZ	2.40	0.56
2:I:83:PHE:CD1	8:I:301:BO2:H252	2.40	0.56
1:D:222:LYS:HB2	6:D:903:ATP:O2B	2.04	0.56
1:B:730:MET:CE	6:B:903:ATP:C4	2.89	0.56
1:F:370:HIS:HD2	1:F:411:ARG:NH2	2.04	0.56
1:A:692:ARG:HH21	2:M:39:GLU:HB3	1.69	0.56
1:E:395:LEU:C	1:E:397:ASP:H	2.09	0.56
1:D:411:ARG:CZ	1:E:241:THR:HG22	2.36	0.56
1:F:390:ILE:HB	1:F:398:LYS:HD2	1.87	0.56
1:F:510:MET:SD	1:F:514:LEU:HG	2.46	0.56
3:T:114:ALA:HB2	3:T:186:VAL:HG11	1.87	0.56
1:A:192:GLY:HA3	1:A:354:HIS:HE1	1.70	0.56
6:B:903:ATP:O3G	1:C:712:ARG:NH2	2.39	0.56
1:D:771:ARG:HD2	7:D:901:ADP:O5'	2.05	0.56
3:S:68:GLY:HA3	3:S:98:SER:HB3	1.87	0.56
3:S:126:LEU:HB2	8:S:201:BO2:O19	2.05	0.56
3:T:96:ALA:O	3:T:101:GLU:HB3	2.06	0.56
1:D:191:ILE:HG13	1:D:361:GLY:HA3	1.88	0.55
1:F:287:ASP:HA	1:F:322:ALA:HB3	1.88	0.55
1:F:742:LEU:HB3	1:F:747:MET:HB2	1.88	0.55
1:C:408:ALA:O	1:C:412:ILE:CG1	2.52	0.55
1:E:337:ALA:O	1:E:341:ARG:NH2	2.39	0.55
2:L:135:HIS:ND1	2:L:186:ASP:OD1	2.40	0.55
1:C:408:ALA:HA	1:C:411:ARG:HG2	1.89	0.55
1:D:369:HIS:HB2	1:E:207:ARG:HH11	1.71	0.55
2:I:184:ASP:O	3:Q:171:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:135:HIS:ND1	2:M:186:ASP:OD1	2.40	0.55
3:N:114:ALA:HB2	3:N:186:VAL:HG11	1.87	0.55
1:B:193:ARG:NH2	1:B:220:VAL:O	2.40	0.55
2:G:135:HIS:ND1	2:G:186:ASP:OD1	2.40	0.55
3:R:143:PHE:CE1	8:R:201:BO2:H5	2.41	0.55
1:B:217:GLU:HB3	1:B:394:PHE:CZ	2.41	0.55
1:F:350:PRO:CG	1:F:396:PRO:HD3	2.36	0.55
3:P:125:PRO:HA	8:P:201:BO2:C22	2.36	0.55
2:G:208:LYS:HB2	2:H:97:ARG:HD2	1.87	0.55
2:I:135:HIS:ND1	2:I:186:ASP:OD1	2.39	0.55
3:N:96:ALA:O	3:N:101:GLU:HB3	2.06	0.55
2:H:135:HIS:ND1	2:H:186:ASP:OD1	2.40	0.55
2:K:138:SER:O	8:K:301:BO2:H17	2.07	0.55
1:D:771:ARG:HA	1:D:774:ARG:HG2	1.89	0.55
3:R:150:MET:CE	8:R:201:BO2:H251	2.35	0.55
1:A:202:GLN:HG2	1:F:412:ILE:CD1	2.36	0.55
1:F:220:VAL:O	1:F:396:PRO:HG2	2.07	0.55
3:O:38:ASP:O	3:O:42:ASN:ND2	2.40	0.55
3:Q:32:LEU:HD11	3:Q:36:VAL:HG22	1.89	0.55
3:T:38:ASP:O	3:T:42:ASN:ND2	2.40	0.55
1:E:394:PHE:O	1:E:398:LYS:HG2	2.07	0.55
2:J:135:HIS:ND1	2:J:186:ASP:OD1	2.40	0.55
2:L:83:PHE:CD1	8:L:301:BO2:H252	2.40	0.55
3:T:32:LEU:HD11	3:T:36:VAL:HG22	1.89	0.55
1:B:206:ARG:HH22	1:B:209:LYS:HB2	1.72	0.54
1:A:273:LEU:HD22	1:A:317:LEU:HD22	1.89	0.54
1:D:298:ALA:H	1:D:301:ALA:HB3	1.72	0.54
3:N:143:PHE:HE1	8:N:201:BO2:H5	1.72	0.54
3:Q:38:ASP:O	3:Q:42:ASN:ND2	2.40	0.54
3:R:38:ASP:O	3:R:42:ASN:ND2	2.40	0.54
3:R:68:GLY:CA	3:R:98:SER:HB3	2.37	0.54
1:B:224:ALA:HA	1:B:227:GLU:HB3	1.90	0.54
1:B:326:ASP:OD1	1:B:329:ARG:NH1	2.40	0.54
3:P:38:ASP:O	3:P:42:ASN:ND2	2.40	0.54
1:F:408:ALA:O	1:F:412:ILE:CG1	2.55	0.54
3:N:38:ASP:O	3:N:42:ASN:ND2	2.40	0.54
1:C:221:GLY:N	6:C:901:ATP:O1A	2.40	0.54
1:C:350:PRO:HD2	1:C:396:PRO:CD	2.28	0.54
1:C:394:PHE:O	1:C:398:LYS:HG2	2.07	0.54
1:F:304:ALA:HA	1:F:307:ILE:HD12	1.89	0.54
2:K:135:HIS:ND1	2:K:186:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:68:GLY:CA	3:P:98:SER:HB3	2.37	0.54
1:B:730:MET:HE1	6:B:903:ATP:C6	2.43	0.54
1:F:350:PRO:HG2	1:F:396:PRO:HD3	1.90	0.54
3:O:32:LEU:HD11	3:O:36:VAL:HG22	1.89	0.54
1:A:308:LEU:O	1:A:312:LEU:N	2.41	0.54
1:B:358:ILE:CD1	6:B:904:ATP:C6	2.89	0.54
1:D:220:VAL:HA	1:D:396:PRO:CG	2.35	0.54
1:F:212:PRO:HG2	1:F:320:ILE:HG23	1.89	0.54
2:G:44:LEU:HD21	2:G:48:VAL:HG22	1.90	0.54
2:J:44:LEU:HD21	2:J:48:VAL:HG22	1.90	0.54
3:S:38:ASP:O	3:S:42:ASN:ND2	2.40	0.54
1:F:775:ARG:NH1	1:F:778:GLN:OE1	2.41	0.54
2:M:138:SER:O	8:M:301:BO2:H17	2.07	0.54
1:B:601:TYR:HB3	1:C:600:GLY:HA2	1.90	0.54
1:F:395:LEU:HD23	1:F:398:LYS:CE	2.30	0.54
2:L:44:LEU:HD21	2:L:48:VAL:HG22	1.90	0.53
3:S:32:LEU:HD11	3:S:36:VAL:HG22	1.90	0.53
1:C:276:ILE:HG23	1:C:282:ILE:HB	1.90	0.53
1:C:369:HIS:HB2	1:D:207:ARG:HH11	1.73	0.53
6:C:904:ATP:PG	1:D:712:ARG:HH22	2.32	0.53
1:D:518:ILE:CG2	7:D:901:ADP:C6	2.92	0.53
1:F:515:HIS:HA	1:F:525:VAL:HG11	1.90	0.53
1:F:518:ILE:HG23	1:F:525:VAL:HG21	1.89	0.53
1:E:290:HIS:HB3	1:E:327:GLU:HB3	1.90	0.53
2:I:107:GLN:HG3	2:I:131:ARG:HD2	1.91	0.53
3:N:32:LEU:HD11	3:N:36:VAL:HG22	1.89	0.53
3:P:32:LEU:HD11	3:P:36:VAL:HG22	1.89	0.53
1:A:370:HIS:ND1	1:A:411:ARG:HD2	2.23	0.53
1:D:561:GLU:HG3	7:D:901:ADP:C2'	2.38	0.53
1:F:681:PHE:HB3	2:L:204:LEU:HD11	1.90	0.53
3:R:32:LEU:HD11	3:R:36:VAL:HG22	1.89	0.53
1:A:315:GLY:HA2	1:A:341:ARG:NH2	2.23	0.53
1:B:370:HIS:ND1	1:B:411:ARG:HD2	2.24	0.53
1:C:221:GLY:CA	6:C:901:ATP:O1A	2.56	0.53
1:D:607:GLY:H	1:D:651:GLN:HE21	1.56	0.53
1:A:751:LEU:HG	1:A:802:VAL:HB	1.91	0.53
1:C:559:LYS:HB2	6:C:904:ATP:O2B	2.08	0.53
2:M:44:LEU:HD21	2:M:48:VAL:HG22	1.90	0.53
1:E:395:LEU:O	1:E:397:ASP:N	2.39	0.53
1:E:411:ARG:NH1	1:F:205:SER:O	2.42	0.53
2:G:107:GLN:HG3	2:G:131:ARG:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:NH2	1:B:241:THR:HG21	2.24	0.53
1:C:411:ARG:NH2	1:D:241:THR:HG21	2.23	0.53
1:D:573:ASP:HB3	1:D:576:ALA:HB2	1.90	0.53
3:N:83:LEU:HD22	3:O:190:ILE:HG22	1.91	0.53
1:A:409:ARG:HH22	1:A:486:GLU:HB2	1.73	0.53
1:B:266:GLU:HG3	1:B:307:ILE:HD11	1.91	0.53
1:C:518:ILE:HD12	6:C:904:ATP:C2	2.38	0.53
2:J:41:ILE:HG12	2:J:73:THR:HB	1.91	0.53
1:A:559:LYS:HB2	6:A:902:ATP:O2B	2.09	0.52
1:C:556:GLY:O	6:C:904:ATP:C8	2.62	0.52
1:D:218:PRO:HD2	1:D:394:PHE:CE2	2.43	0.52
1:E:221:GLY:HA3	7:E:901:ADP:C2	2.44	0.52
2:H:41:ILE:HG12	2:H:73:THR:HB	1.91	0.52
2:L:107:GLN:HG3	2:L:131:ARG:HD2	1.91	0.52
2:L:148:SER:HB3	3:S:124:GLN:HE22	1.74	0.52
3:T:110:GLY:N	3:T:187:ASP:OD2	2.42	0.52
2:H:44:LEU:HD21	2:H:48:VAL:HG22	1.90	0.52
2:I:41:ILE:HG12	2:I:73:THR:HB	1.91	0.52
2:I:44:LEU:HD21	2:I:48:VAL:HG22	1.90	0.52
3:O:28:ARG:NH2	3:O:86:CYS:SG	2.83	0.52
3:Q:28:ARG:NH2	3:Q:86:CYS:SG	2.83	0.52
1:B:276:ILE:HG23	1:B:282:ILE:HB	1.91	0.52
1:C:772:PRO:HG3	1:C:775:ARG:HH21	1.75	0.52
1:D:326:ASP:OD1	1:D:329:ARG:NH1	2.36	0.52
1:D:534:ARG:NH1	1:D:546:SER:O	2.41	0.52
3:R:28:ARG:NH2	3:R:86:CYS:SG	2.83	0.52
1:D:494:ILE:HD11	1:D:618:PRO:HB2	1.91	0.52
1:F:362:LEU:HD11	7:F:901:ADP:N3	2.23	0.52
2:K:44:LEU:HD21	2:K:48:VAL:HG22	1.90	0.52
1:D:780:GLU:O	1:D:784:GLN:NE2	2.40	0.52
2:L:41:ILE:HG12	2:L:73:THR:HB	1.91	0.52
3:T:28:ARG:NH2	3:T:86:CYS:SG	2.83	0.52
1:B:221:GLY:HA3	6:B:904:ATP:C8	2.45	0.52
1:D:518:ILE:HA	7:D:901:ADP:C6	2.38	0.52
2:M:41:ILE:HG12	2:M:73:THR:HB	1.91	0.52
3:P:28:ARG:NH2	3:P:86:CYS:SG	2.83	0.52
3:S:28:ARG:NH2	3:S:86:CYS:SG	2.83	0.52
6:A:902:ATP:O1G	1:B:712:ARG:NH1	2.43	0.52
1:B:730:MET:CE	6:B:903:ATP:C6	2.92	0.52
2:G:41:ILE:HG12	2:G:73:THR:HB	1.91	0.52
2:I:86:LEU:HB2	2:I:111:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:107:GLN:HG3	2:J:131:ARG:HD2	1.91	0.52
2:K:107:GLN:HG3	2:K:131:ARG:HD2	1.91	0.52
3:P:98:SER:OG	8:P:201:BO2:H222	2.09	0.52
1:E:387:ASP:OD1	1:E:395:LEU:HG	2.09	0.52
2:M:107:GLN:HG3	2:M:131:ARG:HD2	1.91	0.52
3:N:28:ARG:NH2	3:N:86:CYS:SG	2.83	0.52
1:B:771:ARG:NH2	6:B:903:ATP:O3G	2.43	0.52
2:I:80:GLY:HA3	2:I:110:SER:HB3	1.92	0.52
8:O:201:BO2:H20	8:O:201:BO2:H243	1.75	0.52
1:B:222:LYS:HD2	6:B:904:ATP:O2B	2.09	0.51
3:O:110:GLY:N	3:O:187:ASP:OD2	2.42	0.51
1:D:561:GLU:OE2	7:D:901:ADP:O3'	2.19	0.51
2:G:110:SER:HB2	8:G:301:BO2:O27	2.09	0.51
1:B:765:ASP:OD1	1:B:772:PRO:HG2	2.11	0.51
1:C:350:PRO:HG2	1:C:396:PRO:HB3	1.92	0.51
1:F:193:ARG:NH1	1:F:220:VAL:O	2.43	0.51
1:F:216:GLY:HA3	1:F:222:LYS:CD	2.40	0.51
2:H:107:GLN:HG3	2:H:131:ARG:HD2	1.91	0.51
2:K:41:ILE:HG12	2:K:73:THR:HB	1.91	0.51
3:R:96:ALA:O	3:R:101:GLU:HB3	2.09	0.51
1:C:601:TYR:HB3	1:D:600:GLY:HA2	1.92	0.51
2:H:157:ILE:HD13	8:H:301:BO2:H6	1.93	0.51
8:R:201:BO2:H3	8:R:201:BO2:H112	1.92	0.51
3:T:160:GLN:NE2	3:T:183:TYR:O	2.41	0.51
1:A:667:ASN:OD1	6:A:902:ATP:O2G	2.28	0.51
1:B:551:PHE:HB2	1:B:665:THR:HG22	1.91	0.51
1:D:730:MET:HE2	7:D:901:ADP:N9	2.25	0.51
1:F:359:LEU:HD11	1:F:399:ALA:HB1	1.93	0.51
2:M:93:MET:HB2	2:M:100:ILE:HG13	1.93	0.51
1:C:555:SER:CB	6:C:904:ATP:O2G	2.59	0.51
2:H:184:ASP:O	3:P:171:ARG:NH1	2.43	0.51
1:B:641:VAL:HG13	1:B:657:PHE:HD2	1.76	0.51
2:K:164:MET:CG	8:K:301:BO2:H251	2.40	0.51
3:N:54:GLU:OE2	3:O:23:ARG:NH2	2.39	0.51
3:N:110:GLY:N	3:N:187:ASP:OD2	2.42	0.51
3:O:71:ILE:HG12	8:O:201:BO2:C7	2.41	0.51
1:D:494:ILE:HG12	1:D:619:PHE:HB2	1.93	0.51
1:F:200:VAL:HG13	1:F:212:PRO:HG3	1.93	0.51
6:C:901:ATP:O3G	1:D:341:ARG:NH2	2.44	0.51
2:H:93:MET:HB2	2:H:100:ILE:HG13	1.93	0.51
2:K:93:MET:HB2	2:K:100:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:HD3	1:B:340:ARG:NH1	2.24	0.51
2:H:110:SER:OG	2:H:111:ALA:N	2.44	0.51
2:H:138:SER:O	8:H:301:BO2:H17	2.10	0.51
1:B:352:VAL:HG22	1:B:395:LEU:HD11	1.94	0.50
1:C:582:MET:HG2	1:C:627:ILE:HG22	1.92	0.50
1:D:679:LEU:HA	2:J:65:SER:HB3	1.94	0.50
1:F:246:GLN:HB2	1:F:282:ILE:HG22	1.93	0.50
3:Q:126:LEU:HB2	8:Q:201:BO2:O19	2.10	0.50
1:F:289:LEU:HD22	1:F:321:GLY:HA3	1.93	0.50
2:G:164:MET:CG	8:G:301:BO2:H251	2.40	0.50
2:I:110:SER:HB2	8:I:301:BO2:O27	2.10	0.50
2:I:157:ILE:HD13	8:I:301:BO2:H6	1.93	0.50
2:I:164:MET:CG	8:I:301:BO2:H251	2.41	0.50
3:P:110:GLY:N	3:P:187:ASP:OD2	2.42	0.50
2:G:157:ILE:HD13	8:G:301:BO2:H6	1.93	0.50
3:P:160:GLN:NE2	3:P:183:TYR:O	2.41	0.50
1:A:276:ILE:HG21	1:A:317:LEU:HA	1.93	0.50
1:F:513:GLU:HA	1:F:516:LYS:HZ2	1.76	0.50
2:G:86:LEU:HB2	2:G:111:ALA:HB1	1.93	0.50
2:H:110:SER:HB2	8:H:301:BO2:O27	2.11	0.50
2:I:93:MET:HB2	2:I:100:ILE:HG13	1.93	0.50
2:L:110:SER:HB2	8:L:301:BO2:O27	2.12	0.50
3:P:83:LEU:HD22	3:Q:190:ILE:HG22	1.93	0.50
3:Q:143:PHE:CE1	8:Q:201:BO2:H5	2.46	0.50
1:D:355:THR:OG1	1:D:395:LEU:HD13	2.10	0.50
2:L:93:MET:HB2	2:L:100:ILE:HG13	1.93	0.50
2:M:110:SER:CB	8:M:301:BO2:O28	2.60	0.50
1:B:544:ARG:HD3	1:B:545:PRO:HD2	1.93	0.50
1:D:518:ILE:CB	7:D:901:ADP:C6	2.94	0.50
1:D:582:MET:HB3	1:D:630:ALA:HB2	1.93	0.50
1:E:289:LEU:HD13	1:E:322:ALA:H	1.77	0.50
1:E:306:SER:HA	1:E:309:LYS:HE2	1.92	0.50
1:F:326:ASP:OD1	1:F:329:ARG:NH1	2.45	0.50
3:S:68:GLY:CA	3:S:98:SER:HB3	2.41	0.50
1:D:769:GLY:O	1:D:772:PRO:HG2	2.12	0.50
2:I:187:LYS:HE2	2:I:189:LEU:HD21	1.94	0.50
2:L:110:SER:OG	2:L:111:ALA:N	2.45	0.50
2:M:187:LYS:HE2	2:M:189:LEU:HD21	1.94	0.50
1:A:355:THR:OG1	1:A:395:LEU:HD13	2.11	0.50
1:E:412:ILE:HD11	1:F:201:MET:O	2.12	0.50
2:J:93:MET:HB2	2:J:100:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:107:GLN:HB2	2:K:84:THR:HB	1.94	0.50
2:J:110:SER:HB2	8:J:301:BO2:O27	2.10	0.50
3:O:28:ARG:HG2	3:O:51:LEU:HD22	1.94	0.50
3:R:28:ARG:HG2	3:R:51:LEU:HD22	1.94	0.50
1:B:411:ARG:HH21	1:C:241:THR:CG2	2.24	0.50
6:C:901:ATP:H5'2	1:D:314:ARG:NH1	2.26	0.50
1:E:363:ARG:NH1	1:E:374:ILE:O	2.45	0.50
2:G:93:MET:HB2	2:G:100:ILE:HG13	1.93	0.50
3:S:146:ILE:HD13	8:S:201:BO2:H6	1.93	0.50
1:B:226:VAL:HG13	1:B:247:LEU:HD21	1.94	0.49
1:B:535:THR:HA	1:B:540:LYS:HB2	1.93	0.49
1:C:559:LYS:N	6:C:904:ATP:O1B	2.37	0.49
1:C:726:GLU:HG2	1:C:729:ARG:HH11	1.77	0.49
1:D:359:LEU:HD11	1:D:399:ALA:HB1	1.93	0.49
1:D:488:LEU:HD23	1:D:496:VAL:HG21	1.94	0.49
1:A:402:LEU:HB3	1:A:484:ILE:HG23	1.94	0.49
3:N:28:ARG:HG2	3:N:51:LEU:HD22	1.94	0.49
1:A:582:MET:HE1	1:A:594:LEU:HD11	1.94	0.49
1:B:412:ILE:O	1:B:412:ILE:CG2	2.59	0.49
1:C:191:ILE:HG13	1:C:361:GLY:HA3	1.94	0.49
1:D:559:LYS:HD2	1:D:665:THR:HG23	1.95	0.49
3:P:143:PHE:CE1	8:P:201:BO2:H5	2.46	0.49
3:R:110:GLY:N	3:R:187:ASP:OD2	2.42	0.49
1:E:396:PRO:O	1:E:400:ILE:HD12	2.12	0.49
1:F:362:LEU:CD1	7:F:901:ADP:H2	2.25	0.49
1:F:510:MET:HA	1:F:569:PHE:HE2	1.78	0.49
2:K:187:LYS:HE2	2:K:189:LEU:HD21	1.94	0.49
3:S:110:GLY:N	3:S:187:ASP:OD2	2.42	0.49
1:D:584:GLU:HG3	1:D:593:ARG:HH12	1.77	0.49
1:F:309:LYS:HE3	1:F:341:ARG:HG3	1.93	0.49
2:L:157:ILE:HD13	8:L:301:BO2:H6	1.93	0.49
3:Q:110:GLY:N	3:Q:187:ASP:OD2	2.42	0.49
2:J:138:SER:O	8:J:301:BO2:H17	2.12	0.49
2:K:107:GLN:HB2	2:L:84:THR:HB	1.93	0.49
2:K:110:SER:OG	2:K:111:ALA:N	2.46	0.49
2:L:109:ALA:HA	2:L:133:LEU:HB3	1.94	0.49
3:S:83:LEU:HD22	3:T:190:ILE:HG22	1.93	0.49
3:S:160:GLN:NE2	3:S:183:TYR:O	2.41	0.49
1:C:606:GLU:HG3	1:D:329:ARG:HH22	1.78	0.49
1:F:375:THR:HG23	1:F:378:ALA:H	1.76	0.49
2:J:187:LYS:HE2	2:J:189:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:HIS:HD2	8:L:301:BO2:O27	1.96	0.49
3:Q:28:ARG:HG2	3:Q:51:LEU:HD22	1.94	0.49
1:A:593:ARG:HH21	1:A:609:GLN:HE22	1.59	0.49
1:D:371:ARG:NH2	1:D:411:ARG:HH21	2.05	0.49
1:D:730:MET:CE	7:D:901:ADP:C2	2.87	0.49
1:E:188:ASP:OD1	1:F:207:ARG:NH1	2.46	0.49
1:F:292:LEU:HD22	1:F:304:ALA:HB3	1.93	0.49
2:M:87:MET:HA	2:M:90:TYR:HB3	1.95	0.49
3:Q:68:GLY:CA	3:Q:98:SER:HB3	2.43	0.49
3:R:71:ILE:H	8:R:201:BO2:HN9	1.59	0.49
3:R:146:ILE:HD13	8:R:201:BO2:H6	1.94	0.49
1:A:681:PHE:HB3	2:M:204:LEU:HD11	1.95	0.49
1:C:397:ASP:OD2	1:D:340:ARG:HD3	2.13	0.49
1:F:395:LEU:O	1:F:396:PRO:C	2.52	0.49
2:G:110:SER:OG	2:G:111:ALA:N	2.46	0.49
2:M:40:ARG:HG2	2:M:63:LEU:HD22	1.95	0.49
3:O:160:GLN:NE2	3:O:183:TYR:O	2.41	0.49
3:R:160:GLN:NE2	3:R:183:TYR:O	2.41	0.49
1:B:182:ALA:HB2	1:B:187:LEU:HD22	1.95	0.49
2:I:110:SER:OG	2:I:111:ALA:N	2.46	0.49
2:J:87:MET:HA	2:J:90:TYR:HB3	1.95	0.49
2:M:150:LEU:HD22	3:T:129:VAL:HG22	1.94	0.49
3:P:28:ARG:HG2	3:P:51:LEU:HD22	1.94	0.49
1:D:350:PRO:CD	1:D:396:PRO:HD3	2.41	0.48
2:H:40:ARG:HG2	2:H:63:LEU:HD22	1.95	0.48
2:J:184:ASP:O	3:R:171:ARG:NH1	2.44	0.48
2:K:147:PHE:HD2	3:R:147:LYS:HB2	1.77	0.48
2:K:147:PHE:HB2	3:R:147:LYS:HD3	1.95	0.48
2:M:77:ASN:HB2	2:M:105:LEU:HD12	1.95	0.48
3:P:54:GLU:OE2	3:Q:23:ARG:NH2	2.43	0.48
1:A:195:LYS:HD2	1:F:490:ASN:HB3	1.95	0.48
3:T:28:ARG:HG2	3:T:51:LEU:HD22	1.94	0.48
3:T:143:PHE:CE1	8:T:201:BO2:H5	2.48	0.48
6:C:904:ATP:O1A	1:D:643:GLU:OE2	2.31	0.48
1:D:350:PRO:HD2	1:D:396:PRO:CD	2.42	0.48
1:F:362:LEU:HD11	7:F:901:ADP:H2	1.78	0.48
1:F:394:PHE:C	1:F:398:LYS:HG3	2.33	0.48
2:G:87:MET:HA	2:G:90:TYR:HB3	1.95	0.48
2:H:31:ASN:H	2:H:34:ASN:HD22	1.62	0.48
2:I:87:MET:HA	2:I:90:TYR:HB3	1.95	0.48
3:R:98:SER:OG	8:R:201:BO2:C22	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:GLY:HA2	7:D:901:ADP:C8	2.49	0.48
1:F:534:ARG:HG3	1:F:535:THR:HG23	1.95	0.48
1:E:411:ARG:CD	1:F:205:SER:CB	2.40	0.48
2:G:137:PRO:HD3	2:G:164:MET:HE2	1.96	0.48
2:H:87:MET:HA	2:H:90:TYR:HB3	1.95	0.48
2:K:31:ASN:H	2:K:34:ASN:HD22	1.62	0.48
2:K:87:MET:HA	2:K:90:TYR:HB3	1.95	0.48
2:L:87:MET:HA	2:L:90:TYR:HB3	1.95	0.48
3:S:28:ARG:HG2	3:S:51:LEU:HD22	1.94	0.48
3:T:68:GLY:CA	3:T:98:SER:HB3	2.43	0.48
1:C:778:GLN:HA	1:C:782:GLU:HB2	1.95	0.48
1:D:222:LYS:H	6:D:903:ATP:PB	2.37	0.48
1:E:411:ARG:NH2	1:F:205:SER:O	2.44	0.48
1:F:218:PRO:HD2	1:F:394:PHE:CE2	2.47	0.48
2:G:77:ASN:HB2	2:G:105:LEU:HD12	1.95	0.48
2:G:187:LYS:HE2	2:G:189:LEU:HD21	1.94	0.48
2:H:77:ASN:HB2	2:H:105:LEU:HD12	1.95	0.48
2:H:187:LYS:HE2	2:H:189:LEU:HD21	1.94	0.48
3:O:125:PRO:HA	8:O:201:BO2:C22	2.34	0.48
3:P:68:GLY:HA3	3:P:98:SER:HB3	1.96	0.48
1:A:312:LEU:O	1:A:341:ARG:NH2	2.46	0.48
1:B:642:LEU:HD21	1:B:662:LEU:HD22	1.96	0.48
1:C:708:GLU:HB2	1:C:712:ARG:HH12	1.79	0.48
1:E:239:PRO:HD2	1:E:242:LEU:HB2	1.94	0.48
1:F:242:LEU:HD22	1:F:245:LYS:HG3	1.94	0.48
1:F:479:VAL:HA	1:F:483:GLN:HG3	1.95	0.48
2:K:40:ARG:HG2	2:K:63:LEU:HD22	1.95	0.48
2:K:110:SER:HB2	8:K:301:BO2:O27	2.14	0.48
1:A:370:HIS:ND1	1:A:411:ARG:CD	2.77	0.48
1:E:340:ARG:NH2	1:E:340:ARG:HG3	2.29	0.48
2:M:31:ASN:H	2:M:34:ASN:HD22	1.62	0.48
3:P:122:MET:HE1	3:P:165:ILE:HG23	1.96	0.48
2:J:77:ASN:HB2	2:J:105:LEU:HD12	1.95	0.48
2:L:42:ILE:HD12	2:L:56:ILE:HG23	1.96	0.48
3:N:30:ILE:HD12	3:N:44:LEU:HD22	1.96	0.48
1:A:560:THR:HG23	6:A:902:ATP:O2B	2.13	0.48
1:D:771:ARG:HG3	7:D:901:ADP:H4'	1.96	0.48
2:I:148:SER:HB3	3:P:124:GLN:HE22	1.79	0.48
8:I:301:BO2:H242	8:I:301:BO2:H21	1.66	0.48
2:M:42:ILE:HD12	2:M:56:ILE:HG23	1.96	0.48
3:R:68:GLY:HA3	3:R:98:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:HB3	1:A:394:PHE:CZ	2.48	0.47
1:E:491:TRP:HE1	1:F:199:ARG:HH22	1.62	0.47
2:I:31:ASN:H	2:I:34:ASN:HD22	1.62	0.47
2:J:40:ARG:HG2	2:J:63:LEU:HD22	1.95	0.47
3:P:30:ILE:HD12	3:P:44:LEU:HD22	1.96	0.47
3:S:68:GLY:HA2	3:S:97:ALA:O	2.14	0.47
1:A:683:LYS:HE3	2:M:125:MET:HE3	1.96	0.47
1:C:411:ARG:HH21	1:D:241:THR:HG21	1.79	0.47
1:C:557:VAL:HA	1:C:722:LEU:HD11	1.96	0.47
2:I:77:ASN:HB2	2:I:105:LEU:HD12	1.95	0.47
2:M:110:SER:HB3	8:M:301:BO2:O28	2.14	0.47
1:A:378:ALA:O	1:A:382:ALA:N	2.47	0.47
1:F:759:LEU:HD21	1:F:777:ILE:HG12	1.96	0.47
1:C:209:LYS:HB3	1:C:343:GLN:HE22	1.79	0.47
1:C:616:ARG:HE	1:D:325:LEU:HB3	1.79	0.47
2:I:42:ILE:HD12	2:I:56:ILE:HG23	1.96	0.47
2:K:77:ASN:HB2	2:K:105:LEU:HD12	1.95	0.47
2:L:184:ASP:O	3:T:171:ARG:NH1	2.47	0.47
3:S:98:SER:CB	8:S:201:BO2:O27	2.62	0.47
1:B:350:PRO:HG3	1:B:396:PRO:HG3	1.97	0.47
1:B:681:PHE:HB3	2:G:204:LEU:HD11	1.96	0.47
2:G:40:ARG:HG2	2:G:63:LEU:HD22	1.95	0.47
2:I:40:ARG:HG2	2:I:63:LEU:HD22	1.95	0.47
2:L:187:LYS:HE2	2:L:189:LEU:HD21	1.94	0.47
2:M:109:ALA:HA	2:M:133:LEU:HB3	1.97	0.47
6:C:901:ATP:PG	1:D:340:ARG:HH21	2.36	0.47
2:G:42:ILE:HD12	2:G:56:ILE:HG23	1.96	0.47
2:J:31:ASN:H	2:J:34:ASN:HD22	1.62	0.47
2:K:207:ARG:NH1	2:L:64:GLU:OE2	2.45	0.47
3:O:30:ILE:HD12	3:O:44:LEU:HD22	1.96	0.47
6:C:901:ATP:H3'	1:D:314:ARG:HH12	1.80	0.47
1:D:276:ILE:HG23	1:D:282:ILE:HB	1.96	0.47
1:E:221:GLY:HA2	7:E:901:ADP:O1A	2.14	0.47
1:F:410:MET:SD	1:F:413:ARG:NH2	2.83	0.47
2:K:86:LEU:HB2	2:K:111:ALA:HB1	1.97	0.47
2:L:40:ARG:HG2	2:L:63:LEU:HD22	1.95	0.47
2:L:208:LYS:HB3	2:M:97:ARG:HA	1.96	0.47
3:N:98:SER:HB2	8:N:201:BO2:O27	2.14	0.47
3:N:143:PHE:CE1	8:N:201:BO2:H5	2.49	0.47
3:R:30:ILE:HD12	3:R:44:LEU:HD22	1.96	0.47
3:T:126:LEU:HB2	8:T:201:BO2:O19	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ILE:HG21	1:B:664:PHE:HB3	1.97	0.47
1:D:190:VAL:HA	6:D:903:ATP:N1	2.30	0.47
1:D:395:LEU:HD23	1:D:395:LEU:HA	1.74	0.47
1:F:411:ARG:O	1:F:411:ARG:HG2	2.15	0.47
2:G:31:ASN:H	2:G:34:ASN:HD22	1.62	0.47
2:L:31:ASN:H	2:L:34:ASN:HD22	1.62	0.47
2:L:77:ASN:HB2	2:L:105:LEU:HD12	1.95	0.47
1:F:385:LEU:HD22	1:F:389:TYR:HE2	1.80	0.47
2:H:150:LEU:HD22	3:O:129:VAL:HG22	1.96	0.47
2:M:140:SER:H	8:M:301:BO2:C17	2.28	0.47
3:T:98:SER:HB2	3:T:123:HIS:HE1	1.79	0.47
1:C:411:ARG:HH21	1:D:241:THR:CG2	2.28	0.47
1:C:727:ILE:HG23	1:C:773:LEU:HD22	1.96	0.47
1:E:405:GLU:OE2	1:F:199:ARG:NH1	2.48	0.47
2:G:135:HIS:HD2	8:G:301:BO2:O27	1.98	0.47
2:G:184:ASP:O	3:O:171:ARG:NH1	2.46	0.47
2:K:42:ILE:HD12	2:K:56:ILE:HG23	1.96	0.47
3:N:150:MET:CE	8:N:201:BO2:H251	2.43	0.47
1:A:190:VAL:HA	6:A:904:ATP:N1	2.29	0.46
2:H:164:MET:CG	8:H:301:BO2:H251	2.43	0.46
3:R:143:PHE:HE1	8:R:201:BO2:H5	1.80	0.46
1:A:176:ARG:HG2	1:B:314:ARG:HH22	1.81	0.46
1:C:694:LYS:HA	1:C:718:VAL:HG11	1.98	0.46
2:H:42:ILE:HD12	2:H:56:ILE:HG23	1.96	0.46
2:M:137:PRO:HD3	2:M:164:MET:HE2	1.96	0.46
8:P:201:BO2:H243	8:P:201:BO2:O28	2.15	0.46
3:R:54:GLU:OE2	3:S:23:ARG:NH2	2.41	0.46
3:S:122:MET:HE1	3:S:165:ILE:HG23	1.97	0.46
1:A:316:GLU:HG3	1:A:317:LEU:HG	1.98	0.46
1:B:204:LEU:HD11	1:B:320:ILE:HD11	1.97	0.46
1:B:616:ARG:HD3	1:C:325:LEU:HD13	1.96	0.46
1:F:511:GLU:HG3	1:F:513:GLU:H	1.81	0.46
2:H:135:HIS:HD2	8:H:301:BO2:O27	1.97	0.46
2:L:138:SER:O	8:L:301:BO2:H17	2.16	0.46
2:M:140:SER:H	8:M:301:BO2:C16	2.29	0.46
3:Q:30:ILE:HD12	3:Q:44:LEU:HD22	1.96	0.46
3:T:30:ILE:HD12	3:T:44:LEU:HD22	1.96	0.46
1:A:340:ARG:CZ	1:A:340:ARG:HA	2.46	0.46
1:C:222:LYS:N	6:C:901:ATP:O1B	2.43	0.46
2:H:109:ALA:HA	2:H:133:LEU:HB3	1.98	0.46
8:H:301:BO2:H242	8:H:301:BO2:H21	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:164:MET:CG	8:L:301:BO2:H251	2.43	0.46
3:O:70:SER:HA	8:O:201:BO2:H111	1.97	0.46
3:S:30:ILE:HD12	3:S:44:LEU:HD22	1.96	0.46
1:B:770:ALA:HB3	6:B:903:ATP:C8	2.51	0.46
1:D:646:ARG:NH2	1:D:654:THR:OG1	2.49	0.46
1:F:517:ARG:NH2	1:F:569:PHE:HB2	2.31	0.46
2:G:137:PRO:HB3	8:G:301:BO2:O19	2.16	0.46
2:I:135:HIS:HD2	8:I:301:BO2:O27	1.98	0.46
3:Q:160:GLN:NE2	3:Q:183:TYR:O	2.41	0.46
1:A:192:GLY:HA3	1:A:354:HIS:CE1	2.51	0.46
1:A:759:LEU:HD13	1:A:777:ILE:HG12	1.97	0.46
1:A:774:ARG:HD2	6:A:902:ATP:O2'	2.16	0.46
1:B:406:ALA:HB1	1:B:483:GLN:HG3	1.97	0.46
1:A:788:LYS:NZ	1:A:793:GLU:OE1	2.42	0.46
1:B:350:PRO:CG	1:B:396:PRO:HG3	2.46	0.46
1:B:579:GLN:NE2	1:C:644:ASP:OD2	2.44	0.46
1:C:402:LEU:HB3	1:C:484:ILE:HG23	1.98	0.46
1:C:551:PHE:HB2	1:C:665:THR:HG22	1.97	0.46
1:E:217:GLU:HB3	1:E:394:PHE:CE2	2.50	0.46
3:O:99:MET:N	8:O:201:BO2:H242	2.31	0.46
1:A:638:LEU:HD23	1:A:664:PHE:HE1	1.81	0.46
1:A:742:LEU:HB3	1:B:539:LEU:HD23	1.98	0.46
1:B:394:PHE:O	1:B:398:LYS:HG2	2.16	0.46
1:C:221:GLY:HA2	6:C:901:ATP:PA	2.56	0.46
1:E:170:VAL:HG21	1:E:284:LEU:HD21	1.98	0.46
1:E:408:ALA:O	1:E:412:ILE:HG13	2.16	0.46
2:J:42:ILE:HD12	2:J:56:ILE:HG23	1.96	0.46
3:N:98:SER:CB	8:N:201:BO2:O27	2.63	0.46
3:P:98:SER:OG	8:P:201:BO2:C22	2.62	0.46
1:A:259:SER:O	1:B:262:ARG:HB2	2.15	0.46
1:A:264:ASP:H	1:B:262:ARG:HH22	1.64	0.46
1:C:218:PRO:HD2	1:C:394:PHE:CE2	2.51	0.46
1:C:771:ARG:NH2	6:C:904:ATP:O1G	2.48	0.46
2:J:137:PRO:HD3	2:J:164:MET:HE2	1.98	0.46
2:J:150:LEU:HD22	3:Q:129:VAL:HG22	1.98	0.46
1:A:314:ARG:O	1:A:315:GLY:C	2.54	0.45
1:A:585:PHE:HE1	1:A:593:ARG:HB2	1.81	0.45
1:A:748:ALA:HB3	1:A:799:VAL:HG22	1.98	0.45
1:B:555:SER:HA	6:B:903:ATP:O1G	2.16	0.45
3:P:68:GLY:HA2	3:P:98:SER:HB3	1.97	0.45
1:B:778:GLN:HA	1:B:782:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:GLU:HG2	6:C:904:ATP:N3	2.31	0.45
1:D:204:LEU:HD11	1:D:320:ILE:HD11	1.98	0.45
1:D:616:ARG:HG3	1:E:329:ARG:HH12	1.80	0.45
1:F:190:VAL:HA	7:F:901:ADP:C2	2.52	0.45
2:H:137:PRO:HD3	2:H:164:MET:HE2	1.98	0.45
3:N:160:GLN:NE2	3:N:183:TYR:O	2.41	0.45
3:O:68:GLY:CA	3:O:98:SER:HB3	2.46	0.45
1:A:210:ASN:HB2	1:A:318:GLN:NE2	2.31	0.45
1:D:771:ARG:C	1:D:773:LEU:H	2.18	0.45
1:E:223:THR:OG1	7:E:901:ADP:O2A	2.23	0.45
1:F:370:HIS:CA	1:F:411:ARG:HH12	2.16	0.45
1:F:510:MET:CE	1:F:529:SER:HA	2.47	0.45
2:K:146:GLN:OE1	3:R:124:GLN:NE2	2.37	0.45
2:L:86:LEU:HB2	2:L:111:ALA:HB1	1.97	0.45
2:M:184:ASP:O	3:N:171:ARG:NH1	2.49	0.45
3:Q:83:LEU:HD22	3:R:190:ILE:HG22	1.99	0.45
3:T:121:LEU:HD13	3:T:174:TRP:CE2	2.52	0.45
3:T:122:MET:HE1	3:T:165:ILE:HG23	1.99	0.45
1:A:517:ARG:NH2	1:A:561:GLU:OE2	2.50	0.45
1:C:177:ASN:HD21	1:C:246:GLN:HE21	1.65	0.45
1:C:622:VAL:HB	1:C:662:LEU:HD23	1.99	0.45
1:C:774:ARG:NH2	1:C:782:GLU:OE2	2.47	0.45
1:D:621:VAL:HG22	1:D:661:VAL:HB	1.97	0.45
2:I:150:LEU:HD22	3:P:129:VAL:HG22	1.99	0.45
2:J:135:HIS:HD2	8:J:301:BO2:O27	1.99	0.45
2:L:147:PHE:HD2	3:S:147:LYS:HB2	1.80	0.45
1:D:730:MET:HE1	7:D:901:ADP:C2	2.26	0.45
2:H:132:VAL:HG11	2:H:199:ILE:HG21	1.99	0.45
2:M:132:VAL:HG11	2:M:199:ILE:HG21	1.99	0.45
3:N:121:LEU:HD13	3:N:174:TRP:CE2	2.52	0.45
3:Q:125:PRO:HA	8:Q:201:BO2:C22	2.28	0.45
3:Q:126:LEU:O	8:Q:201:BO2:H3	2.16	0.45
3:R:68:GLY:HA2	3:R:98:SER:HB3	1.98	0.45
3:S:69:GLY:O	8:S:201:BO2:O28	2.33	0.45
1:A:340:ARG:HE	7:F:901:ADP:H5'2	1.82	0.45
1:A:778:GLN:HA	1:A:782:GLU:HB3	1.97	0.45
1:D:217:GLU:HG2	1:D:394:PHE:CE1	2.52	0.45
1:D:411:ARG:HH22	1:E:241:THR:N	2.15	0.45
1:F:220:VAL:C	1:F:396:PRO:HG2	2.37	0.45
1:F:509:ARG:HD2	1:F:533:ARG:HA	1.99	0.45
2:H:154:ALA:HA	2:H:157:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:99:MET:HE1	8:S:201:BO2:H241	1.98	0.45
3:S:121:LEU:HD13	3:S:174:TRP:CE2	2.52	0.45
1:A:612:GLU:OE1	1:A:615:ARG:NH2	2.50	0.45
1:C:415:MET:HG2	1:D:240:GLU:H	1.81	0.45
1:C:518:ILE:CD1	6:C:904:ATP:N1	2.43	0.45
1:E:221:GLY:HA3	7:E:901:ADP:H2	1.82	0.45
1:F:512:GLU:HA	1:F:515:HIS:CE1	2.52	0.45
3:S:97:ALA:HB1	3:S:121:LEU:HD23	1.98	0.45
1:E:337:ALA:HB1	1:E:341:ARG:HH22	1.82	0.45
2:J:110:SER:OG	2:J:111:ALA:N	2.49	0.45
2:K:135:HIS:HD2	8:K:301:BO2:O27	2.00	0.45
1:B:218:PRO:O	1:B:394:PHE:HD2	2.00	0.45
1:B:555:SER:HG	6:B:903:ATP:PG	2.40	0.45
1:B:612:GLU:HG3	1:C:329:ARG:HH21	1.82	0.45
2:I:132:VAL:HG11	2:I:199:ILE:HG21	1.99	0.45
2:I:138:SER:O	8:I:301:BO2:H17	2.16	0.45
2:L:154:ALA:HA	2:L:157:ILE:HG22	1.99	0.45
3:N:146:ILE:HD13	8:N:201:BO2:H6	1.98	0.45
3:O:122:MET:HE1	3:O:165:ILE:HG23	1.99	0.45
3:Q:121:LEU:HD13	3:Q:174:TRP:CE2	2.52	0.45
1:A:187:LEU:HD13	1:A:227:GLU:HB2	1.99	0.45
1:B:730:MET:CE	6:B:903:ATP:N1	2.76	0.45
2:G:132:VAL:HG11	2:G:199:ILE:HG21	1.99	0.45
3:T:126:LEU:O	8:T:201:BO2:H3	2.16	0.45
1:A:218:PRO:CD	1:A:394:PHE:CE2	2.89	0.44
1:A:679:LEU:HD21	2:M:36:LEU:HG	1.98	0.44
1:C:204:LEU:HD11	1:C:320:ILE:HD11	1.99	0.44
3:R:121:LEU:HD13	3:R:174:TRP:CE2	2.52	0.44
1:F:192:GLY:HA3	1:F:354:HIS:CE1	2.53	0.44
1:F:506:ARG:HD3	1:F:506:ARG:HA	1.65	0.44
2:G:103:VAL:HG22	2:G:125:MET:HB2	1.99	0.44
2:M:154:ALA:HA	2:M:157:ILE:HG22	1.99	0.44
8:O:201:BO2:H243	8:O:201:BO2:N20	2.32	0.44
1:B:390:ILE:HG12	1:B:491:TRP:HZ3	1.81	0.44
1:C:222:LYS:CE	6:C:901:ATP:O2G	2.65	0.44
1:D:242:LEU:HD22	1:D:283:ILE:HD11	1.98	0.44
1:F:218:PRO:HG2	1:F:394:PHE:HE2	1.81	0.44
2:K:103:VAL:HG22	2:K:125:MET:HB2	1.99	0.44
2:M:103:VAL:HG22	2:M:125:MET:HB2	2.00	0.44
1:A:774:ARG:NH2	1:B:544:ARG:NH1	2.65	0.44
1:B:494:ILE:HD11	1:B:618:PRO:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ILE:HG13	1:B:764:PHE:CD1	2.52	0.44
1:D:771:ARG:C	1:D:773:LEU:N	2.71	0.44
2:G:154:ALA:HA	2:G:157:ILE:HG22	1.99	0.44
2:J:154:ALA:HA	2:J:157:ILE:HG22	1.99	0.44
3:P:121:LEU:HD13	3:P:174:TRP:CE2	2.52	0.44
8:Q:201:BO2:H20	8:Q:201:BO2:H253	1.82	0.44
1:C:499:LEU:HD11	1:C:536:ARG:HB3	1.99	0.44
1:E:193:ARG:NH1	1:E:348:GLY:O	2.36	0.44
1:E:369:HIS:CE1	1:E:411:ARG:HH22	2.35	0.44
1:D:351:THR:HG23	1:D:354:HIS:H	1.82	0.44
1:E:286:ILE:HG13	1:E:289:LEU:HD11	1.99	0.44
2:H:86:LEU:HB2	2:H:111:ALA:HB1	2.00	0.44
2:J:132:VAL:HG11	2:J:199:ILE:HG21	1.99	0.44
3:P:76:ALA:HB1	3:Q:93:MET:HG2	2.00	0.44
1:B:559:LYS:NZ	6:B:903:ATP:O3B	2.51	0.44
1:D:371:ARG:NH1	1:D:411:ARG:NE	2.65	0.44
1:E:408:ALA:CA	1:E:411:ARG:HG2	2.44	0.44
3:R:125:PRO:HA	8:R:201:BO2:C22	2.36	0.44
1:D:524:ALA:HB2	1:D:717:ILE:HG21	2.00	0.44
1:E:340:ARG:HG3	1:E:340:ARG:HH21	1.83	0.44
2:I:103:VAL:HG22	2:I:125:MET:HB2	1.99	0.44
2:K:154:ALA:HA	2:K:157:ILE:HG22	1.99	0.44
3:O:98:SER:CB	3:O:123:HIS:CE1	3.01	0.44
3:O:121:LEU:HD13	3:O:174:TRP:CE2	2.52	0.44
3:S:97:ALA:O	3:S:98:SER:HB3	2.17	0.44
1:A:256:VAL:HG12	1:B:263:GLY:HA2	1.99	0.44
1:A:675:LYS:HD2	2:G:68:PRO:HD2	2.00	0.44
1:C:730:MET:HE2	6:C:904:ATP:C6	2.53	0.44
1:D:771:ARG:H	1:D:772:PRO:HD2	1.83	0.44
2:I:154:ALA:HA	2:I:157:ILE:HG22	1.99	0.44
2:K:150:LEU:HD22	3:R:129:VAL:HG22	1.99	0.44
2:L:132:VAL:HG11	2:L:199:ILE:HG21	1.99	0.44
1:A:771:ARG:NE	6:A:902:ATP:C5'	2.66	0.43
1:C:209:LYS:O	1:C:343:GLN:NE2	2.51	0.43
1:D:220:VAL:CA	1:D:396:PRO:HG2	2.38	0.43
3:O:112:ARG:NH2	3:O:187:ASP:OD1	2.47	0.43
1:A:239:PRO:HB2	1:A:241:THR:HG22	2.00	0.43
1:B:722:LEU:O	1:B:764:PHE:HE1	2.01	0.43
1:D:578:ILE:HB	1:D:622:VAL:HG12	2.00	0.43
1:E:362:LEU:HD21	7:E:901:ADP:H8	1.83	0.43
2:G:166:THR:HG22	2:G:170:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:132:VAL:HG11	2:K:199:ILE:HG21	1.99	0.43
1:A:680:GLY:HA2	2:G:61:LEU:HD22	1.99	0.43
1:C:550:ILE:HG12	1:C:664:PHE:HB2	2.00	0.43
1:C:680:GLY:HA2	2:I:61:LEU:HD22	2.00	0.43
1:D:518:ILE:CG2	7:D:901:ADP:N6	2.80	0.43
1:F:508:LEU:HD12	1:F:509:ARG:HD3	2.00	0.43
2:G:138:SER:O	8:G:301:BO2:H17	2.18	0.43
2:H:103:VAL:HG22	2:H:125:MET:HB2	2.00	0.43
2:I:166:THR:HG22	2:I:170:ARG:HH11	1.83	0.43
3:N:112:ARG:NH2	3:N:187:ASP:OD1	2.47	0.43
3:P:71:ILE:HG12	8:P:201:BO2:C7	2.47	0.43
1:C:356:ILE:HG22	1:C:360:LYS:HE2	2.00	0.43
1:D:250:LEU:HD22	1:D:284:LEU:HD21	2.00	0.43
1:D:518:ILE:CB	7:D:901:ADP:HN62	2.06	0.43
1:E:355:THR:OG1	1:E:395:LEU:HD13	2.18	0.43
1:F:218:PRO:CG	1:F:394:PHE:HE2	2.31	0.43
8:J:301:BO2:H242	8:J:301:BO2:H21	1.67	0.43
2:M:166:THR:HG22	2:M:170:ARG:HH11	1.83	0.43
3:R:122:MET:HE1	3:R:165:ILE:HG23	1.99	0.43
1:A:258:GLY:C	1:A:260:ARG:H	2.21	0.43
1:B:288:ALA:O	1:B:291:THR:OG1	2.31	0.43
1:D:524:ALA:HA	1:D:717:ILE:HD13	2.00	0.43
1:D:556:GLY:HA3	1:D:769:GLY:HA3	2.00	0.43
1:E:182:ALA:HB2	1:E:187:LEU:HD12	2.00	0.43
1:F:187:LEU:HD13	1:F:227:GLU:HB2	2.00	0.43
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.69	0.43
3:Q:122:MET:HE1	3:Q:165:ILE:HG23	1.99	0.43
1:B:190:VAL:HG13	6:B:904:ATP:C6	2.52	0.43
2:L:166:THR:HG22	2:L:170:ARG:HH11	1.83	0.43
1:A:350:PRO:HB3	1:A:354:HIS:HD2	1.82	0.43
1:D:337:ALA:O	1:D:341:ARG:NH1	2.51	0.43
1:E:313:ALA:HB1	1:E:340:ARG:HH12	1.83	0.43
2:K:166:THR:HG22	2:K:170:ARG:HH11	1.83	0.43
3:Q:68:GLY:HA3	3:Q:98:SER:HB3	2.01	0.43
3:R:71:ILE:CD1	8:R:201:BO2:H23	2.39	0.43
1:A:746:ASP:HB3	1:A:796:PRO:HB3	2.01	0.43
1:B:359:LEU:HB3	1:B:379:MET:SD	2.59	0.43
1:C:694:LYS:HG3	1:C:718:VAL:HG21	2.01	0.43
2:I:147:PHE:CE2	3:P:125:PRO:HB2	2.54	0.43
2:J:103:VAL:HG22	2:J:125:MET:HB2	1.99	0.43
2:M:147:PHE:CE2	3:T:125:PRO:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:68:GLY:HA3	3:T:98:SER:HB3	2.01	0.43
1:A:411:ARG:NH2	1:B:241:THR:CG2	2.82	0.43
2:J:137:PRO:HB3	8:J:301:BO2:O19	2.19	0.43
3:N:122:MET:HE1	3:N:165:ILE:HG23	2.01	0.43
1:A:669:GLY:HA2	1:A:673:ILE:HD13	2.00	0.43
1:B:402:LEU:HB3	1:B:484:ILE:HG23	2.01	0.43
1:F:276:ILE:HA	1:F:282:ILE:HD11	2.01	0.43
1:F:517:ARG:O	1:F:519:ILE:HG12	2.19	0.43
2:K:137:PRO:HD3	2:K:164:MET:HE2	2.00	0.43
2:L:103:VAL:HG22	2:L:125:MET:HB2	2.00	0.43
1:B:292:LEU:HD21	1:B:308:LEU:HD12	2.00	0.42
1:C:555:SER:HB3	6:C:904:ATP:O2G	2.19	0.42
6:D:903:ATP:PG	1:E:341:ARG:NH1	2.92	0.42
1:F:293:VAL:HG11	1:F:338:LEU:HD22	2.01	0.42
1:F:557:VAL:HG22	1:F:722:LEU:HD11	2.01	0.42
3:Q:112:ARG:NH2	3:Q:187:ASP:OD1	2.47	0.42
3:S:98:SER:OG	3:S:99:MET:N	2.52	0.42
1:A:485:ALA:HB1	1:A:496:VAL:HG13	2.01	0.42
1:D:409:ARG:HH22	1:D:490:ASN:HD22	1.66	0.42
1:E:217:GLU:HG2	1:E:394:PHE:CE1	2.55	0.42
2:K:109:ALA:HA	2:K:133:LEU:HB3	2.01	0.42
1:A:198:GLU:CG	1:A:202:GLN:NE2	2.83	0.42
1:B:411:ARG:HE	1:C:241:THR:HG21	1.84	0.42
1:B:624:PHE:HE2	1:B:662:LEU:HD23	1.84	0.42
1:D:393:ARG:HE	1:E:340:ARG:HA	1.84	0.42
1:D:641:VAL:HG22	1:D:647:LEU:HB2	2.01	0.42
1:E:412:ILE:HD11	1:F:201:MET:C	2.40	0.42
1:F:517:ARG:HB2	1:F:519:ILE:HD11	1.99	0.42
1:A:550:ILE:HD12	1:A:716:ILE:HG12	2.01	0.42
1:C:494:ILE:HG12	1:C:619:PHE:HB2	2.02	0.42
1:E:204:LEU:HD11	1:E:320:ILE:HD11	2.02	0.42
2:L:150:LEU:HD22	3:S:129:VAL:HG22	2.02	0.42
3:N:20:VAL:HG13	3:T:50:LEU:HD22	2.01	0.42
3:S:98:SER:HB2	8:S:201:BO2:O27	2.19	0.42
1:B:706:ARG:NE	1:B:707:PRO:HD2	2.34	0.42
1:C:217:GLU:HB3	1:C:394:PHE:CZ	2.55	0.42
8:L:301:BO2:H242	8:L:301:BO2:H21	1.65	0.42
3:O:98:SER:HB2	3:O:123:HIS:HE1	1.84	0.42
1:A:550:ILE:HG13	1:A:713:ILE:HG21	2.01	0.42
1:C:375:THR:HG22	1:C:377:ALA:H	1.84	0.42
1:F:381:ALA:HA	1:F:384:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:148:SER:HB3	3:N:124:GLN:HE22	1.84	0.42
2:I:208:LYS:HB2	2:J:97:ARG:HD2	2.02	0.42
8:I:301:BO2:O28	8:I:301:BO2:H111	2.19	0.42
8:J:301:BO2:O28	8:J:301:BO2:H111	2.19	0.42
2:K:81:GLY:HA2	8:K:301:BO2:O28	2.20	0.42
3:S:68:GLY:CA	3:S:97:ALA:O	2.67	0.42
3:S:97:ALA:HA	3:S:121:LEU:HB3	2.00	0.42
3:T:98:SER:CB	3:T:123:HIS:CE1	3.02	0.42
1:B:488:LEU:HD23	1:B:496:VAL:HG21	2.02	0.42
1:B:631:HIS:HB3	1:B:634:ILE:HG12	2.02	0.42
1:C:389:TYR:HB2	1:C:488:LEU:HD21	2.00	0.42
1:D:217:GLU:HB3	1:D:394:PHE:CE1	2.55	0.42
1:F:509:ARG:H	1:F:509:ARG:HE	1.68	0.42
8:R:201:BO2:H10	8:R:201:BO2:H17	1.91	0.42
1:B:220:VAL:CA	1:B:396:PRO:HG2	2.45	0.42
1:E:408:ALA:O	1:E:411:ARG:CG	2.64	0.42
1:F:213:VAL:HG23	1:F:289:LEU:HD23	2.02	0.42
1:F:358:ILE:HG23	7:F:901:ADP:C2	2.55	0.42
3:N:97:ALA:CB	3:N:121:LEU:HB3	2.50	0.42
8:T:201:BO2:H20	8:T:201:BO2:H243	1.85	0.42
1:B:249:THR:HA	1:B:285:PHE:HB3	2.00	0.42
1:F:210:ASN:HD21	1:F:312:LEU:HD11	1.85	0.42
2:H:166:THR:HG22	2:H:170:ARG:HH11	1.83	0.42
3:N:152:ARG:HH22	3:O:117:HIS:HE1	1.68	0.42
3:O:98:SER:OG	8:O:201:BO2:C22	2.68	0.42
1:A:386:ALA:HB1	1:A:398:LYS:HG3	2.02	0.42
1:B:627:ILE:HG23	1:B:705:PHE:HZ	1.85	0.42
1:C:222:LYS:HE2	6:C:901:ATP:O2G	2.20	0.42
1:C:225:VAL:O	1:C:229:LEU:N	2.53	0.42
1:C:681:PHE:HB3	2:H:204:LEU:HD11	2.02	0.42
1:F:247:LEU:HD23	1:F:283:ILE:HB	2.01	0.42
1:F:498:LYS:HA	1:F:506:ARG:NH1	2.34	0.42
1:F:510:MET:HG3	1:F:532:ILE:CG2	2.50	0.42
1:F:791:PHE:HD2	1:F:793:GLU:HB2	1.83	0.42
3:N:97:ALA:HB1	3:N:121:LEU:HD23	2.01	0.42
1:A:340:ARG:HA	1:A:340:ARG:HD3	1.71	0.41
1:C:606:GLU:HG2	1:C:608:GLY:H	1.84	0.41
1:D:230:ALA:HB2	1:D:247:LEU:HD23	2.02	0.41
1:D:726:GLU:HB3	1:D:729:ARG:HH11	1.85	0.41
1:D:730:MET:CE	7:D:901:ADP:C1'	2.84	0.41
1:F:190:VAL:CA	7:F:901:ADP:N1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:GLY:HA2	1:F:771:ARG:HH11	1.85	0.41
3:O:71:ILE:HD11	8:O:201:BO2:H20	1.85	0.41
1:A:312:LEU:HA	1:A:316:GLU:O	2.20	0.41
1:B:485:ALA:HB1	1:B:496:VAL:HG23	2.01	0.41
1:C:730:MET:CE	6:C:904:ATP:C6	3.03	0.41
2:H:81:GLY:HA2	8:H:301:BO2:O28	2.19	0.41
2:J:166:THR:HG22	2:J:170:ARG:HH11	1.83	0.41
3:T:98:SER:HB2	3:T:123:HIS:CE1	2.55	0.41
1:A:726:GLU:HG2	1:A:729:ARG:HH21	1.84	0.41
1:B:352:VAL:CG2	1:B:395:LEU:HD11	2.49	0.41
2:K:137:PRO:HB3	8:K:301:BO2:O19	2.20	0.41
3:O:98:SER:HB3	3:O:99:MET:H	1.58	0.41
3:Q:98:SER:OG	8:Q:201:BO2:C22	2.68	0.41
1:B:395:LEU:HD23	1:B:395:LEU:HA	1.75	0.41
2:J:125:MET:SD	2:J:125:MET:N	2.94	0.41
3:Q:68:GLY:HA2	3:Q:98:SER:HB3	2.03	0.41
3:S:97:ALA:CB	3:S:121:LEU:HB3	2.51	0.41
3:T:99:MET:N	8:T:201:BO2:H242	2.35	0.41
1:C:395:LEU:HD23	1:C:395:LEU:HA	1.87	0.41
1:C:579:GLN:HG2	1:C:623:LEU:HD23	2.03	0.41
1:F:508:LEU:HD13	1:F:508:LEU:HA	1.84	0.41
3:P:52:ALA:HB1	3:P:85:PRO:HD2	2.03	0.41
1:A:325:LEU:HD11	1:A:329:ARG:HH21	1.85	0.41
1:A:740:GLY:O	1:A:744:SER:N	2.54	0.41
1:A:774:ARG:HH12	1:B:544:ARG:HH11	1.67	0.41
1:E:370:HIS:HA	1:E:411:ARG:NH2	2.35	0.41
1:E:411:ARG:HD2	1:F:205:SER:OG	2.11	0.41
2:L:137:PRO:HB3	8:L:301:BO2:O19	2.21	0.41
3:Q:54:GLU:OE2	3:R:23:ARG:NH2	2.46	0.41
3:R:52:ALA:HB1	3:R:85:PRO:HD2	2.03	0.41
1:D:768:LEU:HB3	1:D:772:PRO:CG	2.50	0.41
1:F:218:PRO:HG2	1:F:394:PHE:CE2	2.55	0.41
2:I:125:MET:SD	2:I:125:MET:N	2.94	0.41
3:S:112:ARG:NH2	3:S:187:ASP:OD1	2.47	0.41
3:T:98:SER:C	3:T:100:GLY:N	2.74	0.41
1:A:526:LYS:HG2	1:A:530:LYS:HE2	2.03	0.41
1:A:583:GLY:O	1:B:637:SER:HA	2.21	0.41
1:C:507:LEU:HD11	1:C:536:ARG:HG3	2.03	0.41
1:D:382:ALA:HB2	1:D:484:ILE:HD13	2.03	0.41
1:E:312:LEU:HB2	1:E:341:ARG:HD3	2.01	0.41
1:E:395:LEU:HA	1:E:398:LYS:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:ASP:HB2	1:F:395:LEU:HD21	2.02	0.41
1:F:508:LEU:HB3	1:F:509:ARG:H	1.60	0.41
2:H:125:MET:SD	2:H:125:MET:N	2.94	0.41
2:I:110:SER:CB	8:I:301:BO2:O27	2.67	0.41
2:I:124:ARG:NH2	2:I:201:ASP:OD1	2.51	0.41
2:M:101:GLN:HA	2:M:123:LYS:HB3	2.03	0.41
2:M:124:ARG:NH2	2:M:201:ASP:OD1	2.51	0.41
1:A:212:PRO:HG2	1:A:320:ILE:HG12	2.03	0.41
1:A:542:PRO:HD3	1:F:741:GLN:NE2	2.36	0.41
1:B:727:ILE:HG23	1:B:773:LEU:HD22	2.03	0.41
1:C:554:PRO:HG2	1:C:557:VAL:HG11	2.03	0.41
1:C:731:VAL:HG22	1:C:773:LEU:HD11	2.02	0.41
1:D:359:LEU:HB3	1:D:379:MET:SD	2.61	0.41
1:F:306:SER:HA	1:F:309:LYS:HD3	2.03	0.41
1:F:627:ILE:HD12	1:F:627:ILE:HA	1.95	0.41
2:G:81:GLY:HA2	8:G:301:BO2:O28	2.21	0.41
2:G:109:ALA:HA	2:G:133:LEU:HB3	2.02	0.41
2:G:125:MET:N	2:G:125:MET:SD	2.94	0.41
2:G:126:ALA:HB3	2:G:200:ILE:HD13	2.03	0.41
2:J:131:ARG:HH11	2:K:84:THR:HG21	1.85	0.41
2:K:184:ASP:O	3:S:171:ARG:NH1	2.52	0.41
2:M:125:MET:SD	2:M:125:MET:N	2.94	0.41
3:R:83:LEU:HD11	3:S:116:PRO:HD3	2.03	0.41
3:R:123:HIS:O	8:R:201:BO2:H253	2.20	0.41
3:S:52:ALA:HB1	3:S:85:PRO:HD2	2.03	0.41
3:T:68:GLY:HA2	3:T:98:SER:HB3	2.02	0.41
3:T:125:PRO:HA	8:T:201:BO2:C22	2.31	0.41
1:B:230:ALA:HB2	1:B:247:LEU:HD23	2.02	0.41
1:B:393:ARG:NH1	1:C:342:PHE:O	2.51	0.41
1:B:739:ALA:HB2	1:B:749:LEU:HB3	2.02	0.41
1:C:629:LYS:HZ2	1:C:667:ASN:HD22	1.69	0.41
1:E:370:HIS:HE1	1:F:206:ARG:HA	1.86	0.41
1:F:512:GLU:O	1:F:515:HIS:N	2.54	0.41
2:G:101:GLN:HA	2:G:123:LYS:HB3	2.03	0.41
2:H:57:MET:HG3	2:H:89:ILE:HG22	2.03	0.41
2:H:126:ALA:HB3	2:H:200:ILE:HD13	2.03	0.41
2:H:137:PRO:HB3	8:H:301:BO2:O19	2.21	0.41
2:H:195:LYS:HB3	2:H:200:ILE:HG13	2.03	0.41
2:I:101:GLN:HA	2:I:123:LYS:HB3	2.03	0.41
2:J:105:LEU:HB3	2:K:57:MET:SD	2.61	0.41
2:K:125:MET:SD	2:K:125:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:57:MET:HG3	2:L:89:ILE:HG22	2.03	0.41
2:M:57:MET:HG3	2:M:89:ILE:HG22	2.03	0.41
3:N:70:SER:O	3:N:99:MET:HG3	2.21	0.41
1:A:191:ILE:HG13	1:A:361:GLY:HA3	2.02	0.40
1:A:264:ASP:H	1:B:262:ARG:NH2	2.18	0.40
1:A:309:LYS:N	1:A:310:PRO:HD2	2.37	0.40
1:A:395:LEU:O	1:A:396:PRO:C	2.59	0.40
1:B:649:ASP:OD1	1:B:650:GLY:N	2.54	0.40
1:C:648:THR:HA	1:C:654:THR:HA	2.02	0.40
1:F:408:ALA:O	1:F:412:ILE:CD1	2.69	0.40
3:O:52:ALA:HB1	3:O:85:PRO:HD2	2.03	0.40
1:E:363:ARG:NH2	1:E:376:ASP:OD1	2.52	0.40
1:F:507:LEU:O	1:F:508:LEU:C	2.58	0.40
2:I:57:MET:HG3	2:I:89:ILE:HG22	2.03	0.40
2:K:126:ALA:HB3	2:K:200:ILE:HD13	2.03	0.40
2:L:125:MET:SD	2:L:125:MET:N	2.94	0.40
8:L:301:BO2:H111	8:L:301:BO2:O28	2.20	0.40
2:M:195:LYS:HB3	2:M:200:ILE:HG13	2.03	0.40
1:A:683:LYS:HD3	2:M:202:THR:HG21	2.04	0.40
1:C:265:PHE:CZ	1:C:304:ALA:HB2	2.56	0.40
1:D:362:LEU:HD11	6:D:903:ATP:N3	2.36	0.40
1:E:414:ARG:NH1	1:F:240:GLU:OE2	2.51	0.40
1:F:518:ILE:HD13	1:F:525:VAL:HB	2.04	0.40
2:K:195:LYS:HB3	2:K:200:ILE:HG13	2.03	0.40
3:N:190:ILE:HG22	3:T:83:LEU:HD22	2.02	0.40
3:Q:98:SER:HB3	3:Q:99:MET:H	1.60	0.40
3:Q:99:MET:N	8:Q:201:BO2:H252	2.37	0.40
8:G:301:BO2:H242	8:G:301:BO2:H21	1.65	0.40
3:N:98:SER:OG	3:N:99:MET:N	2.53	0.40
3:P:126:LEU:HB2	8:P:201:BO2:O19	2.21	0.40
1:A:404:ASP:HB3	1:B:206:ARG:HE	1.86	0.40
1:A:588:ARG:HB3	1:A:631:HIS:CE1	2.57	0.40
1:A:589:PHE:HE1	1:C:601:TYR:HH	1.67	0.40
1:D:771:ARG:N	1:D:772:PRO:CD	2.84	0.40
1:E:408:ALA:C	1:E:411:ARG:HG2	2.41	0.40
1:F:286:ILE:HG22	1:F:288:ALA:H	1.87	0.40
2:L:81:GLY:HA2	8:L:301:BO2:O28	2.21	0.40
2:M:148:SER:HB3	3:T:124:GLN:HE22	1.87	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	567/657 (86%)	531 (94%)	36 (6%)	0	100	100
1	B	556/657 (85%)	535 (96%)	21 (4%)	0	100	100
1	C	562/657 (86%)	537 (96%)	24 (4%)	1 (0%)	44	71
1	D	536/657 (82%)	508 (95%)	27 (5%)	1 (0%)	44	71
1	E	264/657 (40%)	244 (92%)	19 (7%)	1 (0%)	30	59
1	F	432/657 (66%)	402 (93%)	27 (6%)	3 (1%)	19	46
2	G	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	H	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	I	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	J	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	K	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	L	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
2	M	179/181 (99%)	167 (93%)	12 (7%)	0	100	100
3	N	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
3	O	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
3	P	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
3	Q	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
3	R	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
3	S	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
3	T	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
4	a	22/24 (92%)	19 (86%)	3 (14%)	0	100	100
All	All	5424/6479 (84%)	5123 (94%)	295 (5%)	6 (0%)	50	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	485	ALA
1	C	397	ASP
1	D	397	ASP
1	F	507	LEU
1	F	519	ILE
1	E	396	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	476/543 (88%)	467 (98%)	9 (2%)	52	81
1	B	467/543 (86%)	462 (99%)	5 (1%)	70	90
1	C	474/543 (87%)	473 (100%)	1 (0%)	92	97
1	D	450/543 (83%)	443 (98%)	7 (2%)	58	84
1	E	216/543 (40%)	212 (98%)	4 (2%)	52	81
1	F	383/543 (70%)	366 (96%)	17 (4%)	24	55
2	G	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	H	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	I	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	J	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	K	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	L	149/149 (100%)	148 (99%)	1 (1%)	81	94
2	M	149/149 (100%)	147 (99%)	2 (1%)	65	88
3	N	139/139 (100%)	138 (99%)	1 (1%)	81	94
3	O	139/139 (100%)	137 (99%)	2 (1%)	62	86
3	P	139/139 (100%)	137 (99%)	2 (1%)	62	86
3	Q	139/139 (100%)	137 (99%)	2 (1%)	62	86
3	R	139/139 (100%)	137 (99%)	2 (1%)	62	86
3	S	139/139 (100%)	139 (100%)	0	100	100
3	T	139/139 (100%)	137 (99%)	2 (1%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	a	20/20 (100%)	20 (100%)	0	100 100
All	All	4502/5294 (85%)	4440 (99%)	62 (1%)	62 86

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	LYS
1	A	259	SER
1	A	260	ARG
1	A	314	ARG
1	A	317	LEU
1	A	340	ARG
1	A	395	LEU
1	A	588	ARG
1	A	745	LYS
1	B	222	LYS
1	B	388	ARG
1	B	397	ASP
1	B	588	ARG
1	B	646	ARG
1	C	397	ASP
1	D	371	ARG
1	D	395	LEU
1	D	410	MET
1	D	615	ARG
1	D	646	ARG
1	D	747	MET
1	D	771	ARG
1	E	176	ARG
1	E	340	ARG
1	E	395	LEU
1	E	397	ASP
1	F	176	ARG
1	F	222	LYS
1	F	223	THR
1	F	242	LEU
1	F	340	ARG
1	F	498	LYS
1	F	505	THR
1	F	506	ARG
1	F	507	LEU
1	F	508	LEU

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Mol	Chain	Res	Type
1	F	509	ARG
1	F	510	MET
1	F	515	HIS
1	F	517	ARG
1	F	518	ILE
1	F	530	LYS
1	F	636	ASN
2	G	131	ARG
2	H	131	ARG
2	I	131	ARG
2	J	131	ARG
2	K	131	ARG
2	L	131	ARG
2	M	110	SER
2	M	131	ARG
3	N	99	MET
3	O	98	SER
3	O	99	MET
3	P	98	SER
3	P	99	MET
3	Q	98	SER
3	Q	99	MET
3	R	98	SER
3	R	99	MET
3	T	98	SER
3	T	99	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	211	ASN
1	A	354	HIS
1	A	609	GLN
1	A	659	ASN
1	B	211	ASN
1	B	667	ASN
1	B	720	HIS
1	C	246	GLN
1	C	354	HIS
1	C	798	GLN
1	D	490	ASN

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Mol	Chain	Res	Type
1	D	631	HIS
1	D	651	GLN
1	E	235	HIS
1	F	354	HIS
1	F	370	HIS
1	F	636	ASN
2	G	34	ASN
2	G	135	HIS
2	H	34	ASN
2	H	135	HIS
2	I	34	ASN
2	I	135	HIS
2	J	34	ASN
2	J	135	HIS
2	K	34	ASN
2	K	54	ASN
2	K	77	ASN
2	K	135	HIS
2	L	34	ASN
2	L	54	ASN
2	L	135	HIS
2	M	34	ASN
3	O	142	GLN
3	P	142	GLN
3	Q	142	GLN
3	R	142	GLN
3	S	142	GLN
3	T	142	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 7 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
8	BO2	G	301	-	25,29,29	0.22	0	32,38,38	0.36	0
6	ATP	A	902	5	26,33,33	0.68	0	31,52,52	0.85	1 (3%)
8	BO2	J	301	-	25,29,29	0.22	0	32,38,38	0.35	0
8	BO2	M	301	-	25,29,29	0.23	0	32,38,38	0.43	0
8	BO2	K	301	-	25,29,29	0.21	0	32,38,38	0.35	0
8	BO2	S	201	-	25,29,29	0.23	0	32,38,38	0.39	0
8	BO2	I	301	-	25,29,29	0.22	0	32,38,38	0.38	0
6	ATP	A	904	-	26,33,33	0.68	0	31,52,52	0.73	1 (3%)
8	BO2	O	201	-	25,29,29	0.25	0	32,38,38	0.58	1 (3%)
8	BO2	T	201	-	25,29,29	0.24	0	32,38,38	0.62	1 (3%)
8	BO2	Q	201	-	25,29,29	0.23	0	32,38,38	0.57	1 (3%)
6	ATP	C	904	5	26,33,33	0.71	0	31,52,52	0.80	1 (3%)
6	ATP	B	904	5	26,33,33	0.70	0	31,52,52	0.77	1 (3%)
8	BO2	N	201	-	25,29,29	0.26	0	32,38,38	0.38	0
7	ADP	D	901	-	24,29,29	0.70	1 (4%)	29,45,45	0.70	1 (3%)
7	ADP	F	901	-	24,29,29	0.68	0	29,45,45	0.72	1 (3%)
8	BO2	R	201	-	25,29,29	0.24	0	32,38,38	0.42	0
8	BO2	L	301	-	25,29,29	0.22	0	32,38,38	0.37	0
6	ATP	C	901	5	26,33,33	0.71	0	31,52,52	0.84	1 (3%)
8	BO2	P	201	-	25,29,29	0.24	0	32,38,38	0.41	0
8	BO2	H	301	-	25,29,29	0.21	0	32,38,38	0.38	0
6	ATP	B	903	5	26,33,33	0.74	0	31,52,52	0.76	1 (3%)
6	ATP	D	903	5	26,33,33	0.69	0	31,52,52	0.74	1 (3%)
7	ADP	E	901	-	24,29,29	0.73	0	29,45,45	0.94	3 (10%)

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
8	BO2	G	301	-	-	8/22/28/28	0/2/2/2
6	ATP	A	902	5	-	4/18/38/38	0/3/3/3
8	BO2	J	301	-	-	8/22/28/28	0/2/2/2
8	BO2	M	301	-	-	5/22/28/28	0/2/2/2
8	BO2	K	301	-	-	8/22/28/28	0/2/2/2
8	BO2	S	201	-	-	16/22/28/28	0/2/2/2
8	BO2	I	301	-	-	8/22/28/28	0/2/2/2
6	ATP	A	904	-	-	5/18/38/38	0/3/3/3
8	BO2	O	201	-	-	9/22/28/28	0/2/2/2
8	BO2	T	201	-	-	15/22/28/28	0/2/2/2
8	BO2	Q	201	-	-	15/22/28/28	0/2/2/2
6	ATP	C	904	5	-	7/18/38/38	0/3/3/3
6	ATP	B	904	5	-	5/18/38/38	0/3/3/3
8	BO2	N	201	-	-	7/22/28/28	0/2/2/2
7	ADP	D	901	-	-	5/12/32/32	0/3/3/3
7	ADP	F	901	-	-	0/12/32/32	0/3/3/3
8	BO2	R	201	-	-	12/22/28/28	0/2/2/2
8	BO2	L	301	-	-	8/22/28/28	0/2/2/2
6	ATP	C	901	5	-	8/18/38/38	0/3/3/3
8	BO2	P	201	-	-	9/22/28/28	0/2/2/2
8	BO2	H	301	-	-	8/22/28/28	0/2/2/2
6	ATP	B	903	5	-	6/18/38/38	0/3/3/3
6	ATP	D	903	5	-	2/18/38/38	0/3/3/3
7	ADP	E	901	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	901	ADP	C8-N7	-2.04	1.31	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	T	201	BO2	C21-C22-C23	2.91	119.06	115.39
8	O	201	BO2	C21-C22-C23	2.56	118.61	115.39
8	Q	201	BO2	C21-C22-C23	2.54	118.59	115.39
7	E	901	ADP	C5-C6-N6	2.32	123.87	120.35
6	A	902	ATP	C5-C6-N6	2.30	123.85	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	901	ATP	C5-C6-N6	2.28	123.82	120.35
6	B	904	ATP	C5-C6-N6	2.27	123.81	120.35
6	C	904	ATP	C5-C6-N6	2.25	123.77	120.35
7	E	901	ADP	O2B-PB-O1B	2.25	119.48	110.68
6	D	903	ATP	C5-C6-N6	2.19	123.68	120.35
6	B	903	ATP	C5-C6-N6	2.19	123.67	120.35
6	A	904	ATP	C5-C6-N6	2.18	123.66	120.35
7	F	901	ADP	C5-C6-N6	2.17	123.65	120.35
7	E	901	ADP	O4'-C1'-C2'	-2.14	103.80	106.93
7	D	901	ADP	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	902	ATP	PB-O3B-PG-O3G
6	B	903	ATP	PB-O3B-PG-O2G
6	B	903	ATP	PB-O3B-PG-O3G
6	C	901	ATP	C5'-O5'-PA-O1A
6	C	901	ATP	C5'-O5'-PA-O2A
6	C	904	ATP	C5'-O5'-PA-O1A
6	C	904	ATP	O4'-C4'-C5'-O5'
7	D	901	ADP	C5'-O5'-PA-O2A
7	D	901	ADP	C5'-O5'-PA-O3A
7	D	901	ADP	O4'-C4'-C5'-O5'
7	E	901	ADP	C3'-C4'-C5'-O5'
8	G	301	BO2	C10-C18-N20-C21
8	G	301	BO2	O19-C18-N20-C21
8	G	301	BO2	C22-C21-N20-C18
8	G	301	BO2	C21-C22-C23-C24
8	G	301	BO2	C21-C22-C23-C25
8	H	301	BO2	C10-C18-N20-C21
8	H	301	BO2	O19-C18-N20-C21
8	H	301	BO2	C22-C21-N20-C18
8	H	301	BO2	C21-C22-C23-C24
8	H	301	BO2	C21-C22-C23-C25
8	I	301	BO2	C10-C18-N20-C21
8	I	301	BO2	O19-C18-N20-C21
8	I	301	BO2	C22-C21-N20-C18
8	I	301	BO2	C21-C22-C23-C24
8	I	301	BO2	C21-C22-C23-C25
8	J	301	BO2	C10-C18-N20-C21

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Mol	Chain	Res	Type	Atoms
8	J	301	BO2	O19-C18-N20-C21
8	J	301	BO2	C22-C21-N20-C18
8	J	301	BO2	C21-C22-C23-C25
8	K	301	BO2	C10-C18-N20-C21
8	K	301	BO2	O19-C18-N20-C21
8	K	301	BO2	C22-C21-N20-C18
8	K	301	BO2	C21-C22-C23-C25
8	L	301	BO2	C10-C18-N20-C21
8	L	301	BO2	O19-C18-N20-C21
8	L	301	BO2	C22-C21-N20-C18
8	L	301	BO2	C21-C22-C23-C25
8	N	201	BO2	C3-C2-C7-O8
8	N	201	BO2	C10-C18-N20-C21
8	N	201	BO2	O19-C18-N20-C21
8	N	201	BO2	N20-C21-C22-C23
8	O	201	BO2	C3-C2-C7-O8
8	O	201	BO2	C3-C2-C7-N9
8	O	201	BO2	C21-C22-C23-C24
8	O	201	BO2	C21-C22-C23-C25
8	P	201	BO2	C3-C2-C7-O8
8	P	201	BO2	C18-C10-C11-C12
8	P	201	BO2	O19-C18-N20-C21
8	Q	201	BO2	C3-C2-C7-O8
8	Q	201	BO2	C3-C2-C7-N9
8	Q	201	BO2	C21-C22-C23-C24
8	Q	201	BO2	C21-C22-C23-C25
8	R	201	BO2	N1-C2-C7-O8
8	R	201	BO2	N1-C2-C7-N9
8	R	201	BO2	C3-C2-C7-O8
8	R	201	BO2	C3-C2-C7-N9
8	R	201	BO2	C2-C7-N9-C10
8	R	201	BO2	C11-C10-N9-C7
8	R	201	BO2	C10-C18-N20-C21
8	R	201	BO2	O19-C18-N20-C21
8	S	201	BO2	C3-C2-C7-O8
8	S	201	BO2	C3-C2-C7-N9
8	S	201	BO2	O19-C18-N20-C21
8	S	201	BO2	N20-C21-C22-C23
8	T	201	BO2	C3-C2-C7-O8
8	T	201	BO2	C3-C2-C7-N9
8	T	201	BO2	C21-C22-C23-C24
8	T	201	BO2	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
8	Q	201	BO2	N1-C2-C7-O8
8	S	201	BO2	N1-C2-C7-O8
8	T	201	BO2	N1-C2-C7-O8
8	Q	201	BO2	N1-C2-C7-N9
8	S	201	BO2	N1-C2-C7-N9
8	T	201	BO2	N1-C2-C7-N9
8	N	201	BO2	N1-C2-C7-O8
8	P	201	BO2	N1-C2-C7-O8
8	P	201	BO2	N9-C10-C11-C12
8	R	201	BO2	N20-C21-C22-C23
8	R	201	BO2	O8-C7-N9-C10
8	N	201	BO2	N1-C2-C7-N9
8	P	201	BO2	N1-C2-C7-N9
8	O	201	BO2	N9-C10-C11-C12
8	Q	201	BO2	C18-C10-C11-C12
8	S	201	BO2	C18-C10-C11-C12
8	T	201	BO2	C18-C10-C11-C12
8	I	301	BO2	C11-C10-C18-O19
8	G	301	BO2	C11-C10-C18-N20
8	I	301	BO2	C11-C10-C18-N20
8	J	301	BO2	C11-C10-C18-N20
8	H	301	BO2	C11-C10-C18-N20
8	K	301	BO2	C11-C10-C18-N20
8	L	301	BO2	C11-C10-C18-N20
8	Q	201	BO2	N9-C10-C11-C12
8	T	201	BO2	N9-C10-C11-C12
8	G	301	BO2	N20-C21-C22-C23
8	H	301	BO2	N20-C21-C22-C23
8	J	301	BO2	N20-C21-C22-C23
8	K	301	BO2	N20-C21-C22-C23
8	L	301	BO2	N20-C21-C22-C23
8	G	301	BO2	C11-C10-C18-O19
8	H	301	BO2	C11-C10-C18-O19
8	J	301	BO2	C11-C10-C18-O19
8	K	301	BO2	C11-C10-C18-O19
8	L	301	BO2	C11-C10-C18-O19
6	B	904	ATP	O4'-C4'-C5'-O5'
6	C	904	ATP	C3'-C4'-C5'-O5'
8	M	301	BO2	N9-C10-C11-C12
8	S	201	BO2	N9-C10-C11-C12
8	I	301	BO2	N20-C21-C22-C23
8	Q	201	BO2	C18-C10-N9-C7

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Mol	Chain	Res	Type	Atoms
8	Q	201	BO2	O8-C7-N9-C10
8	S	201	BO2	O8-C7-N9-C10
8	P	201	BO2	C10-C18-N20-C21
8	S	201	BO2	C18-C10-N9-C7
8	O	201	BO2	N1-C2-C7-N9
6	B	904	ATP	C3'-C4'-C5'-O5'
6	C	901	ATP	O4'-C4'-C5'-O5'
7	E	901	ADP	O4'-C4'-C5'-O5'
8	O	201	BO2	N1-C2-C7-O8
8	N	201	BO2	C3-C2-C7-N9
8	P	201	BO2	C3-C2-C7-N9
8	T	201	BO2	C18-C10-N9-C7
8	O	201	BO2	C18-C10-C11-C12
8	T	201	BO2	O8-C7-N9-C10
6	B	903	ATP	C3'-C4'-C5'-O5'
6	C	901	ATP	C3'-C4'-C5'-O5'
8	P	201	BO2	N20-C21-C22-C23
6	B	903	ATP	O4'-C4'-C5'-O5'
8	S	201	BO2	C10-C18-N20-C21
8	S	201	BO2	N9-C10-C18-N20
8	S	201	BO2	N9-C10-C18-O19
7	E	901	ADP	C4'-C5'-O5'-PA
8	T	201	BO2	N9-C10-C18-O19
8	T	201	BO2	N9-C10-C18-N20
8	S	201	BO2	C11-C10-N9-C7
8	S	201	BO2	C2-C7-N9-C10
6	A	902	ATP	PB-O3B-PG-O1G
8	Q	201	BO2	C11-C10-N9-C7
8	Q	201	BO2	N9-C10-C18-N20
6	C	901	ATP	C4'-C5'-O5'-PA
8	Q	201	BO2	N9-C10-C18-O19
6	C	904	ATP	C5'-O5'-PA-O3A
6	A	902	ATP	PG-O3B-PB-O2B
6	A	904	ATP	PG-O3B-PB-O1B
6	B	904	ATP	PA-O3A-PB-O2B
6	C	901	ATP	PG-O3B-PB-O2B
6	C	904	ATP	PB-O3A-PA-O2A
8	R	201	BO2	C10-C11-C12-C17
8	M	301	BO2	C22-C21-N20-C18
8	Q	201	BO2	C2-C7-N9-C10
6	C	904	ATP	C5'-O5'-PA-O2A
8	J	301	BO2	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	K	301	BO2	C21-C22-C23-C24
8	L	301	BO2	C21-C22-C23-C24
8	M	301	BO2	C21-C22-C23-C25
8	R	201	BO2	C10-C11-C12-C13
6	A	902	ATP	PG-O3B-PB-O1B
6	A	904	ATP	PG-O3B-PB-O2B
6	B	903	ATP	PG-O3B-PB-O2B
8	T	201	BO2	C11-C10-N9-C7
8	T	201	BO2	C2-C7-N9-C10
8	M	301	BO2	C18-C10-C11-C12
6	A	904	ATP	C4'-C5'-O5'-PA
7	D	901	ADP	C3'-C4'-C5'-O5'
8	O	201	BO2	C18-C10-N9-C7
6	D	903	ATP	PB-O3A-PA-O1A
6	A	904	ATP	O4'-C4'-C5'-O5'
6	D	903	ATP	O4'-C4'-C5'-O5'
6	C	901	ATP	C5'-O5'-PA-O3A
6	B	903	ATP	PG-O3B-PB-O1B
6	B	904	ATP	PG-O3B-PB-O2B
6	C	901	ATP	PG-O3B-PB-O1B
6	C	904	ATP	PB-O3A-PA-O1A
7	D	901	ADP	PB-O3A-PA-O1A
8	Q	201	BO2	C11-C10-C18-O19
8	T	201	BO2	C11-C10-C18-O19
8	S	201	BO2	C11-C10-C18-O19
6	B	904	ATP	C5'-O5'-PA-O1A
7	E	901	ADP	C5'-O5'-PA-O1A
6	A	904	ATP	C3'-C4'-C5'-O5'
8	M	301	BO2	C21-C22-C23-C24

There are no ring outliers.

24 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	301	BO2	13	0
6	A	902	ATP	26	0
8	J	301	BO2	12	0
8	M	301	BO2	7	0
8	K	301	BO2	11	0
8	S	201	BO2	13	0
8	I	301	BO2	13	0
6	A	904	ATP	9	0

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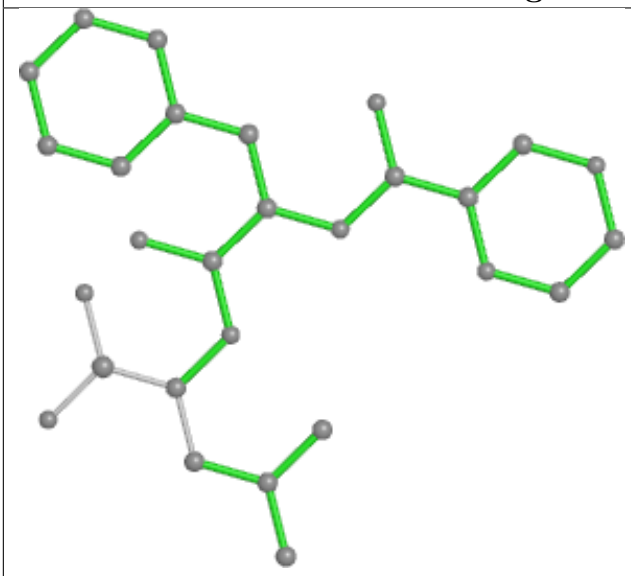
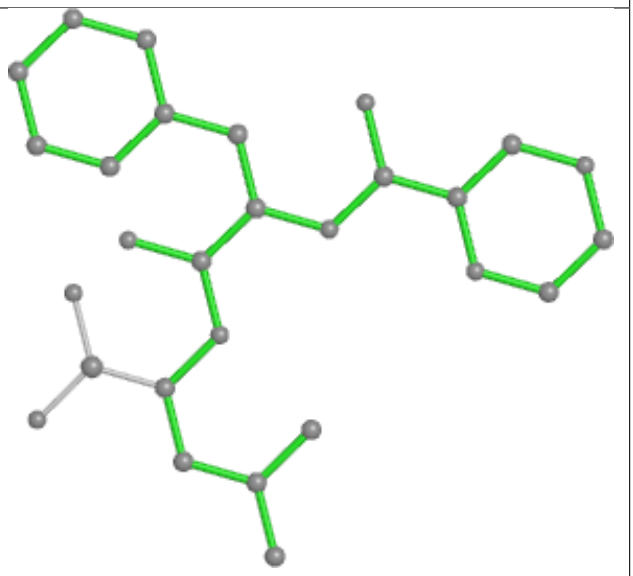
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	201	BO2	12	0
8	T	201	BO2	11	0
8	Q	201	BO2	12	0
6	C	904	ATP	30	0
6	B	904	ATP	8	0
8	N	201	BO2	8	0
7	D	901	ADP	41	0
7	F	901	ADP	14	0
8	R	201	BO2	18	0
8	L	301	BO2	14	0
6	C	901	ATP	16	0
8	P	201	BO2	12	0
8	H	301	BO2	13	0
6	B	903	ATP	26	0
6	D	903	ATP	11	0
7	E	901	ADP	8	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.

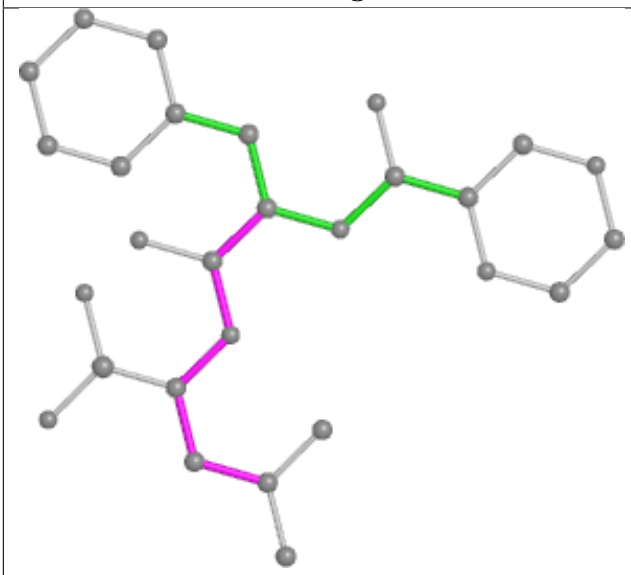
Ligand BO2 G 301



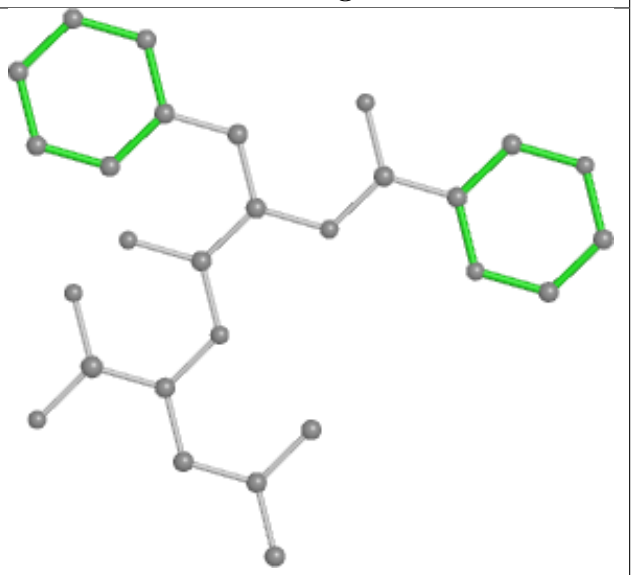
Bond lengths



Bond angles

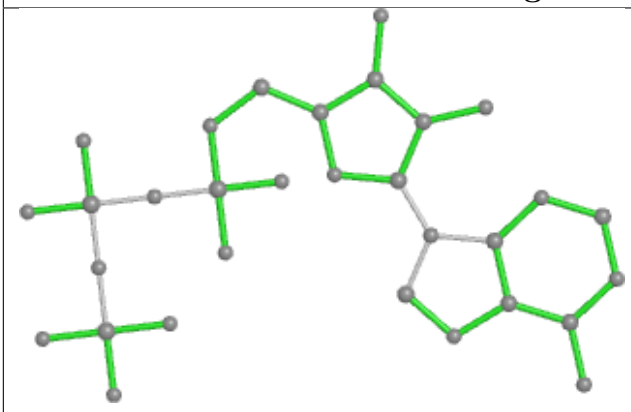


Torsions

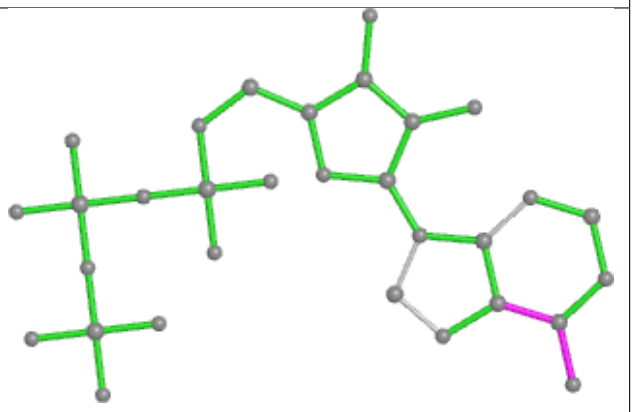


Rings

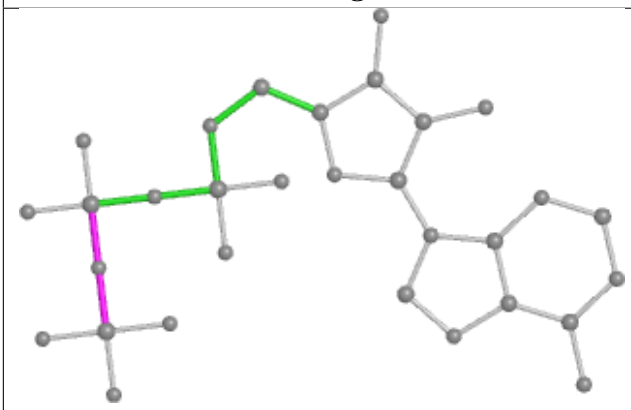
Ligand ATP A 902



Bond lengths



Bond angles



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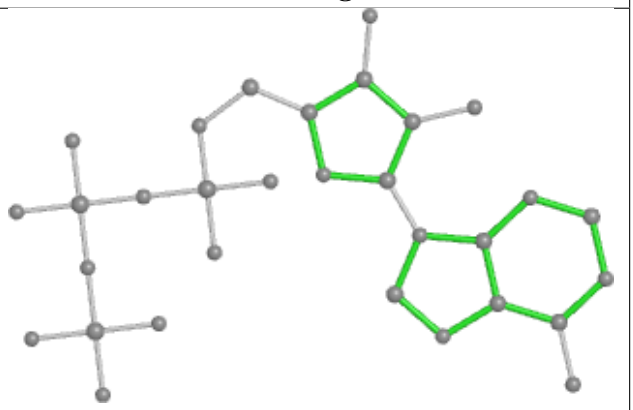
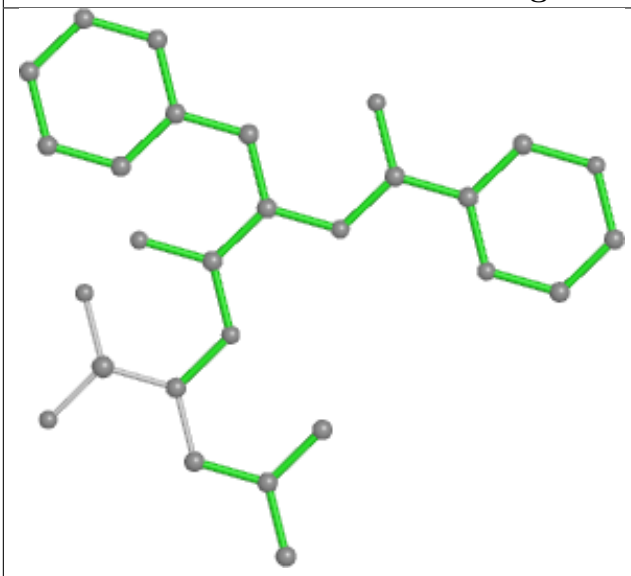
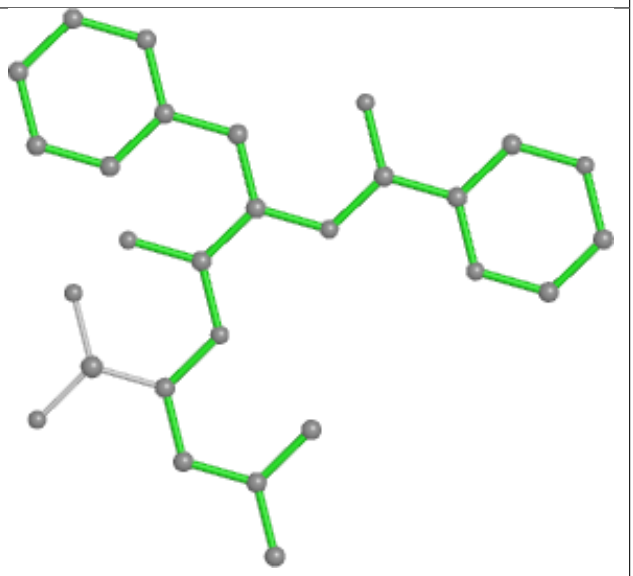


Rings

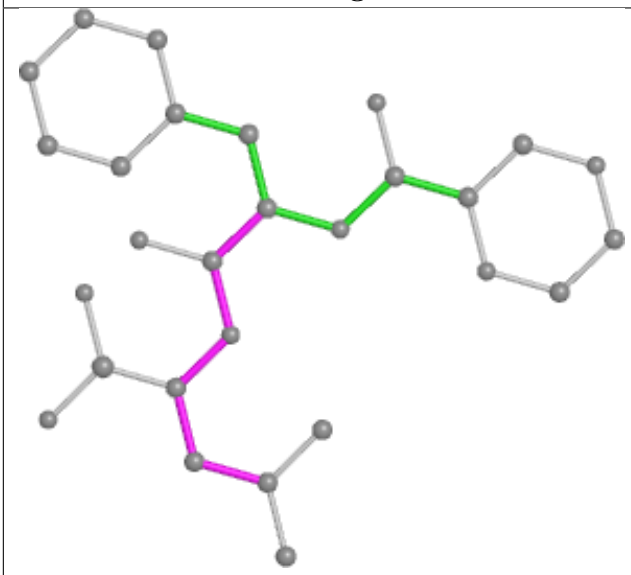
Ligand BO2 J 301



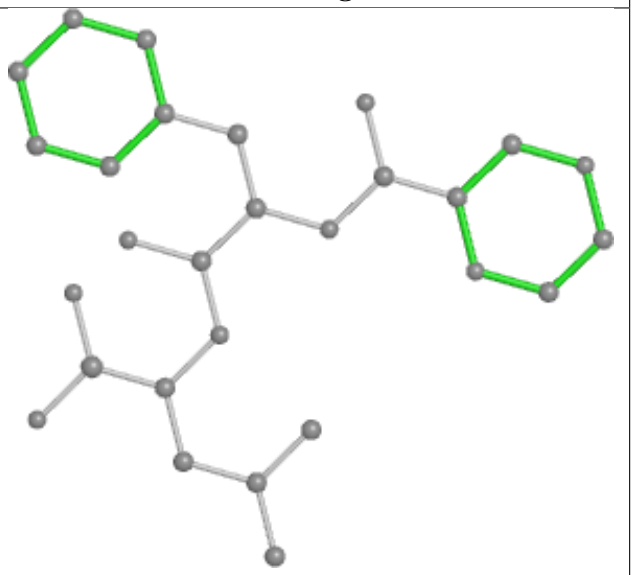
Bond lengths



Bond angles

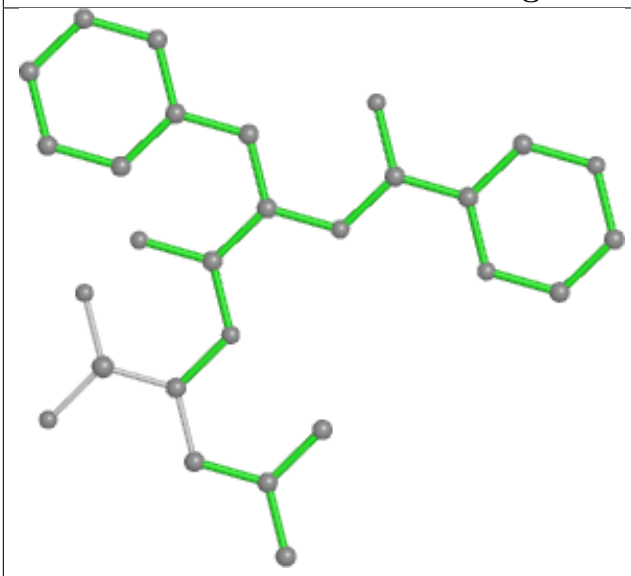


Torsions

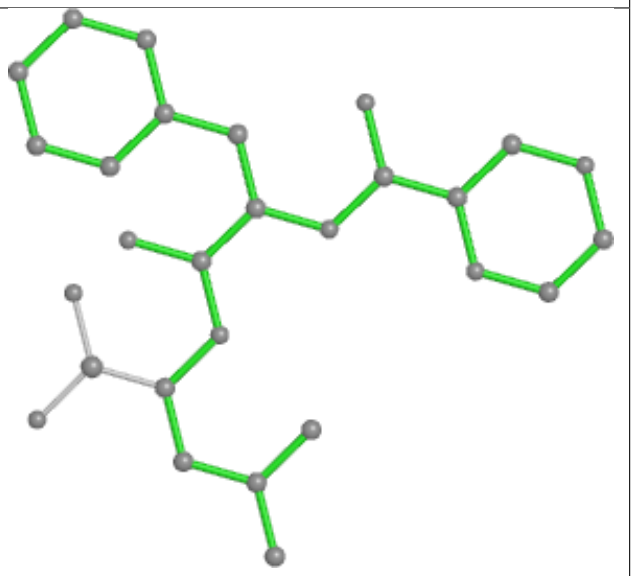


Rings

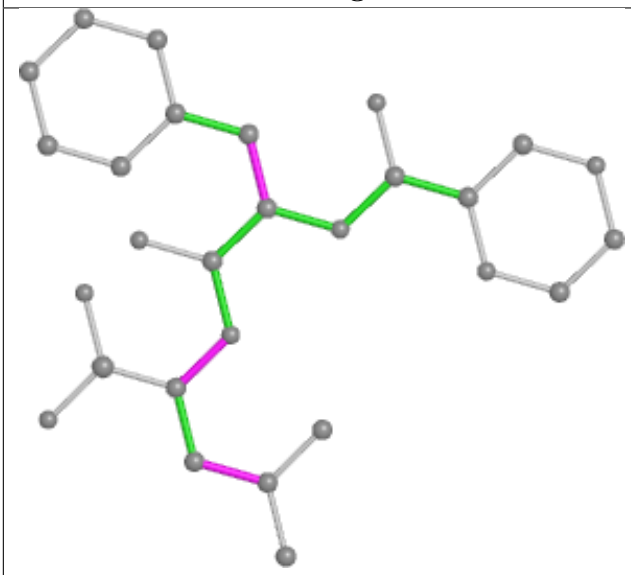
Ligand BO2 M 301



Bond lengths



Bond angles



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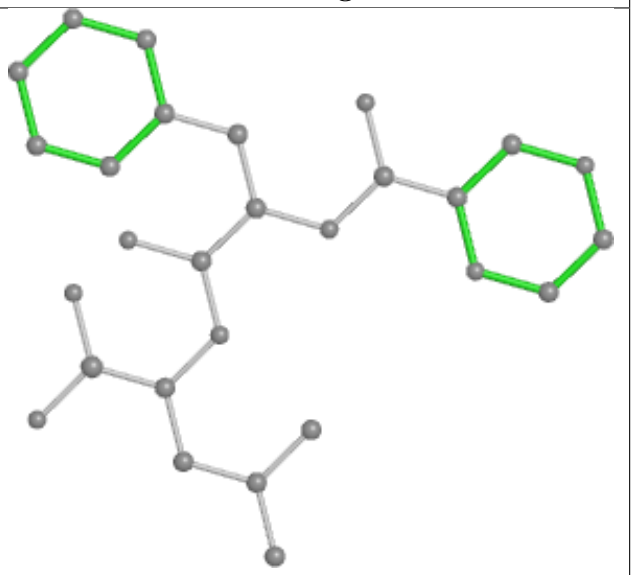
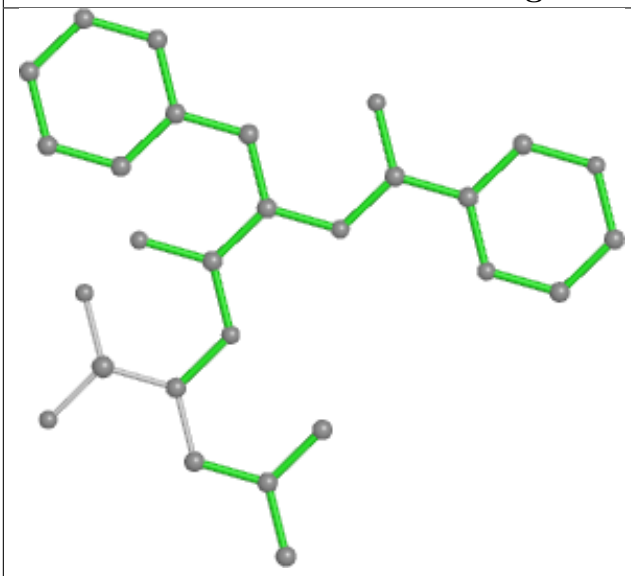
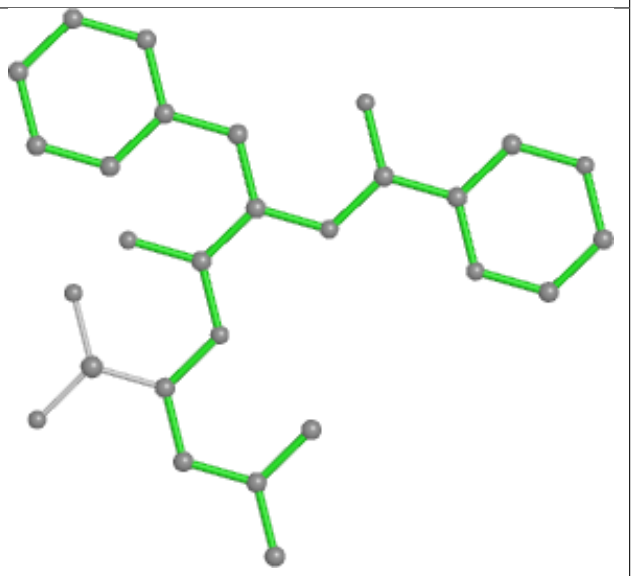


Rings

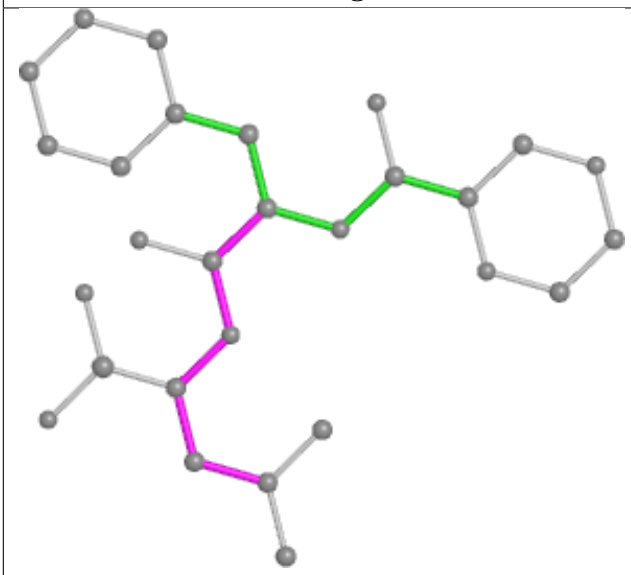
Ligand BO2 K 301



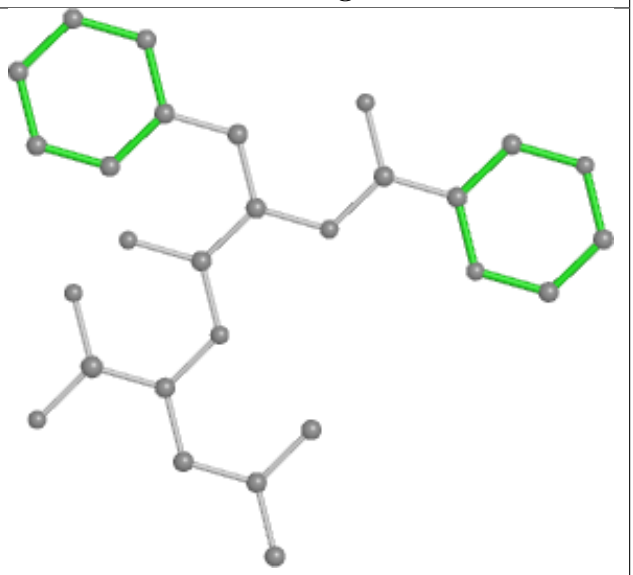
Bond lengths



Bond angles

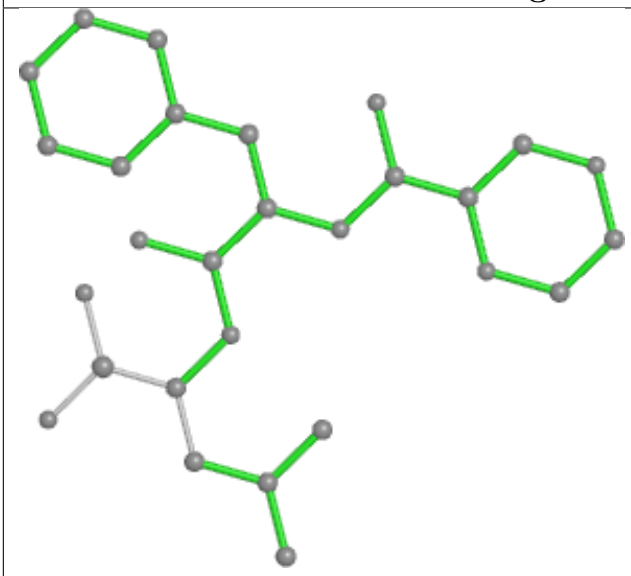


Torsions

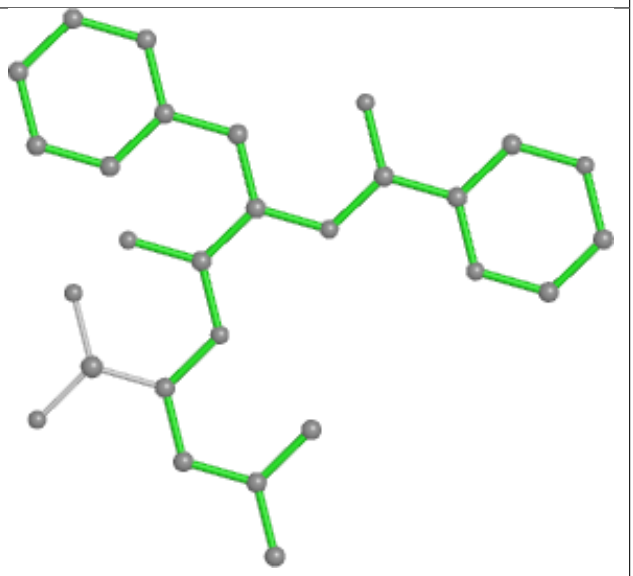


Rings

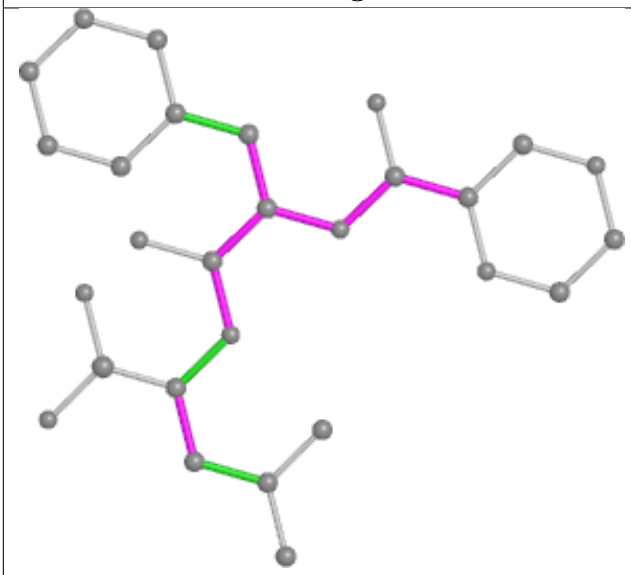
Ligand BO2 S 201



Bond lengths



Bond angles



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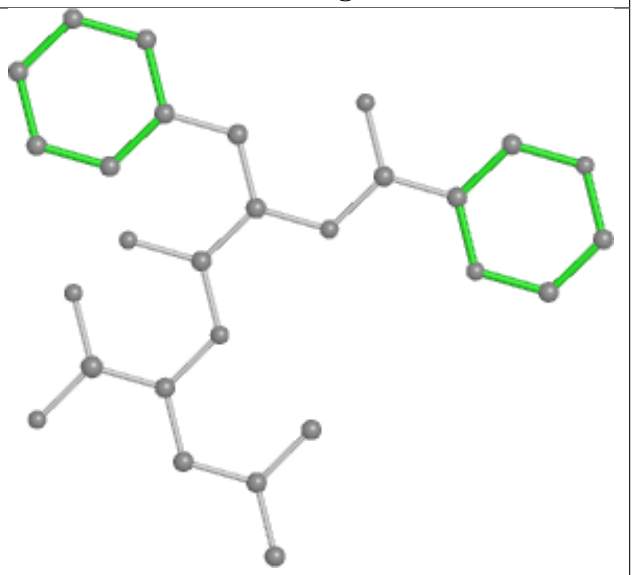
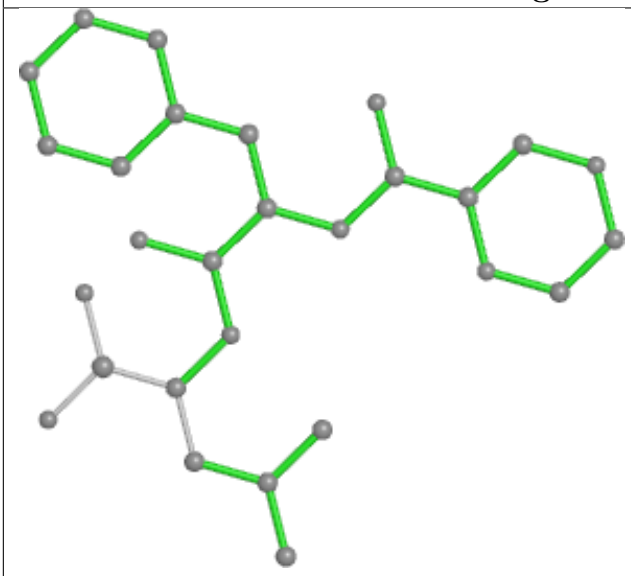


Rings

Ligand BO2 I 301



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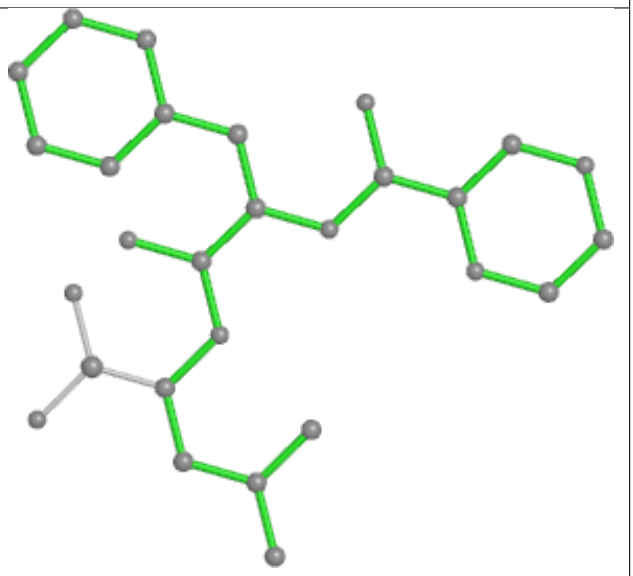

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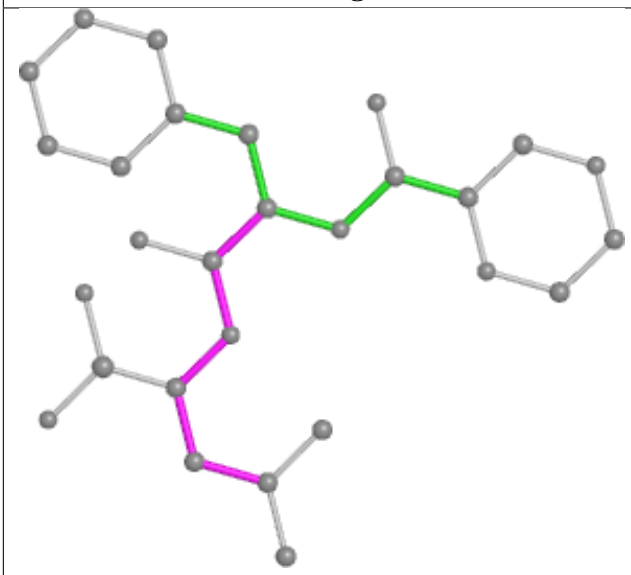

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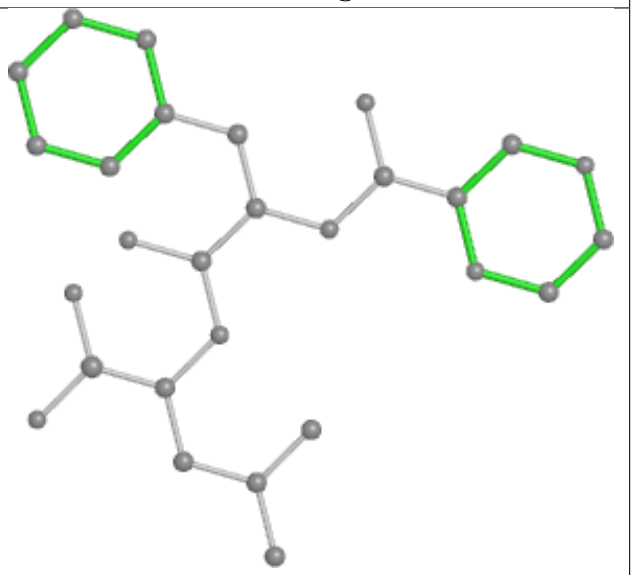
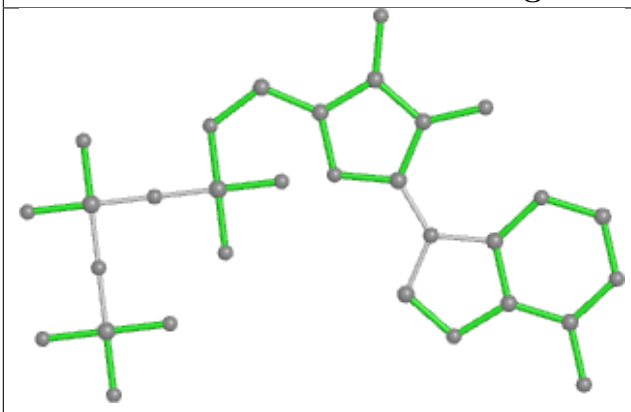


Rings

Ligand ATP A 904



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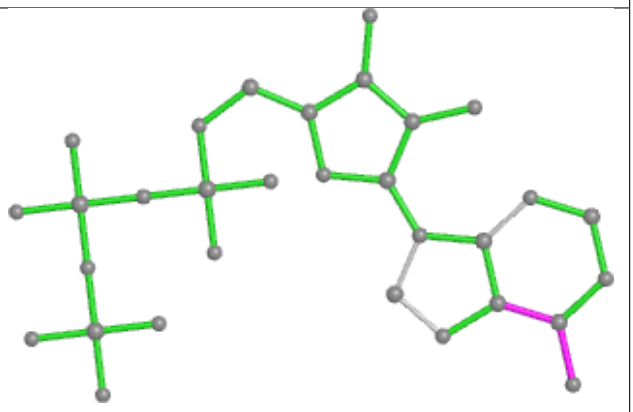

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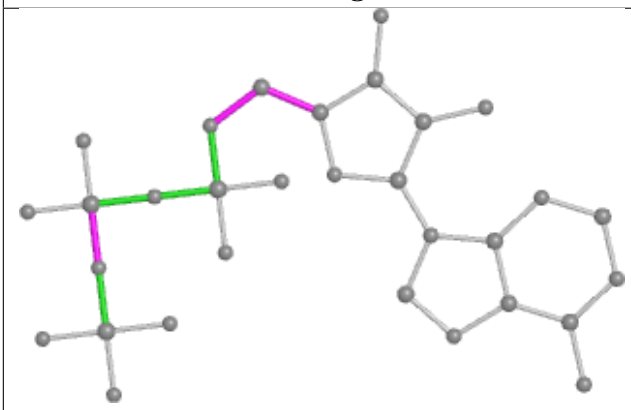

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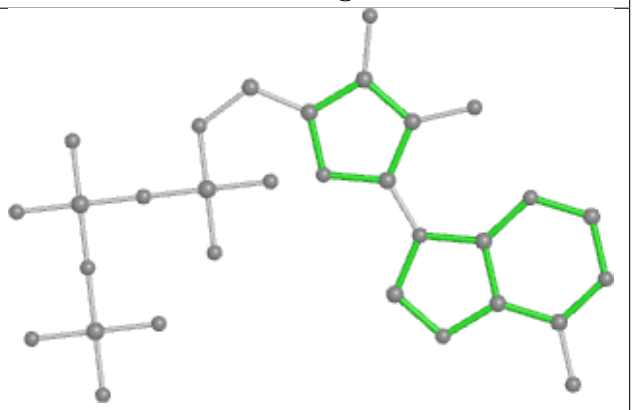
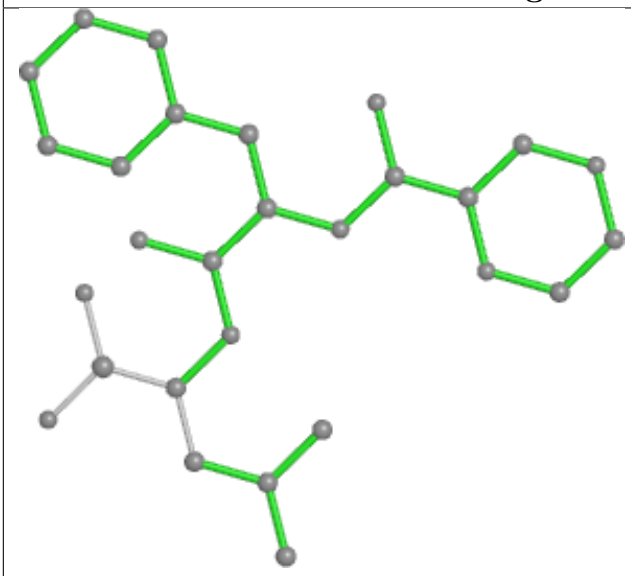


Rings

Ligand BO2 O 201



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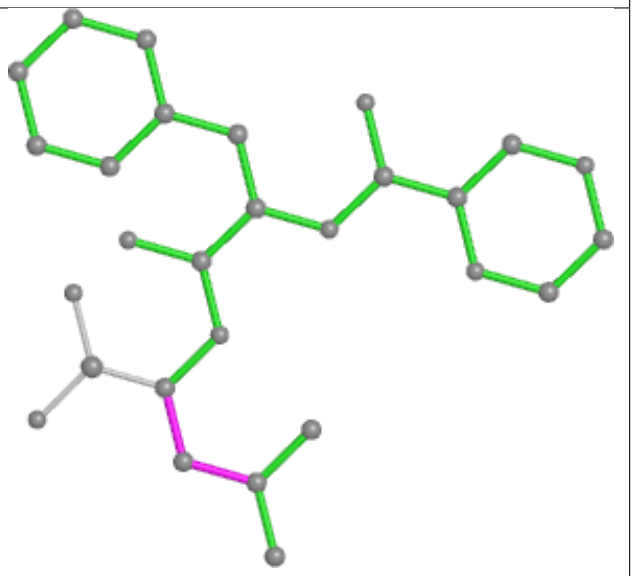

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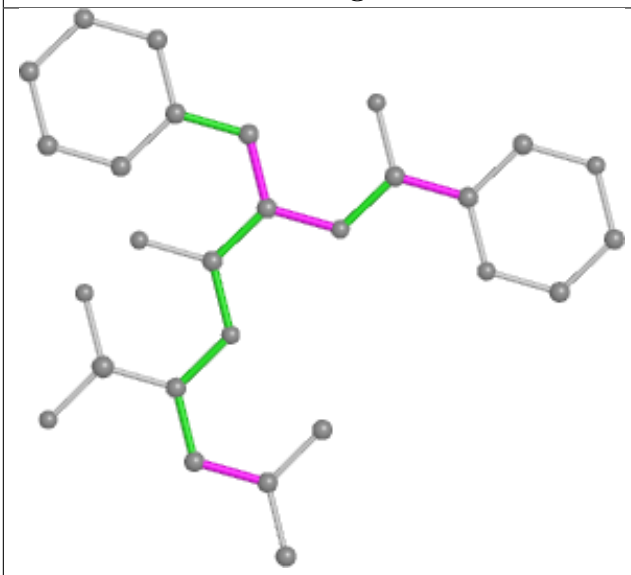

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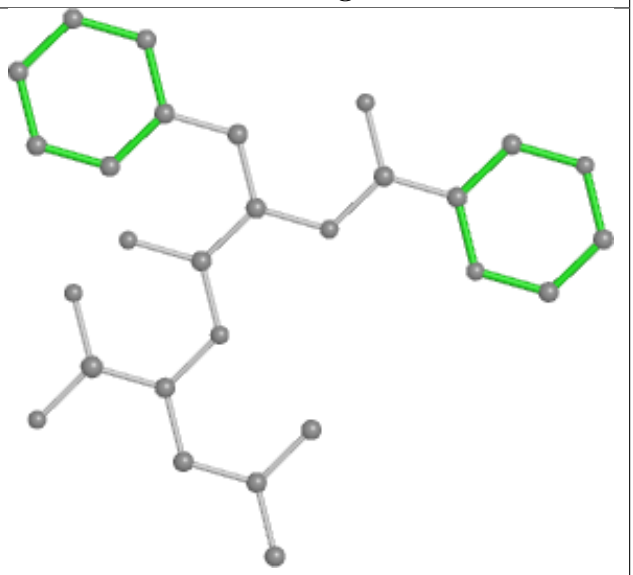
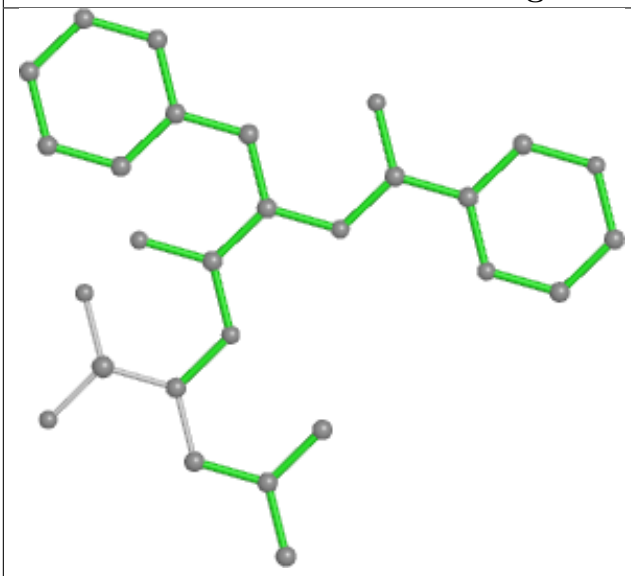


Rings

Ligand BO2 T 201



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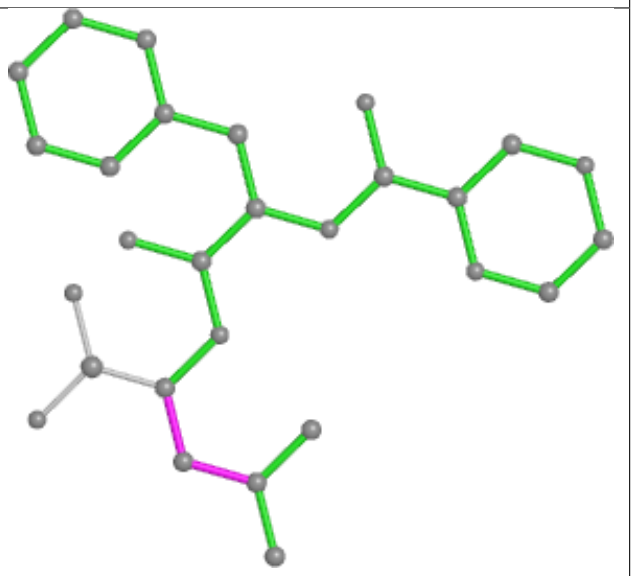

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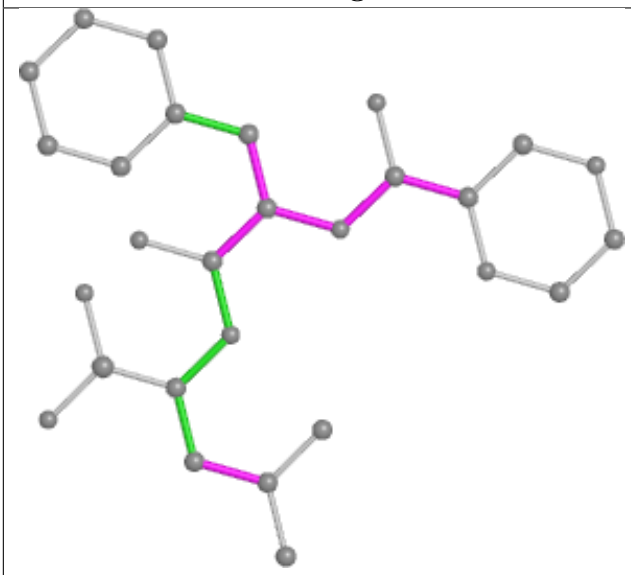

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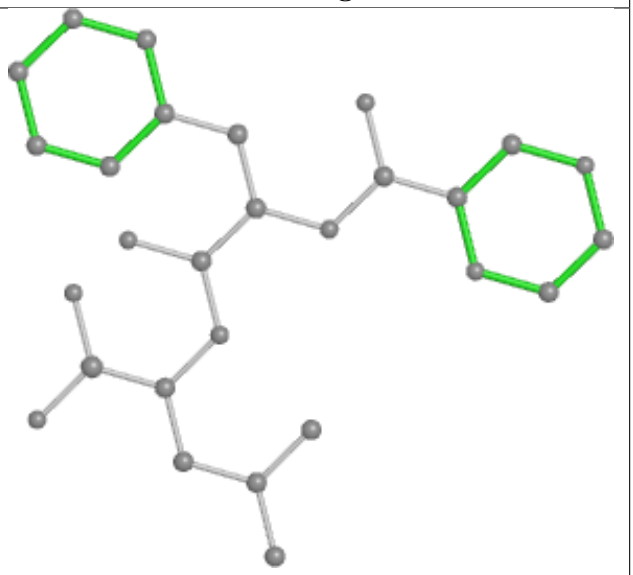
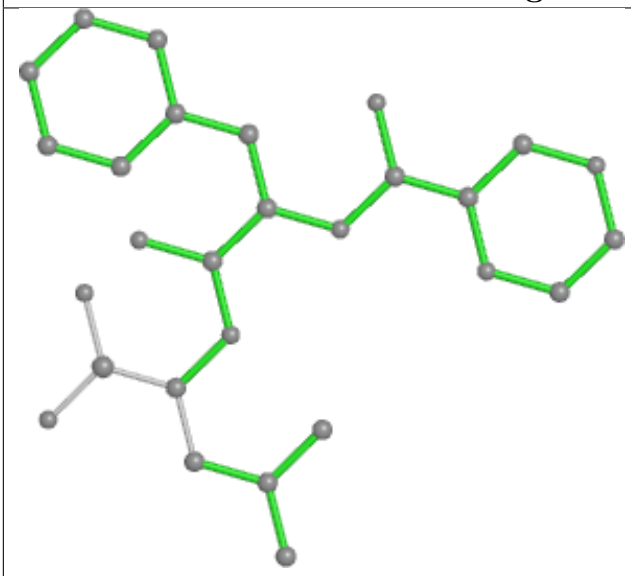


Rings

Ligand BO2 Q 201



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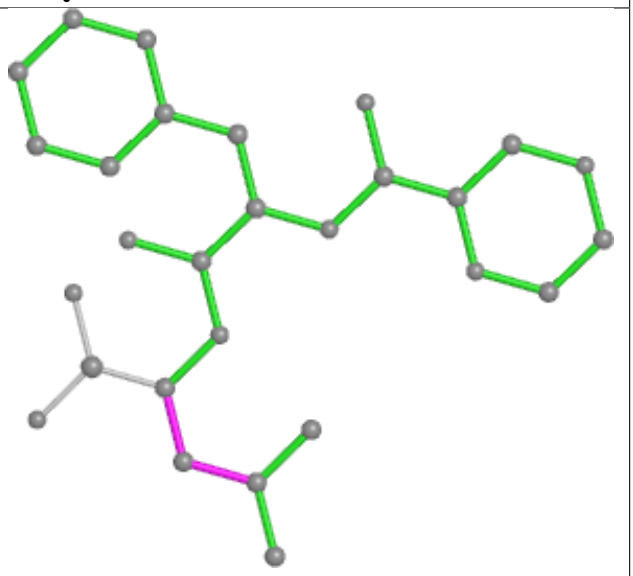
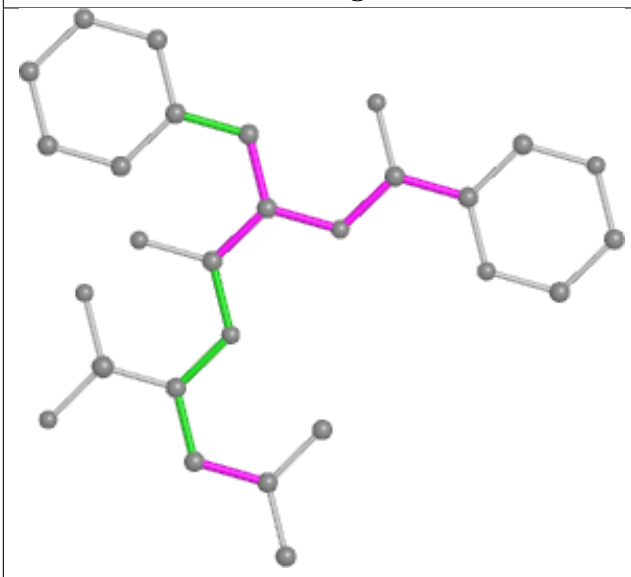


Bond angles



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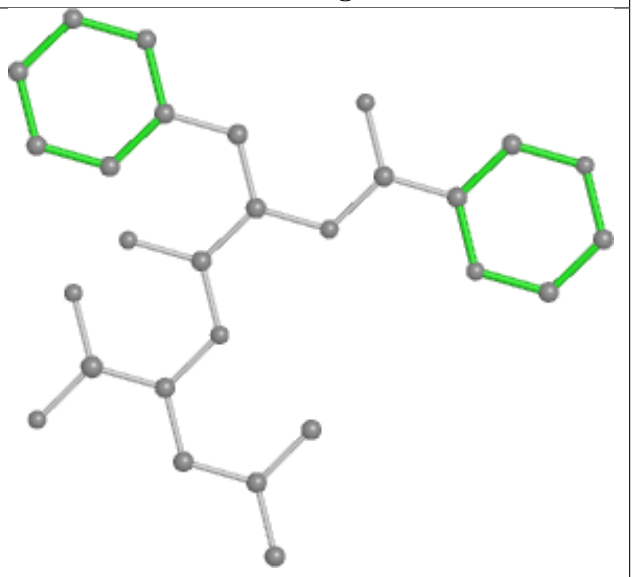
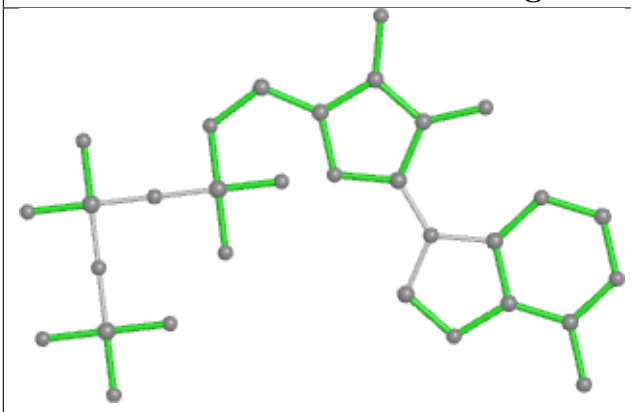


Rings

Ligand ATP C 904



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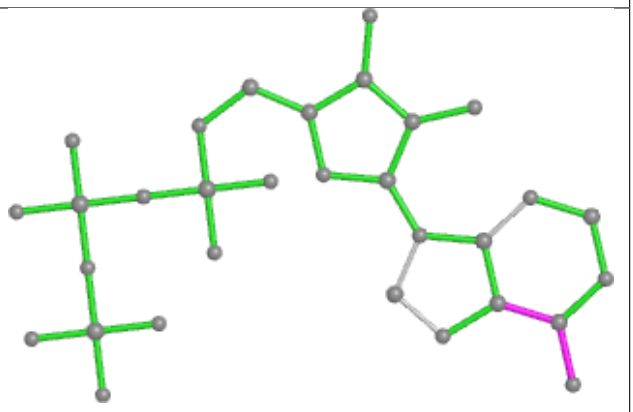

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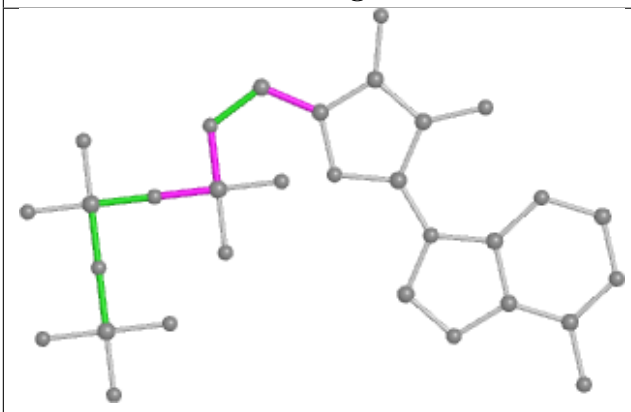

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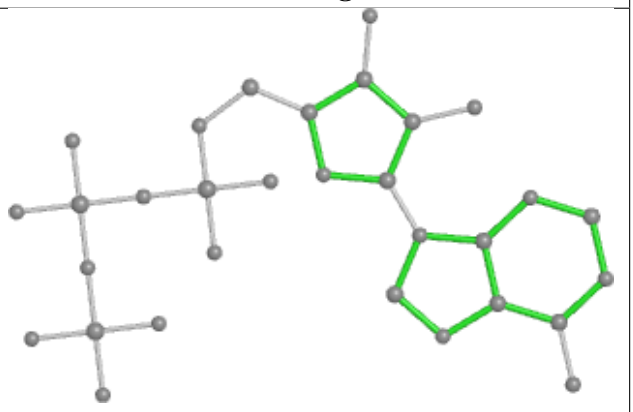
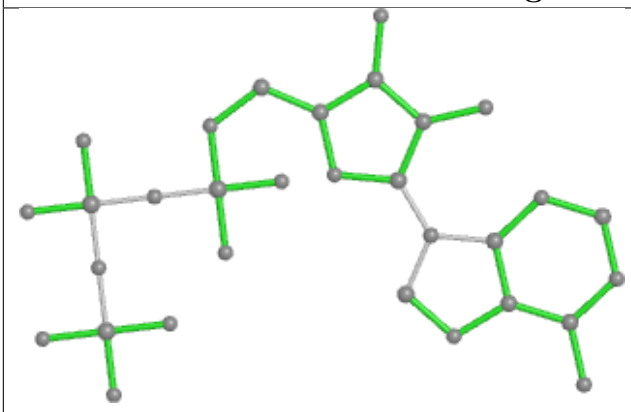


Rings

Ligand ATP B 904



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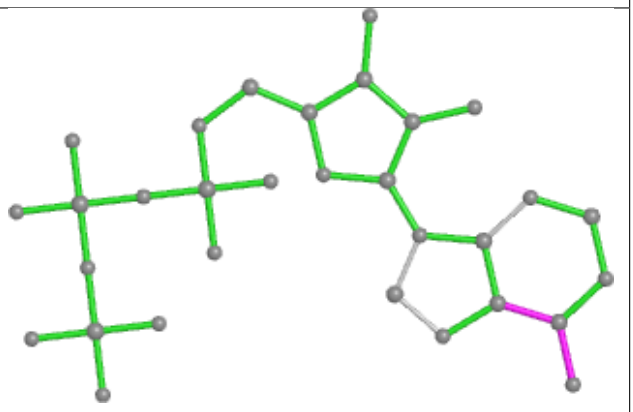

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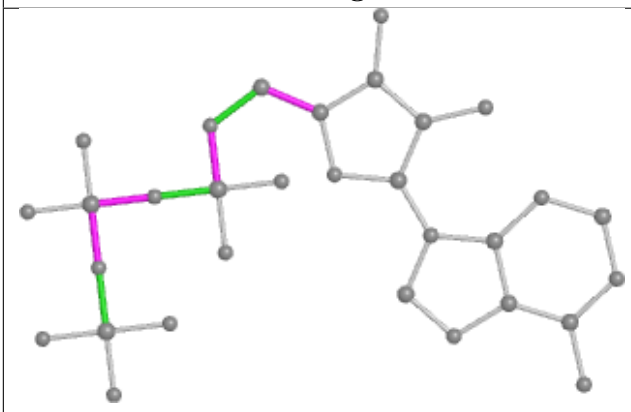

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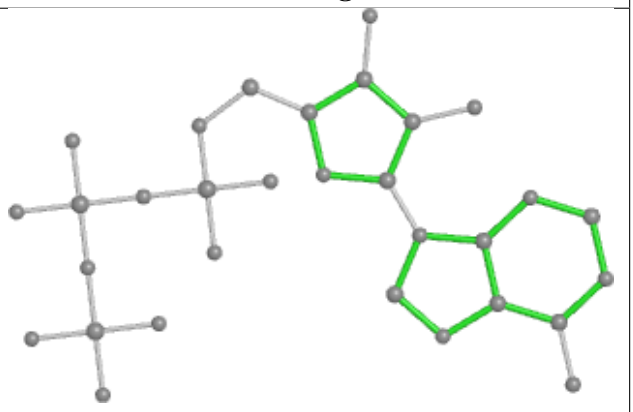
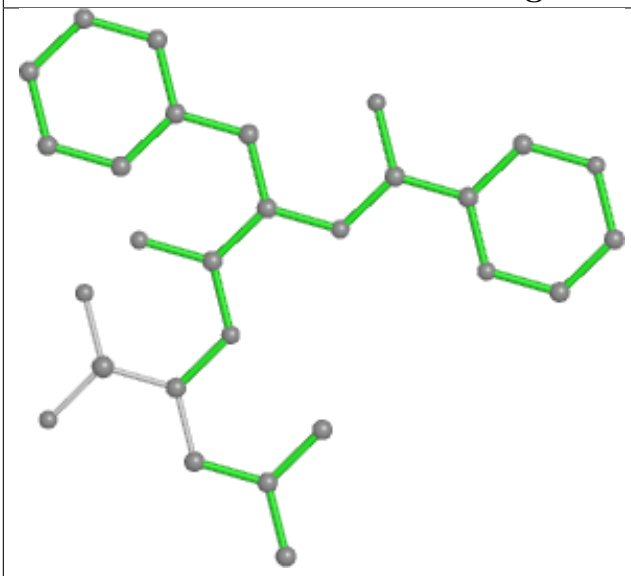


Rings

Ligand BO2 N 201



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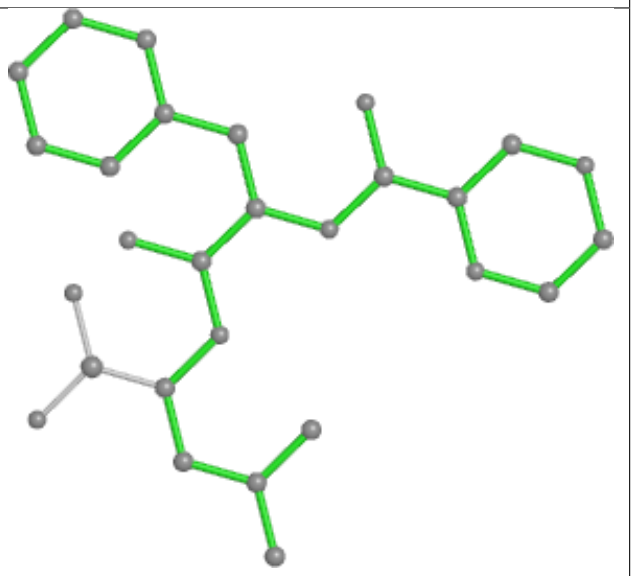
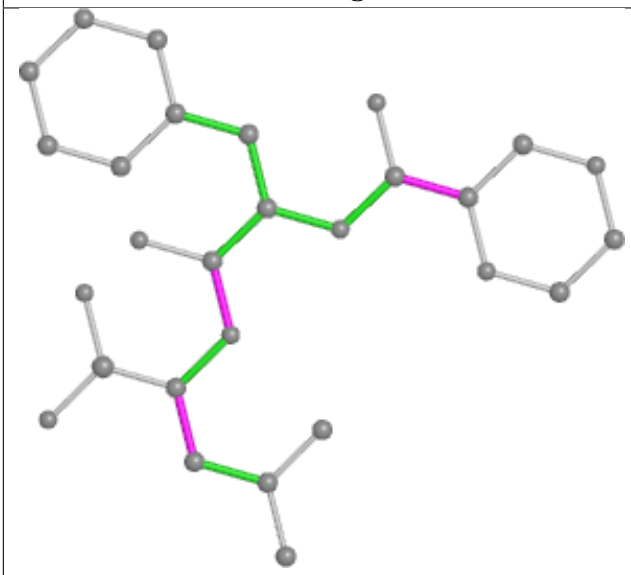
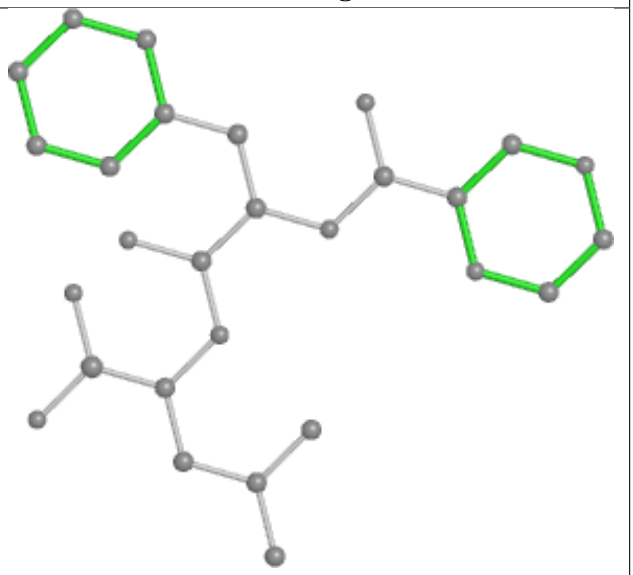


Bond angles

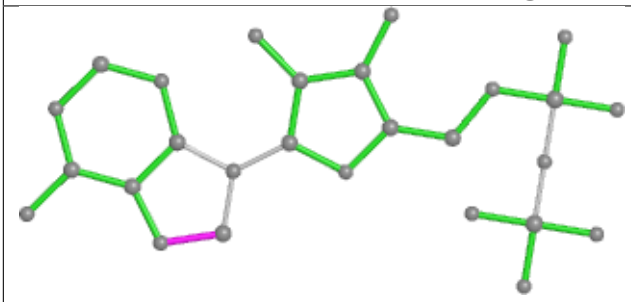


Torsions



Rings

Ligand ADP D 901



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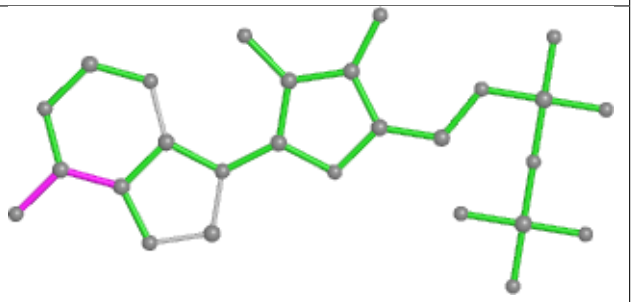
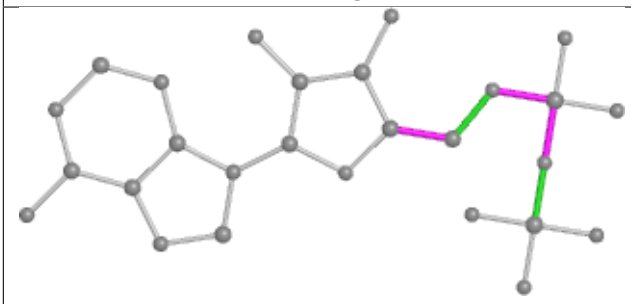


Bond angles



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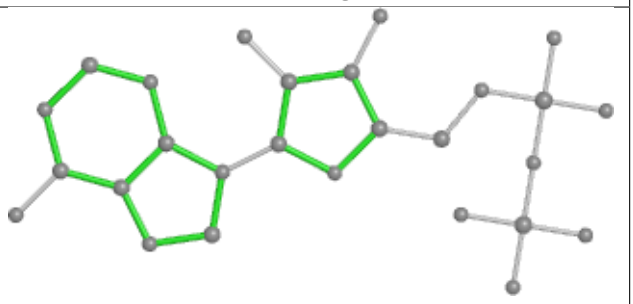
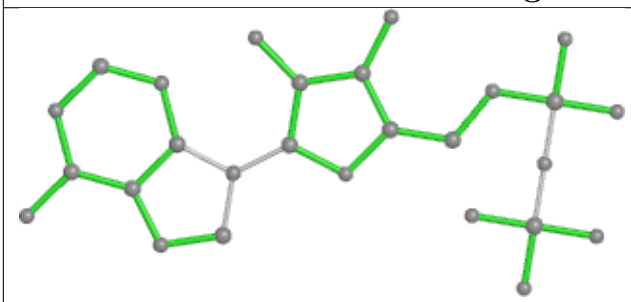


Rings

Ligand ADP F 901



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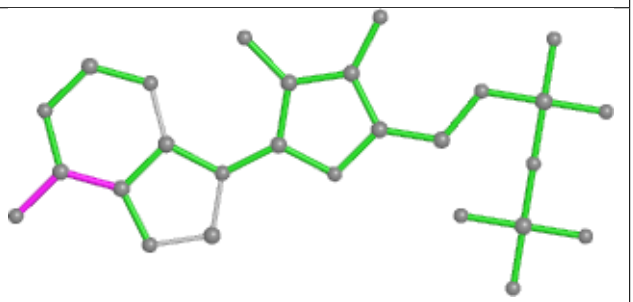
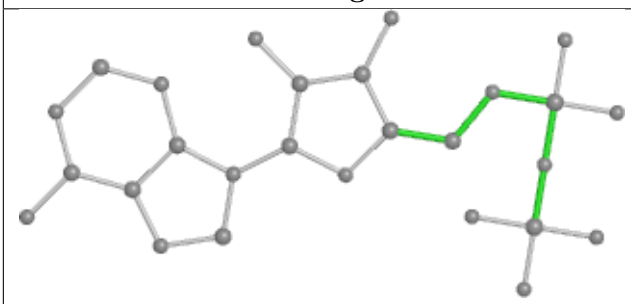


Bond angles



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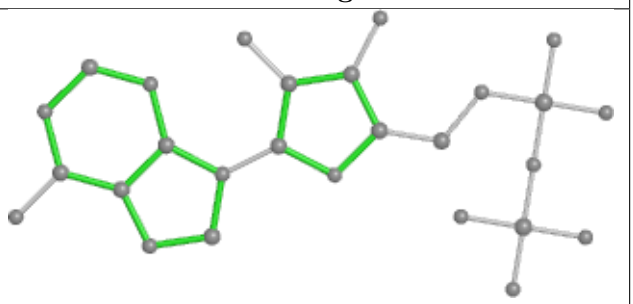
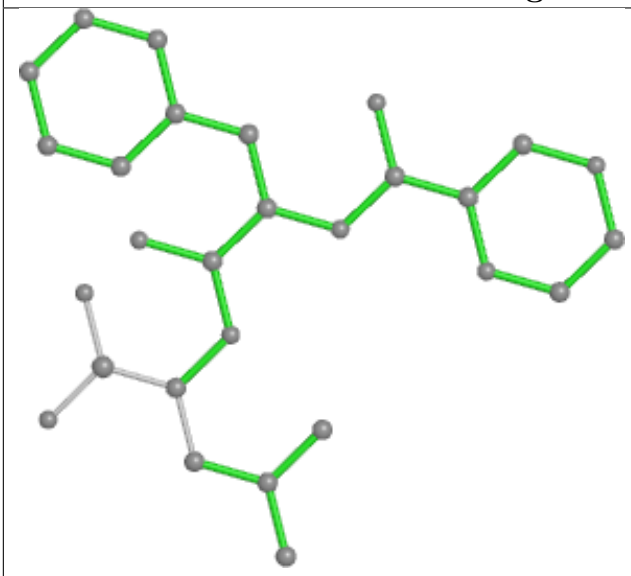


Rings

Ligand BO2 R 201



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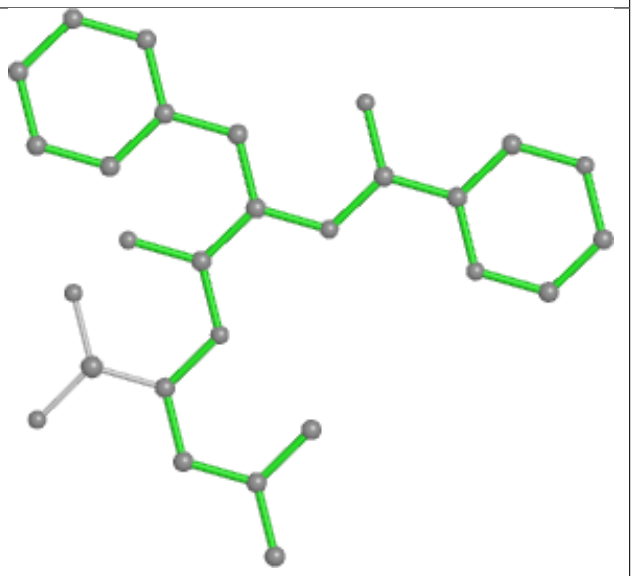
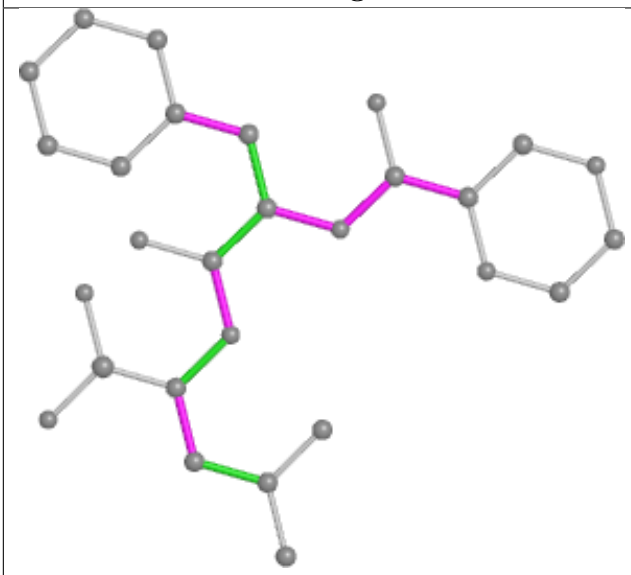


Bond angles



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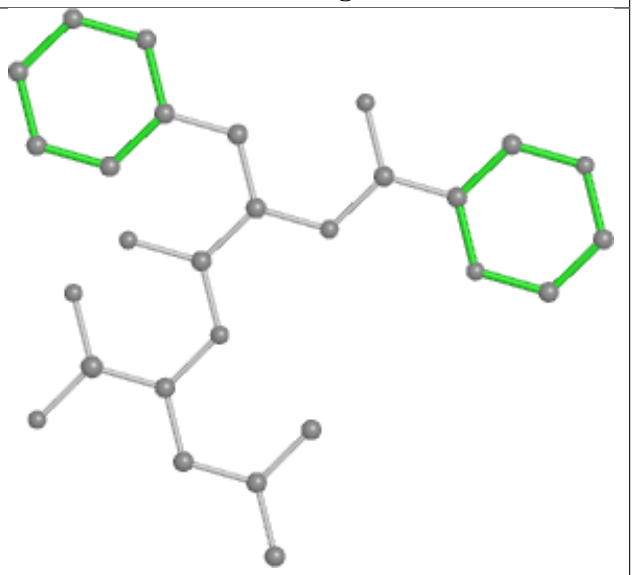
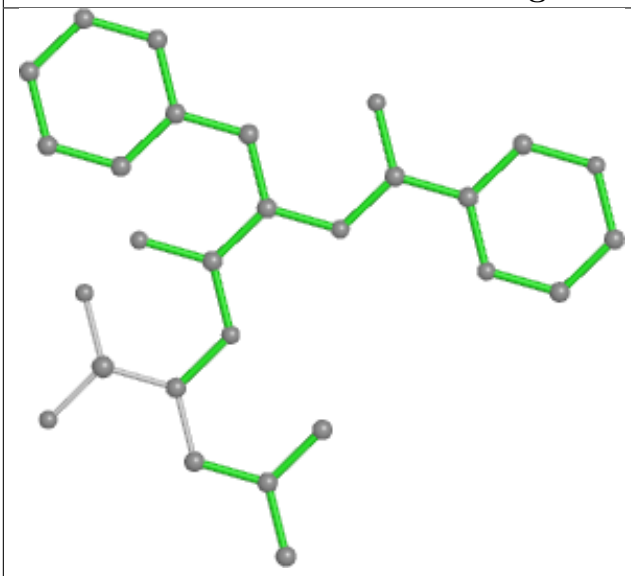
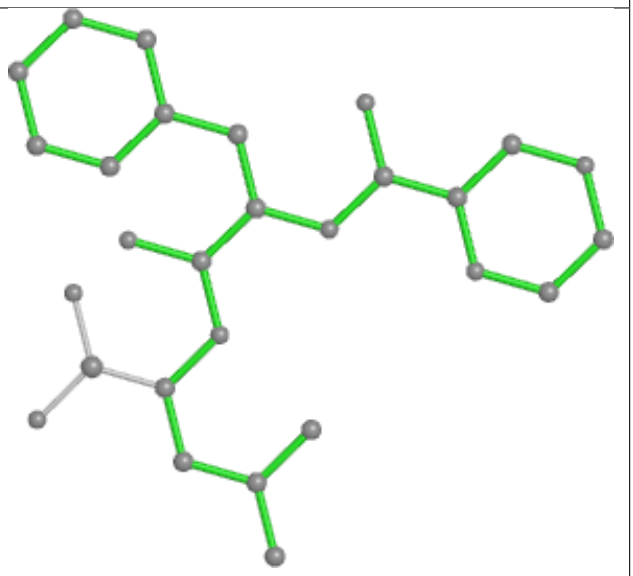


Rings

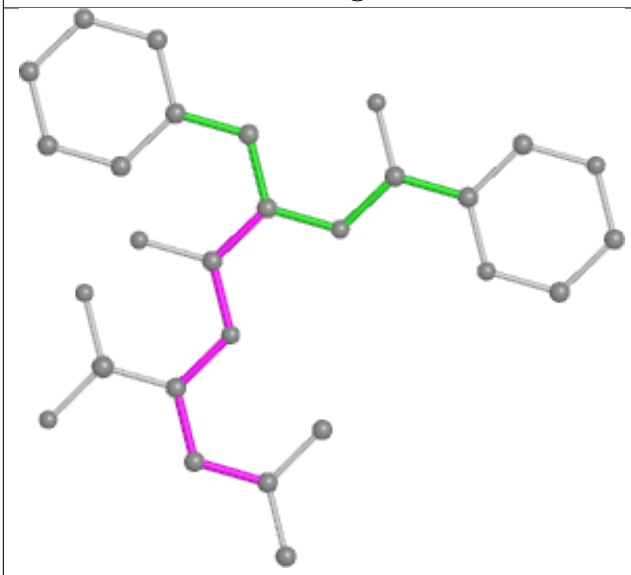
Ligand BO2 L 301



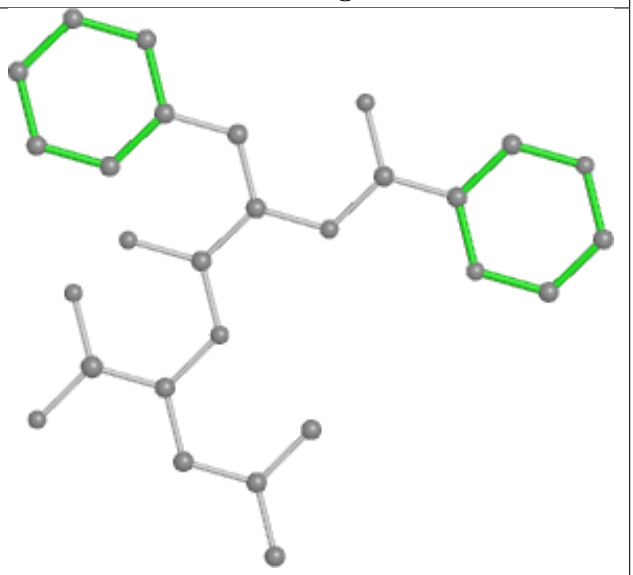
Bond lengths



Bond angles

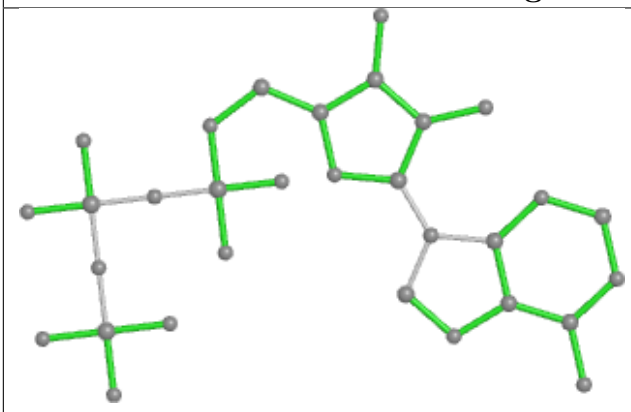


Torsions

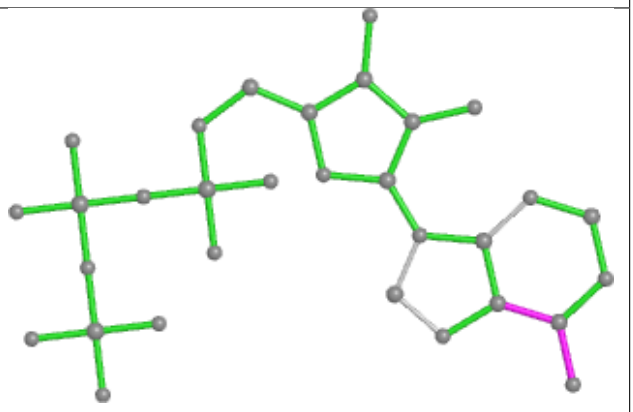


Rings

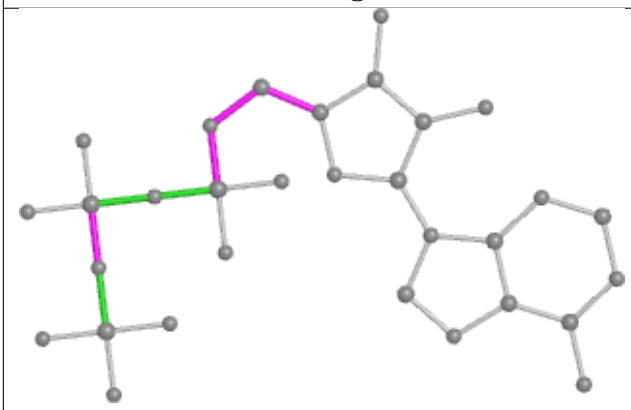
Ligand ATP C 901



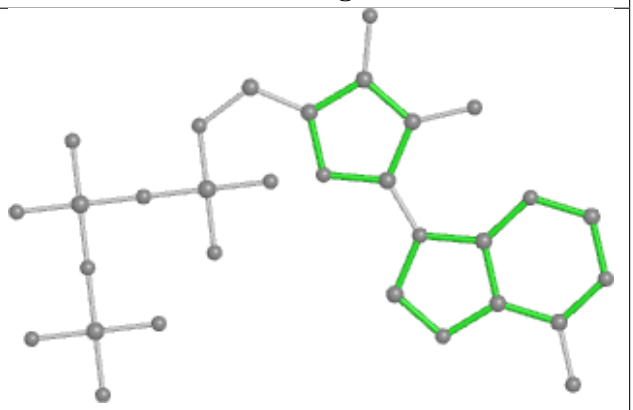
Bond lengths



Bond angles

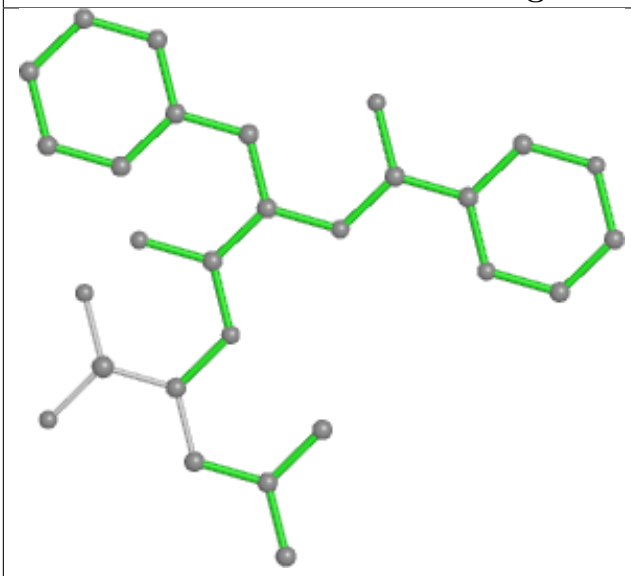


Torsions

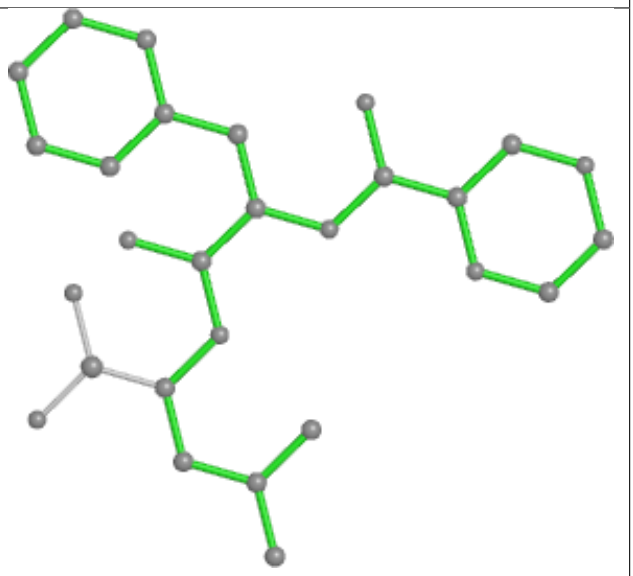


Rings

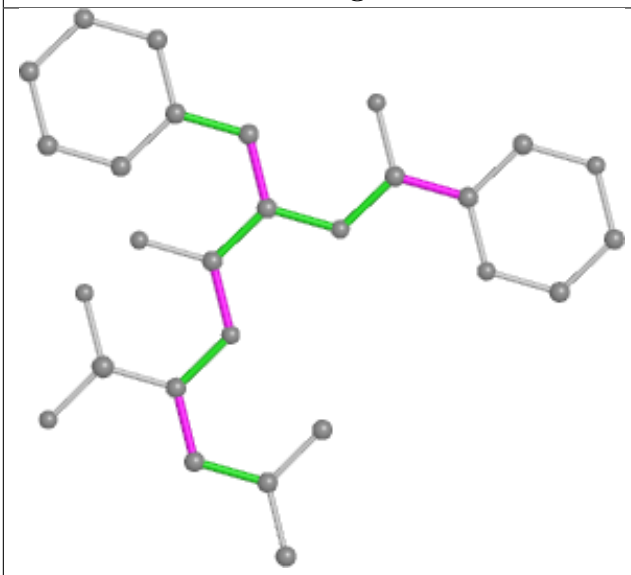
Ligand BO2 P 201



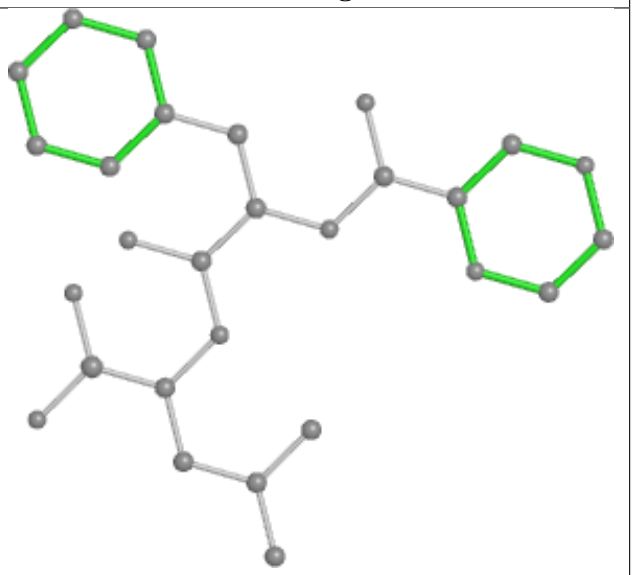
Bond lengths



Bond angles

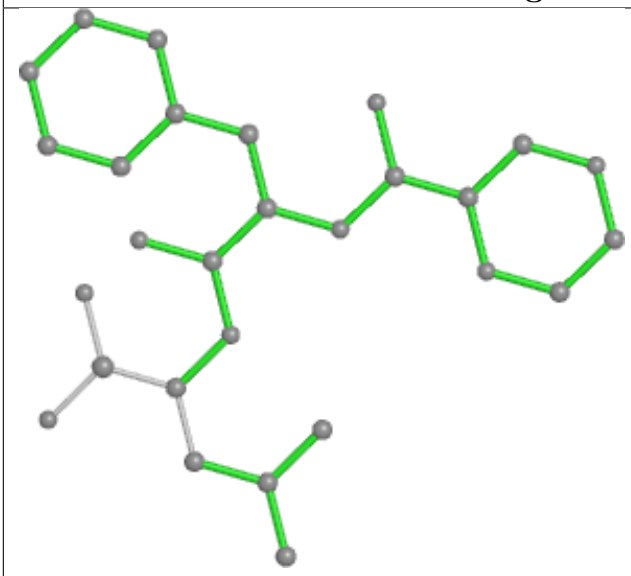


Torsions

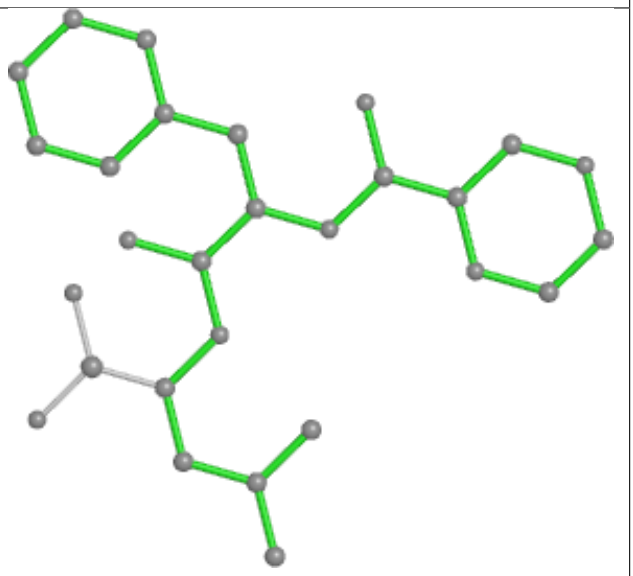


Rings

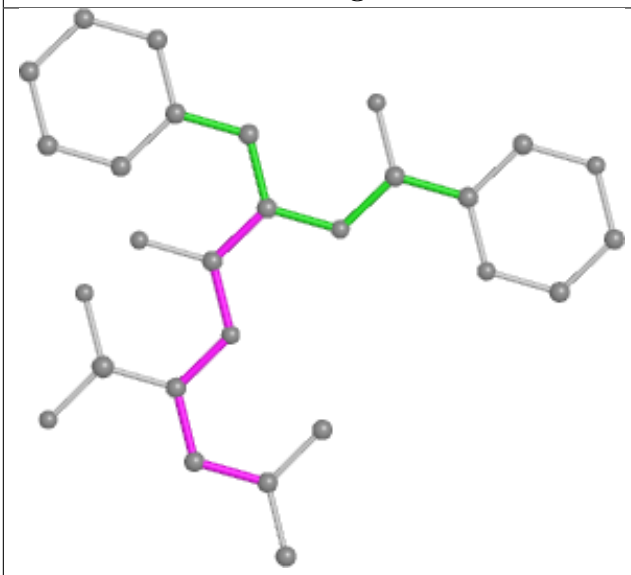
Ligand BO2 H 301



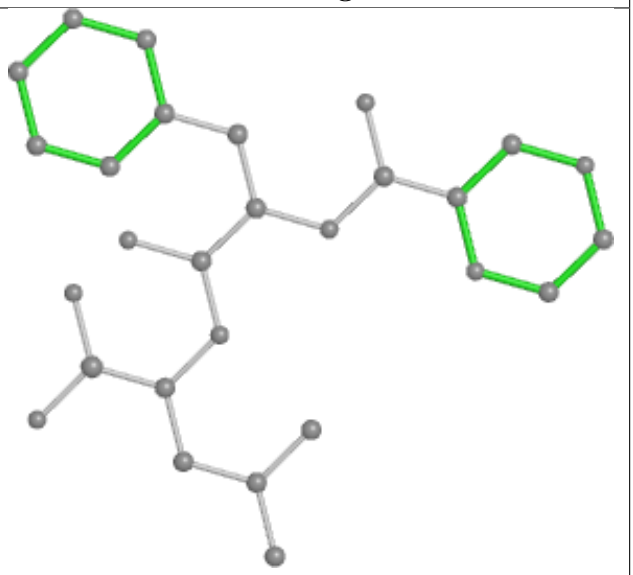
Bond lengths



Bond angles

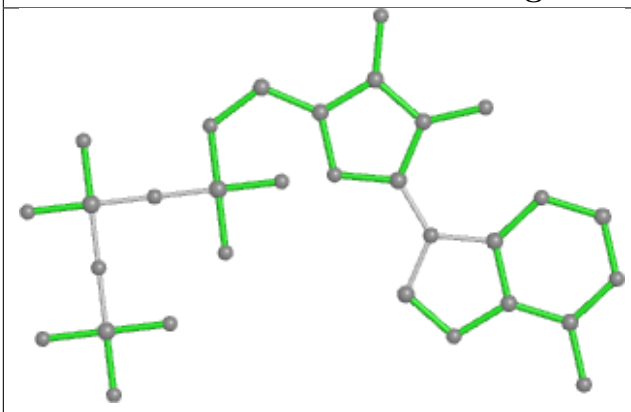


Torsions

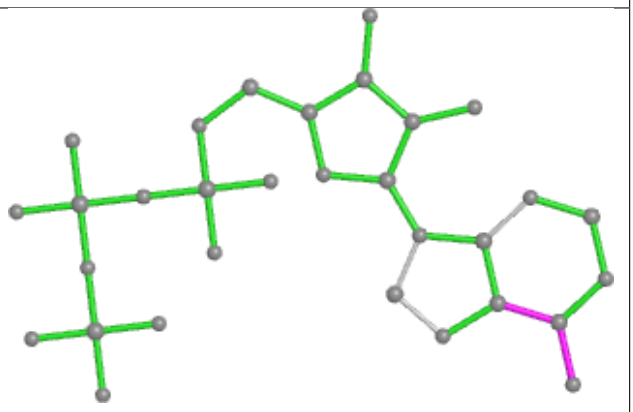


Rings

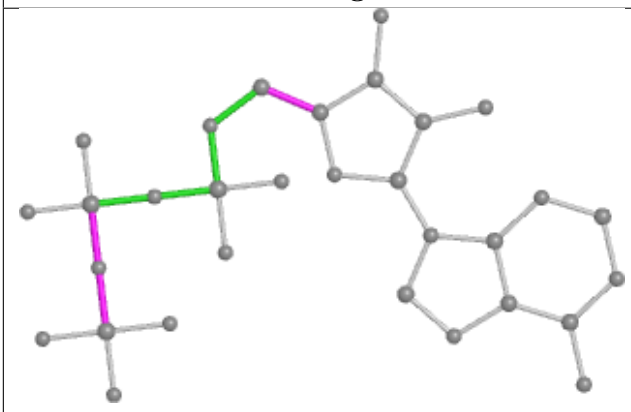
Ligand ATP B 903



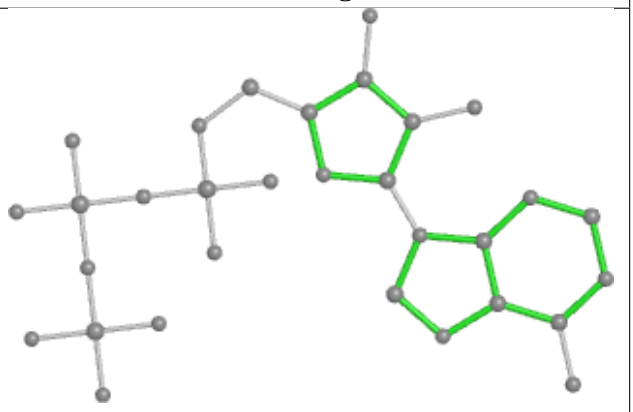
Bond lengths



Bond angles

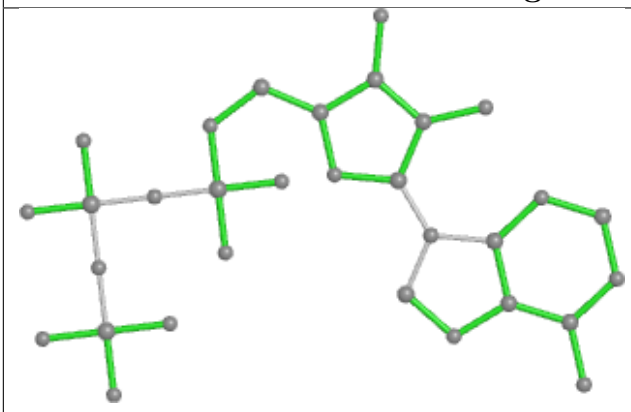


Torsions

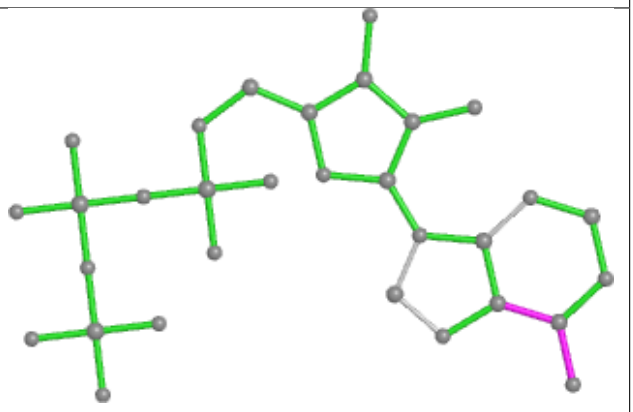


Rings

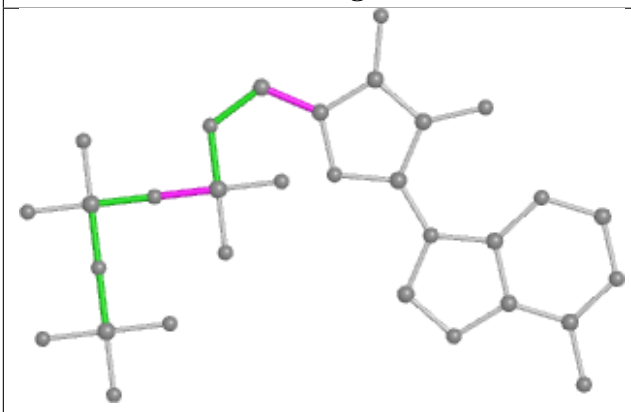
Ligand ATP D 903



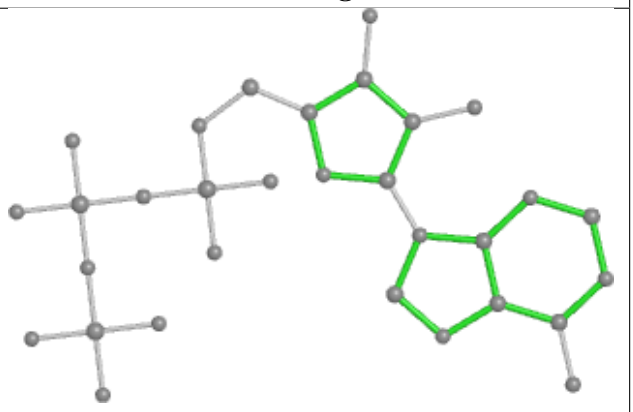
Bond lengths



Bond angles

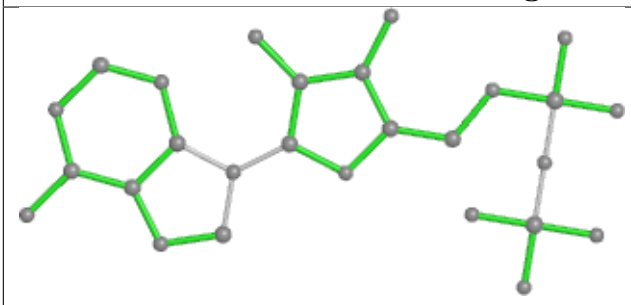


Torsions

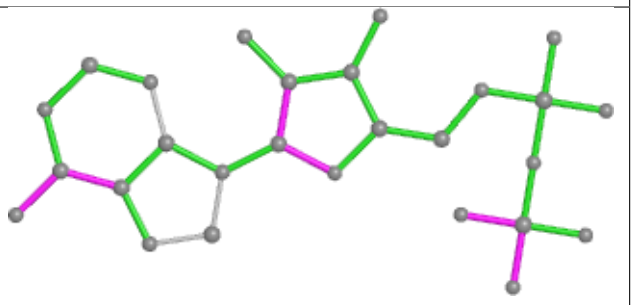


Rings

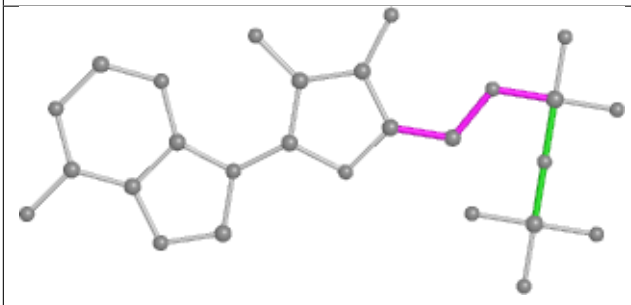
Ligand ADP E 901



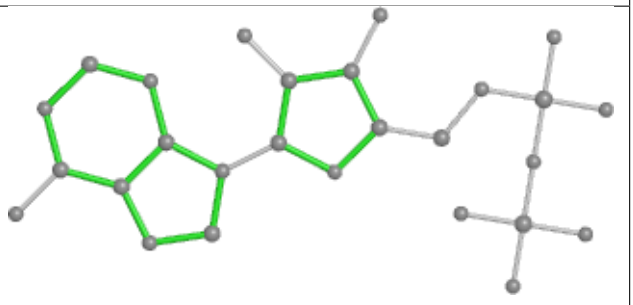
Bond lengths



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.

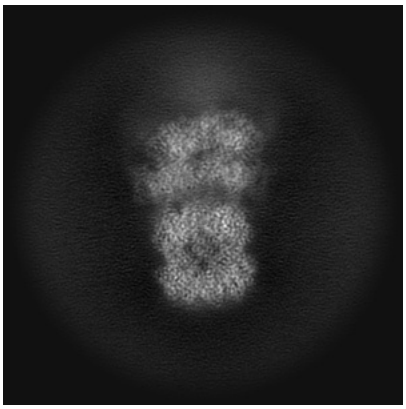
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39162. These allow visual inspection of the internal detail of the map and identification of artifacts.

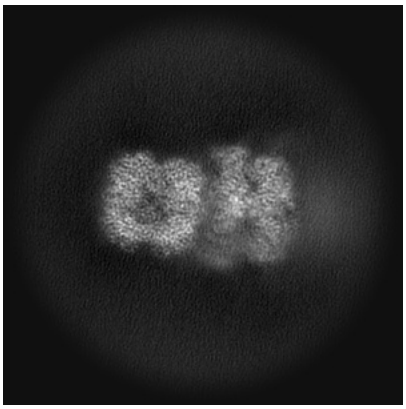
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

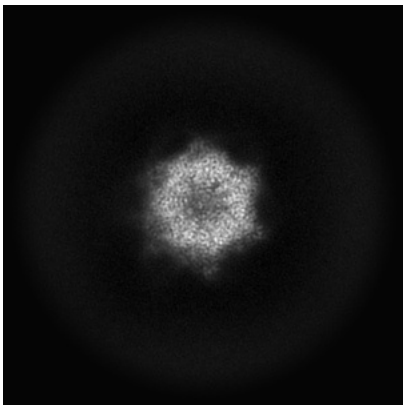
6.1.1 Primary map



X

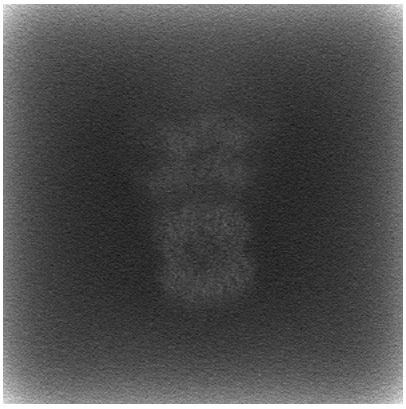


Y

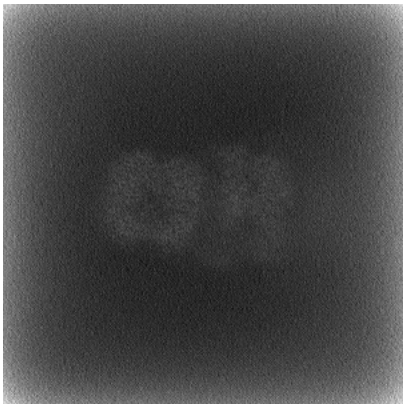


Z

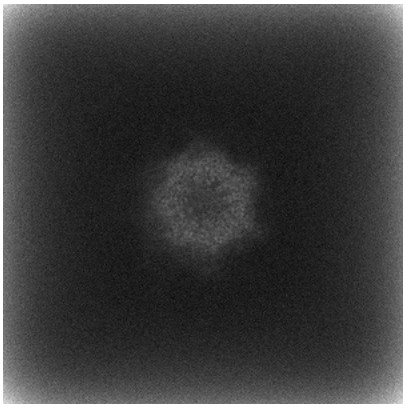
6.1.2 Raw map



X



Y

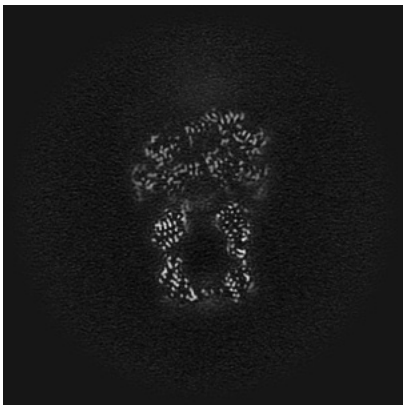


Z

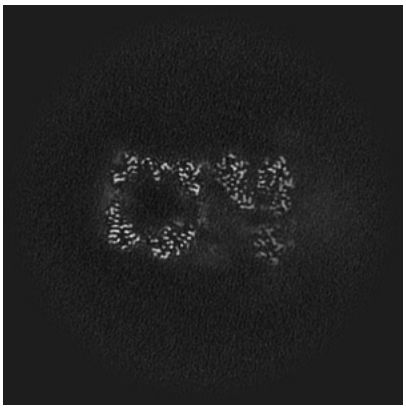
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

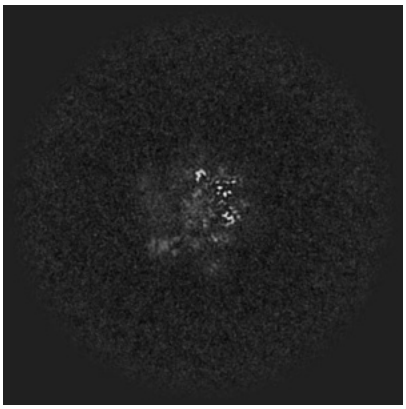
6.2.1 Primary map



X Index: 256

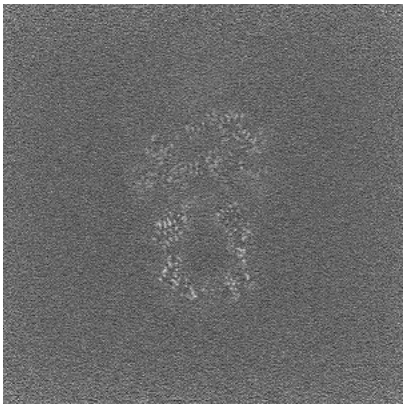


Y Index: 256

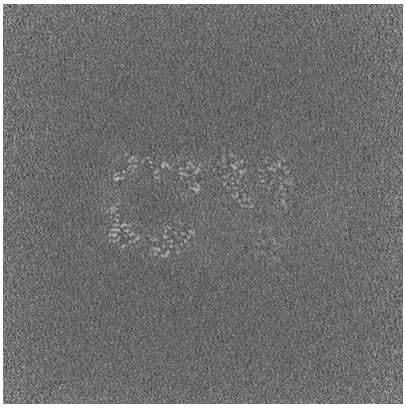


Z Index: 256

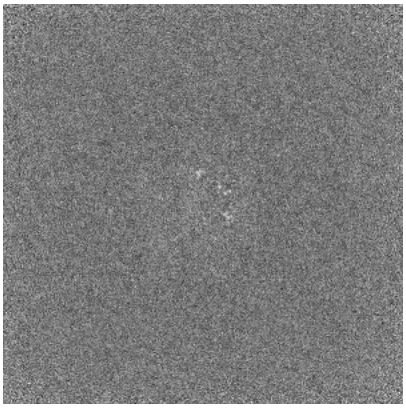
6.2.2 Raw map



X Index: 256



Y Index: 256

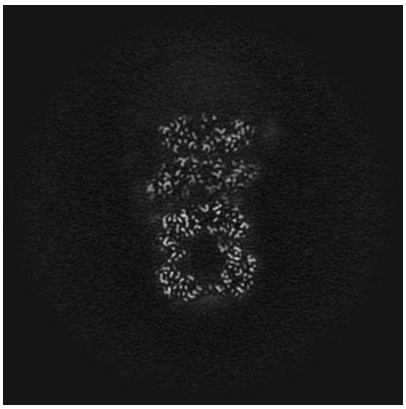


Z Index: 256

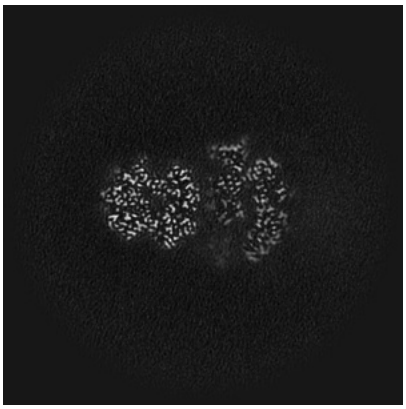
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

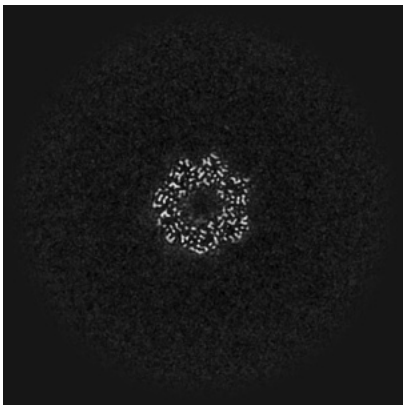
6.3.1 Primary map



X Index: 279

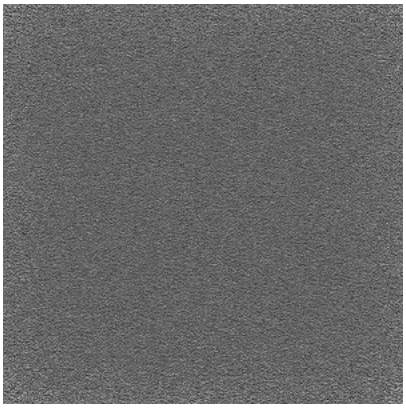


Y Index: 219

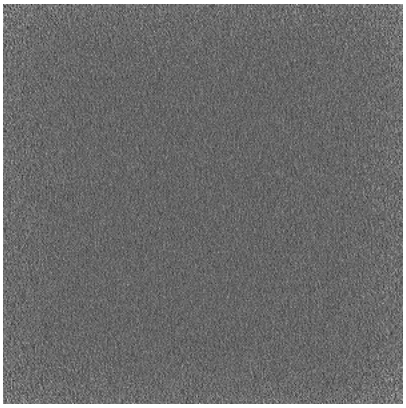


Z Index: 223

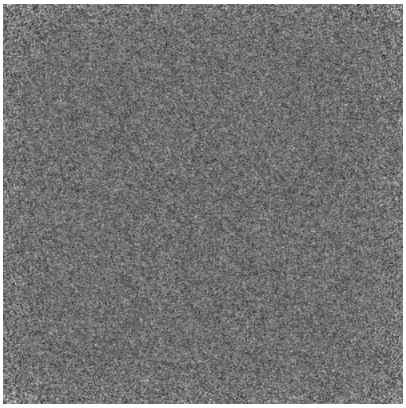
6.3.2 Raw map



X Index: 0



Y Index: 0

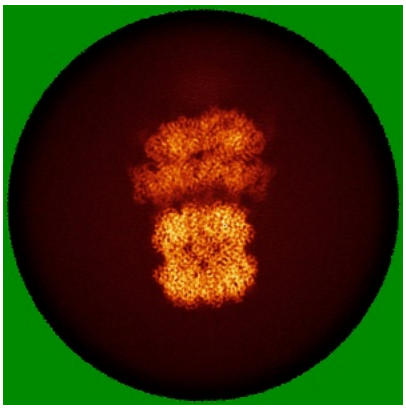


Z Index: 511

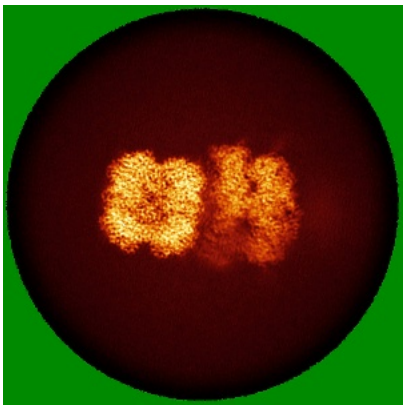
The images above show the largest variance slices of the map in three orthogonal directions.

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

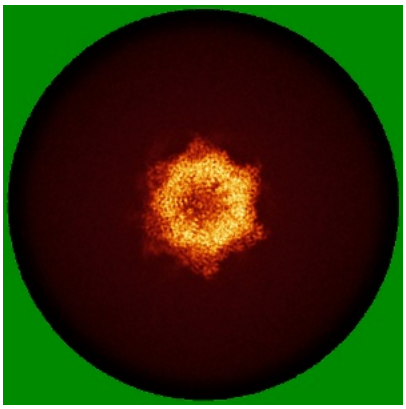
6.4.1 Primary map



X

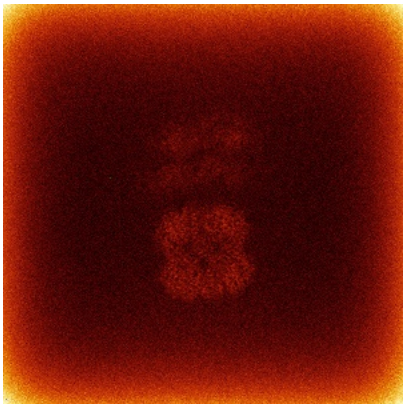


Y

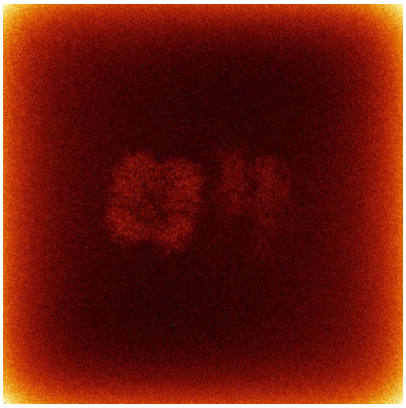


Z

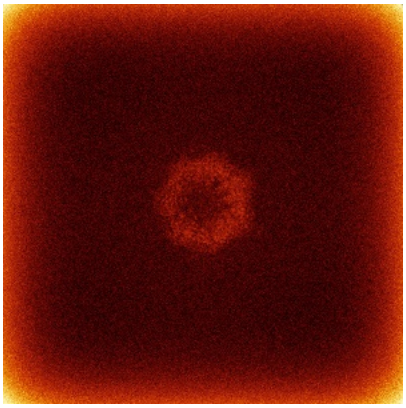
6.4.2 Raw map



X



Y



Z

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

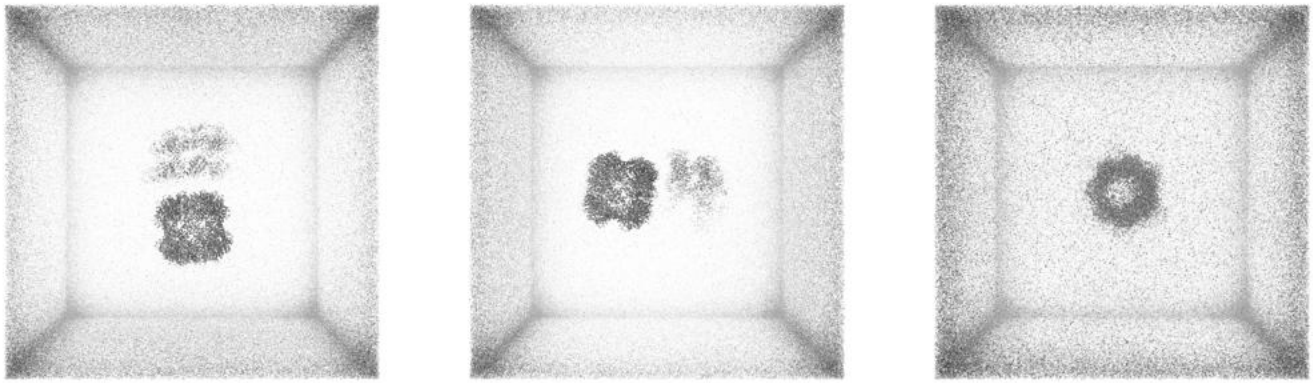
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

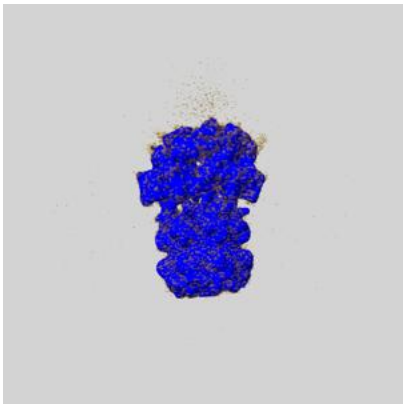
6.6 Mask visualisation (i)

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:

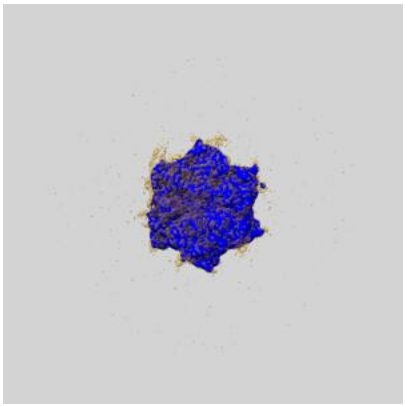
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_39162_msk_1.map (i)



X

Y

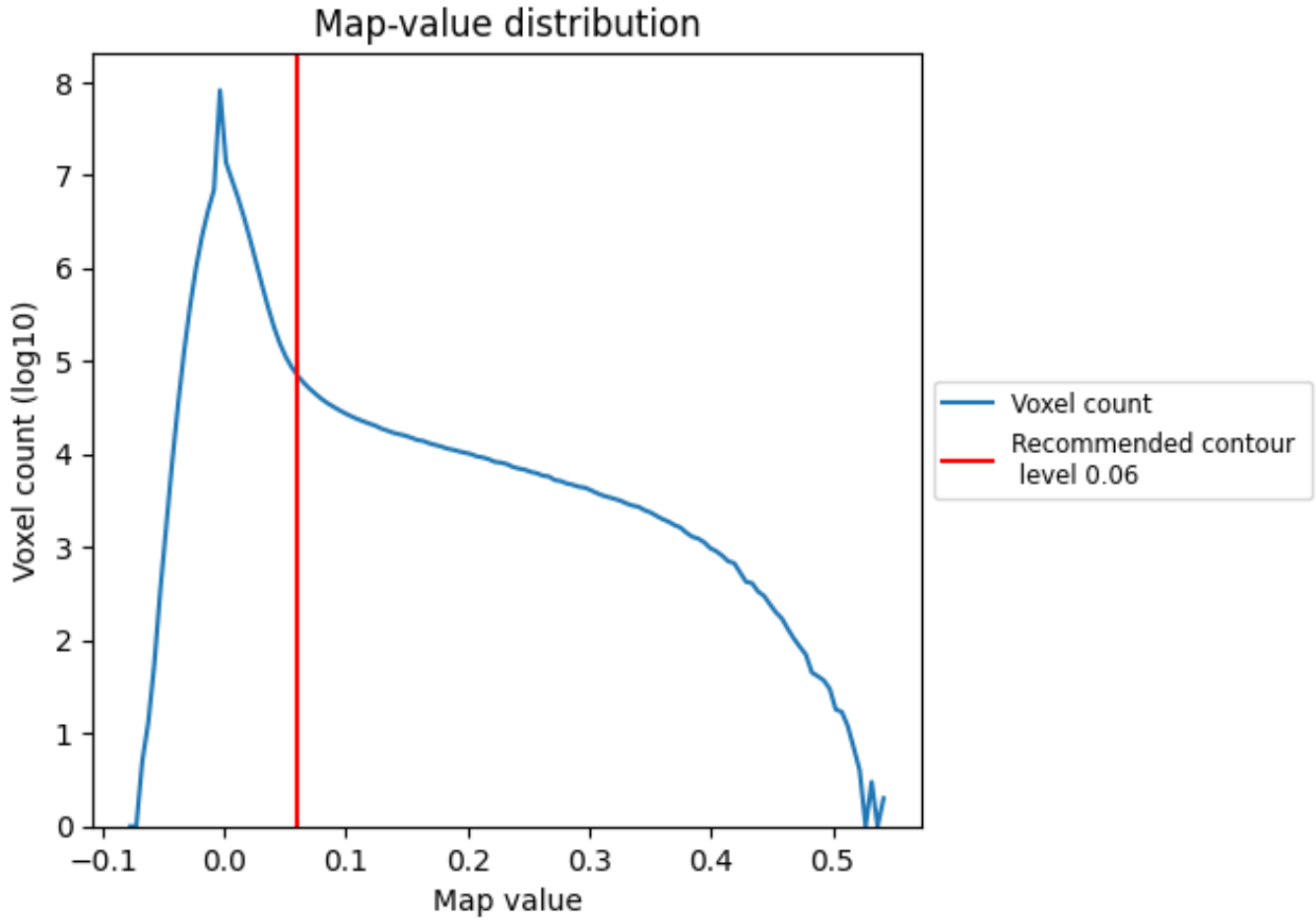


Z

7 Map analysis

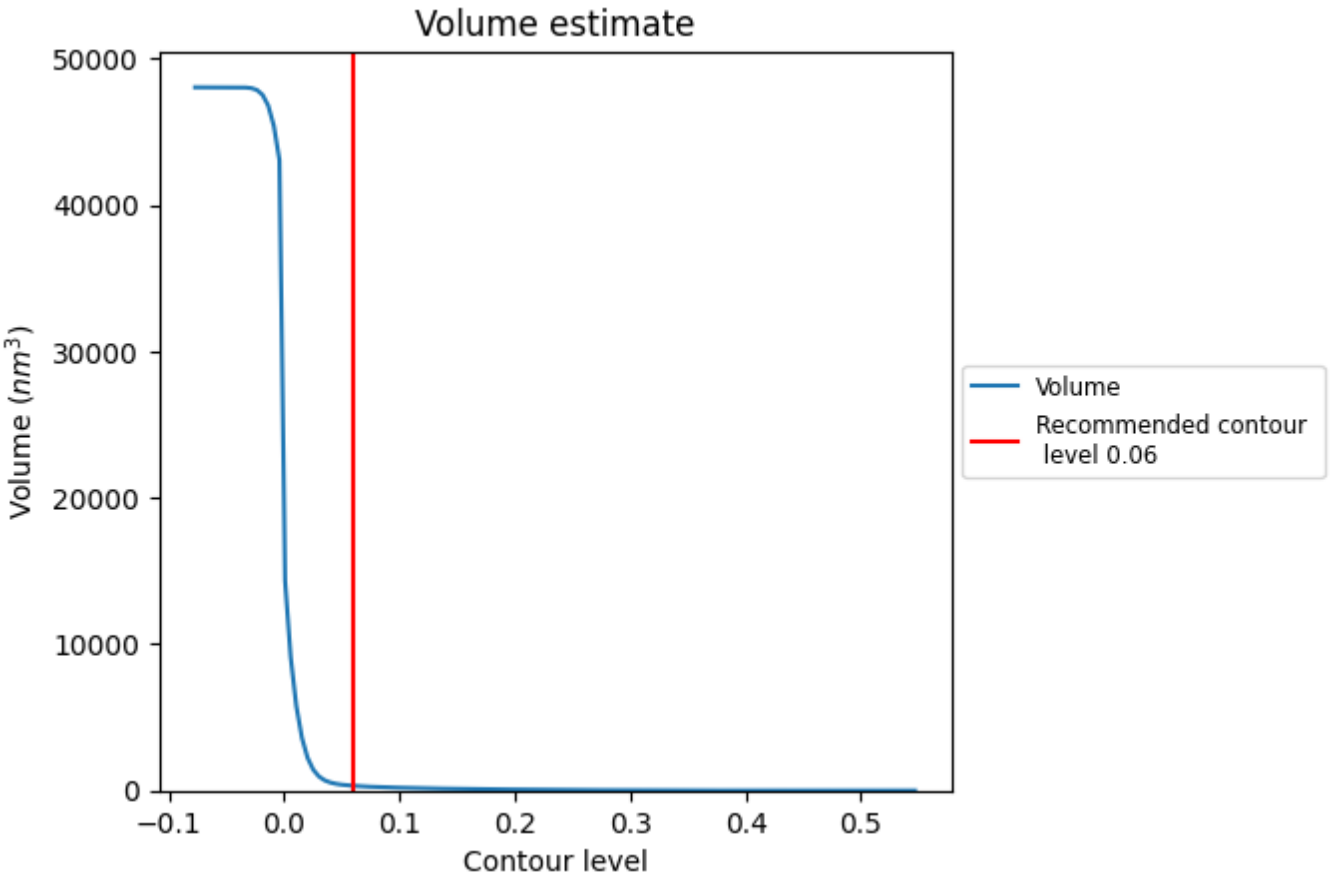
This section contains the results of statistical analysis of the map.

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.

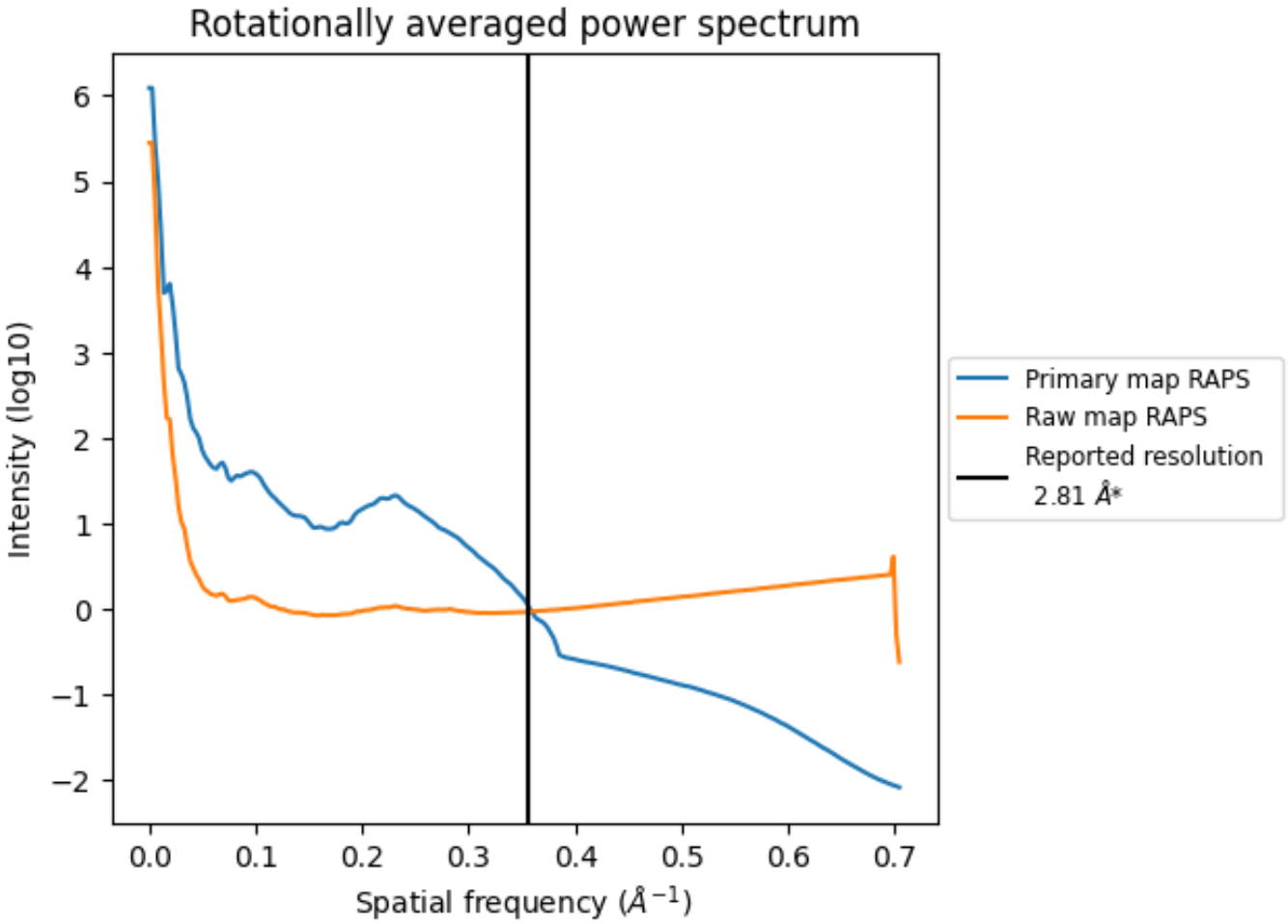
7.2 Volume estimate



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 294 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)

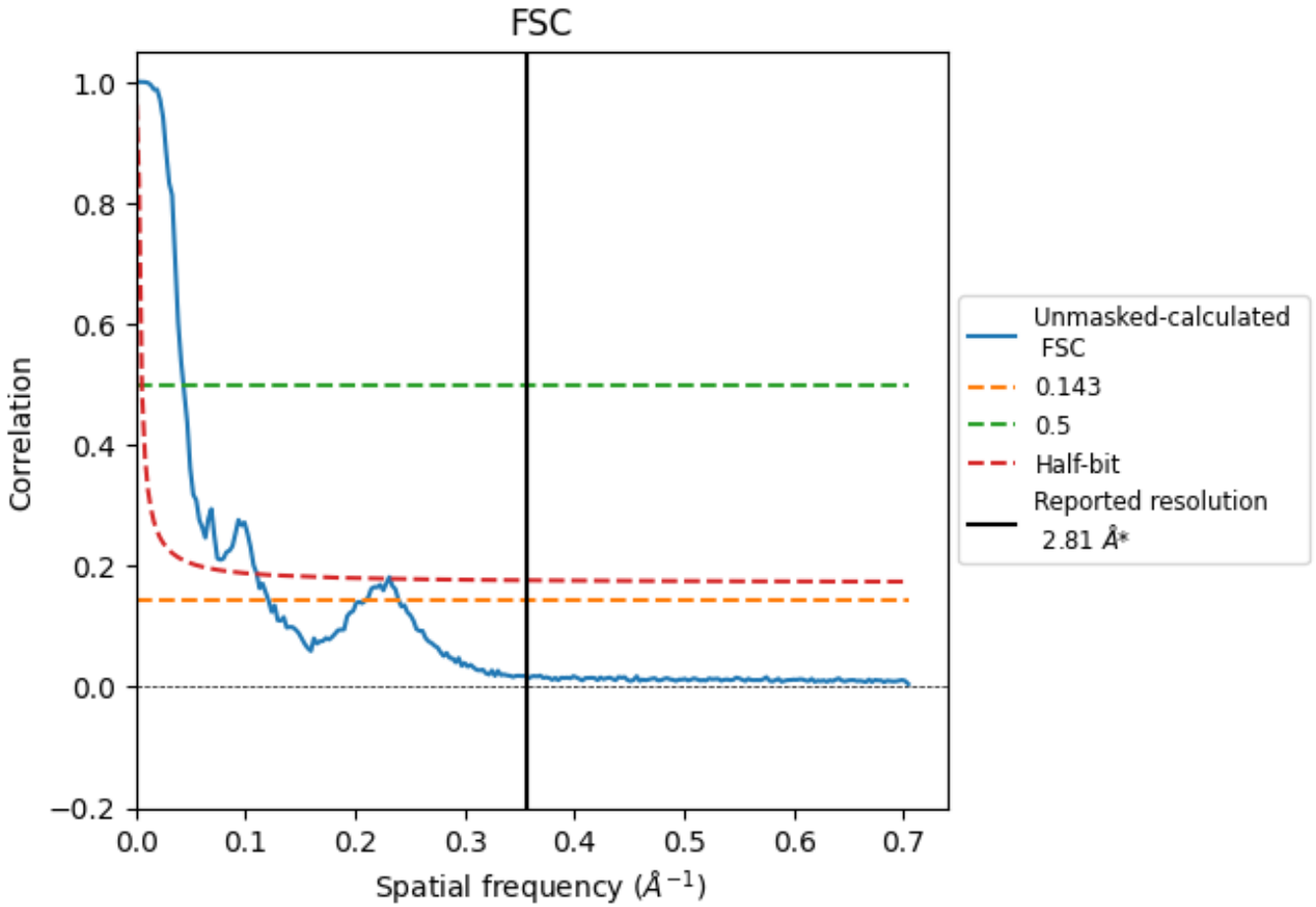


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

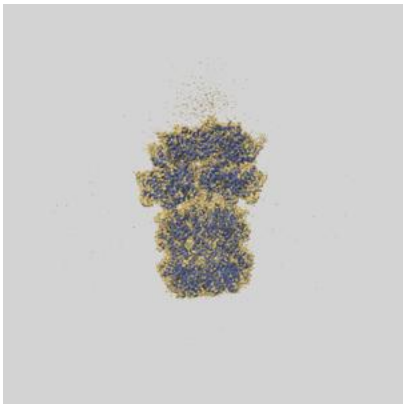
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.27	23.15	9.07

*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 8.27 differs from the reported value 2.81 by more than 10 %

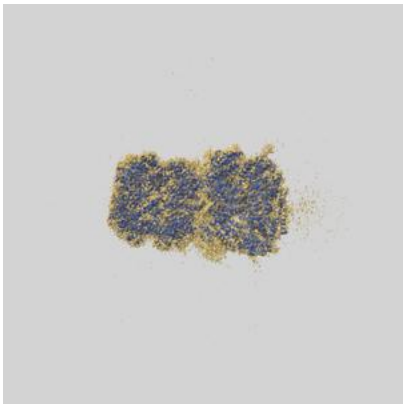
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39162 and PDB model 8YD1. Per-residue inclusion information can be found in section 3 on page 10.

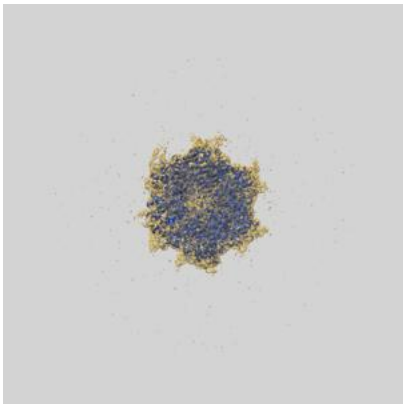
9.1 Map-model overlay



X



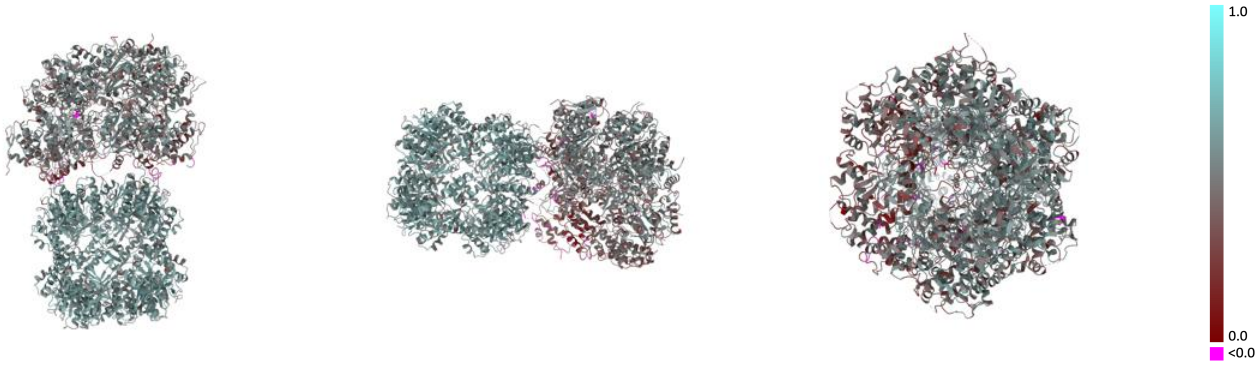
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

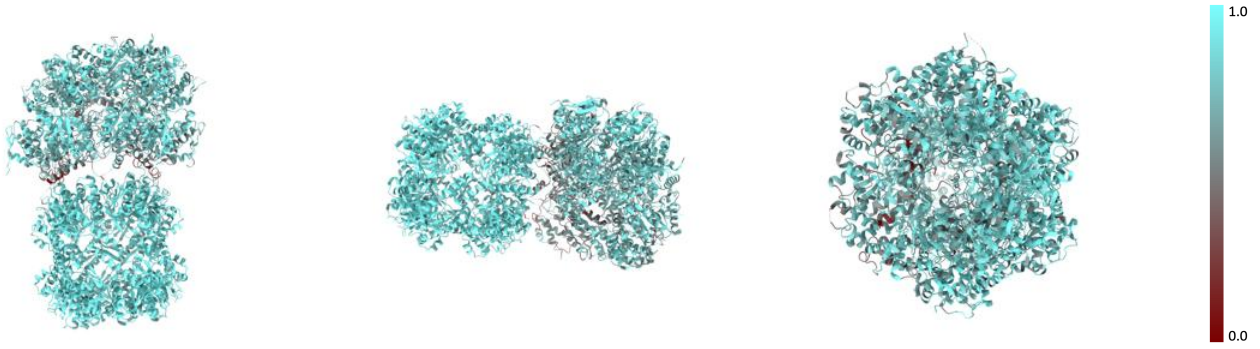
9.2 Q-score mapped to coordinate model



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.

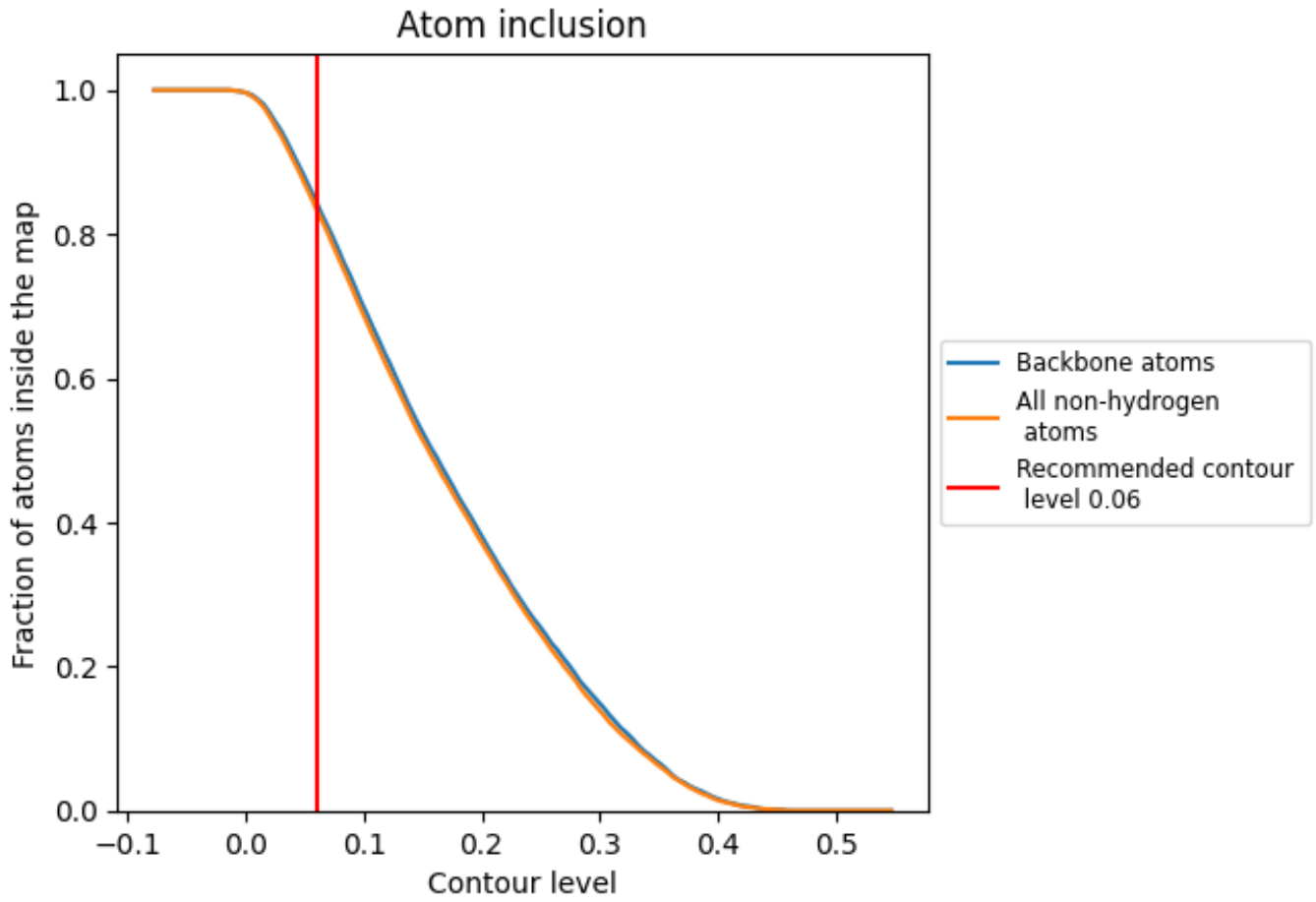
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.4960
A	0.7650	0.4420
B	0.8260	0.4830
C	0.8180	0.4740
D	0.7380	0.4190
E	0.7480	0.4170
F	0.6520	0.3360
G	0.9380	0.5700
H	0.9380	0.5720
I	0.9390	0.5690
J	0.9370	0.5640
K	0.9320	0.5620
L	0.9420	0.5710
M	0.9340	0.5650
N	0.9440	0.5810
O	0.9460	0.5820
P	0.9420	0.5820
Q	0.9420	0.5810
R	0.9430	0.5790
S	0.9400	0.5820
T	0.9420	0.5760
a	0.5980	0.3260