



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:28 PM UTC

PDB ID : 6RKD / pdb_00006rkd
EMDB ID : EMD-4907
Title : Molybdenum storage protein under turnover conditions
Authors : Bruenle, S.; Mills, D.J.; Vonck, J.; Ermler, U.
Deposited on : 2019-04-30
Resolution : 3.20 Å(reported)
Based on initial model : 4F6T

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:

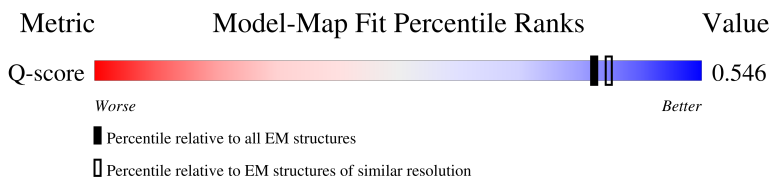
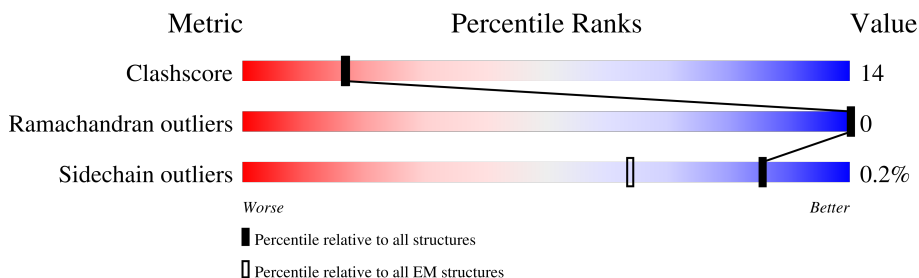
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. 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	276	9% 82% 16% .
1	C	276	9% 83% 16% .
1	E	276	8% 82% 16% .
1	G	276	9% 82% 16% .

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Mol	Chain	Length	Quality of chain
1	I	276	
1	K	276	
2	B	270	
2	D	270	
2	F	270	
2	H	270	
2	J	270	
2	L	270	

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	8M0	B	806	-	-	X	-
5	8M0	D	907	-	-	X	-
5	8M0	F	906	-	-	X	-
5	8M0	H	806	-	-	X	-
5	8M0	J	805	-	-	X	-
5	8M0	L	906	-	-	X	-
7	MOO	A	305	-	-	X	-
7	MOO	A	306	-	-	X	-
7	MOO	A	308	-	-	X	-
7	MOO	B	801	-	-	X	-
7	MOO	B	802	-	-	X	-
7	MOO	B	803	-	-	X	-
7	MOO	B	804	-	-	X	-
7	MOO	B	807	-	-	X	-
7	MOO	C	305	-	-	X	-
7	MOO	C	306	-	-	X	-
7	MOO	D	902	-	-	X	-
7	MOO	D	903	-	-	X	-
7	MOO	D	904	-	-	X	-
7	MOO	D	905	-	-	X	-
7	MOO	D	908	-	-	X	-
7	MOO	E	306	-	-	X	-
7	MOO	E	307	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MOO	F	902	-	-	X	-
7	MOO	F	903	-	-	X	-
7	MOO	F	904	-	-	X	-
7	MOO	F	907	-	-	X	-
7	MOO	G	305	-	-	X	-
7	MOO	G	306	-	-	X	-
7	MOO	G	307	-	-	X	-
7	MOO	H	801	-	-	X	-
7	MOO	H	802	-	-	X	-
7	MOO	H	803	-	-	X	-
7	MOO	H	804	-	-	X	-
7	MOO	H	807	-	-	X	-
7	MOO	I	306	-	-	X	-
7	MOO	I	307	-	-	X	-
7	MOO	I	308	-	-	X	-
7	MOO	J	801	-	-	X	-
7	MOO	J	802	-	-	X	-
7	MOO	J	803	-	-	X	-
7	MOO	J	806	-	-	X	-
7	MOO	K	306	-	-	X	-
7	MOO	K	307	-	-	X	-
7	MOO	L	902	-	-	X	-
7	MOO	L	903	-	-	X	-
7	MOO	L	904	-	-	X	-
7	MOO	L	907	-	-	X	-
8	OMO	A	307	-	-	X	-
8	OMO	C	307	-	-	X	-
8	OMO	E	301	-	-	X	-
8	OMO	G	308	-	-	X	-
8	OMO	I	301	-	-	X	-
8	OMO	K	301	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Molybdenum storage protein subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		
1	C	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		
1	E	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		
1	G	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		
1	I	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		
1	K	271	Total	C	N	O	S	1	0
			2033	1283	382	365	3		

- Molecule 2 is a protein called Molybdenum storage protein subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		
2	D	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		
2	F	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		
2	H	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		
2	J	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		
2	L	268	Total	C	N	O	S	3	0
			1982	1258	347	369	8		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

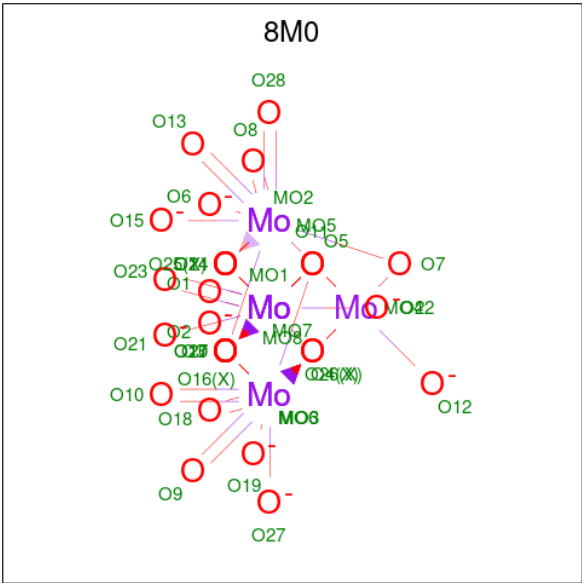


Id	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	J	1	Total 31	C 10	N 5	O 13	P 3	0
3	K	1	Total 31	C 10	N 5	O 13	P 3	0
3	L	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	

- Molecule 5 is bis(mu4-oxo)-tetrakis(mu3-oxo)-hexakis(mu2-oxo)-hexadeca-oxo-octamolybdenum (VI) (CCD ID: 8M0) (formula: Mo₈O₂₈).



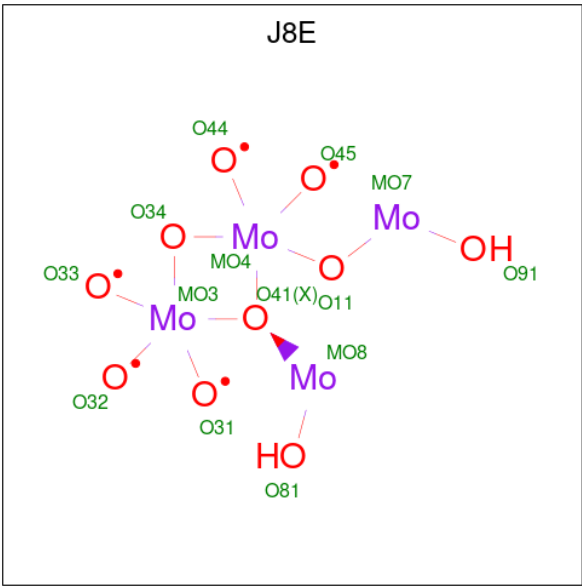
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Mo	O	0
			34	8	26	
5	B	1	Total	Mo	O	0
			36	8	28	
5	C	1	Total	Mo	O	0
			34	8	26	
5	D	1	Total	Mo	O	0
			36	8	28	
5	E	1	Total	Mo	O	0
			34	8	26	

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Mol	Chain	Residues	Atoms			AltConf
5	F	1	Total	Mo	O	0
			36	8	28	
5	G	1	Total	Mo	O	0
			34	8	26	
5	H	1	Total	Mo	O	0
			36	8	28	
5	I	1	Total	Mo	O	0
			34	8	26	
5	J	1	Total	Mo	O	0
			36	8	28	
5	K	1	Total	Mo	O	0
			34	8	26	
5	L	1	Total	Mo	O	0
			36	8	28	

- Molecule 6 is oxidanyl-[[2,2,4,4,4-pentakis($\text{l}^{\wedge}\{1\}$ -oxidanyl)-1-(oxidanylmolybdenio)-1 $\text{l}^{\wedge}\{3\}$,3-dioxa-2 $\text{l}^{\wedge}\{5\}$,4 $\text{l}^{\wedge}\{5\}$ -dimolybdacyclobut-2-yl]oxy]molybdenum (CCD ID: J8E) (formula: $\text{H}_2\text{Mo}_4\text{O}_{10}$).



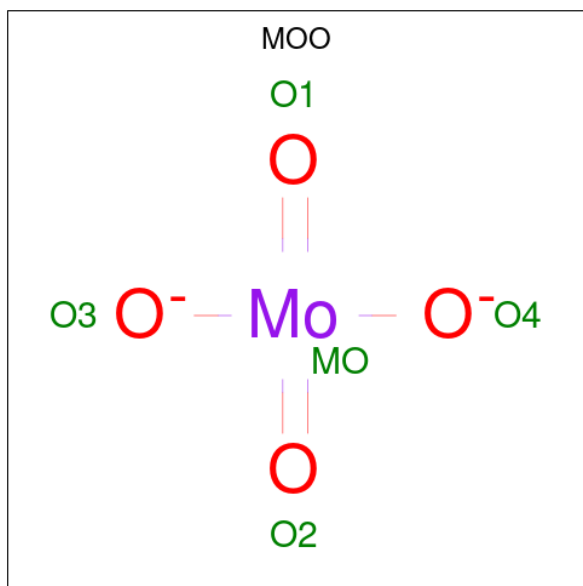
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	Mo	O	0
			14	4	10	
6	B	1	Total	Mo	O	0
			14	4	10	
6	C	1	Total	Mo	O	0
			14	4	10	

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Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	Mo	O	0
			14	4	10	
6	E	1	Total	Mo	O	0
			14	4	10	
6	F	1	Total	Mo	O	0
			14	4	10	
6	G	1	Total	Mo	O	0
			14	4	10	
6	H	1	Total	Mo	O	0
			14	4	10	
6	I	1	Total	Mo	O	0
			14	4	10	
6	J	1	Total	Mo	O	0
			14	4	10	
6	K	1	Total	Mo	O	0
			14	4	10	
6	L	1	Total	Mo	O	0
			14	4	10	

- Molecule 7 is MOLYBDATE ION (CCD ID: MOO) (formula: MoO_4).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Mo	O	0
			5	1	4	
7	A	1	Total	Mo	O	0
			5	1	4	

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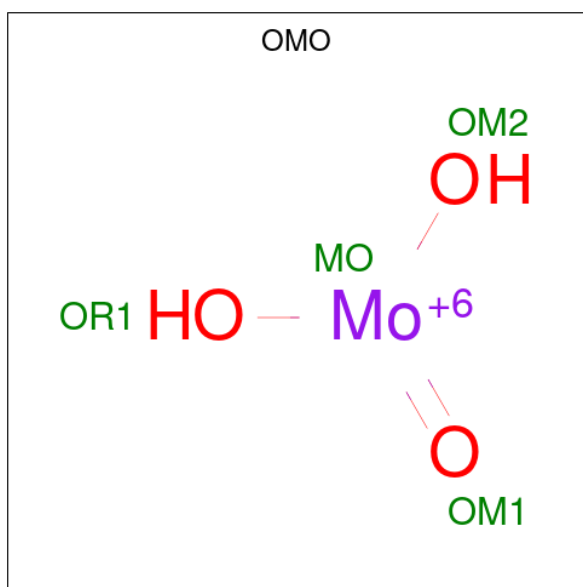
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total 5	Mo 1	O 4	0
7	B	1	Total 5	Mo 1	O 4	0
7	B	1	Total 5	Mo 1	O 4	0
7	B	1	Total 5	Mo 1	O 4	0
7	B	1	Total 5	Mo 1	O 4	0
7	B	1	Total 5	Mo 1	O 4	0
7	C	1	Total 5	Mo 1	O 4	0
7	C	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	D	1	Total 5	Mo 1	O 4	0
7	E	1	Total 5	Mo 1	O 4	0
7	E	1	Total 5	Mo 1	O 4	0
7	F	1	Total 5	Mo 1	O 4	0
7	F	1	Total 5	Mo 1	O 4	0
7	F	1	Total 5	Mo 1	O 4	0
7	F	1	Total 5	Mo 1	O 4	0
7	F	1	Total 5	Mo 1	O 4	0
7	G	1	Total 5	Mo 1	O 4	0
7	G	1	Total 5	Mo 1	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total	Mo	O	0
			5	1	4	
7	H	1	Total	Mo	O	0
			5	1	4	
7	H	1	Total	Mo	O	0
			5	1	4	
7	H	1	Total	Mo	O	0
			5	1	4	
7	H	1	Total	Mo	O	0
			5	1	4	
7	H	1	Total	Mo	O	0
			5	1	4	
7	I	1	Total	Mo	O	0
			5	1	4	
7	I	1	Total	Mo	O	0
			5	1	4	
7	I	1	Total	Mo	O	0
			5	1	4	
7	J	1	Total	Mo	O	0
			5	1	4	
7	J	1	Total	Mo	O	0
			5	1	4	
7	J	1	Total	Mo	O	0
			5	1	4	
7	J	1	Total	Mo	O	0
			5	1	4	
7	K	1	Total	Mo	O	0
			5	1	4	
7	K	1	Total	Mo	O	0
			5	1	4	
7	L	1	Total	Mo	O	0
			5	1	4	
7	L	1	Total	Mo	O	0
			5	1	4	
7	L	1	Total	Mo	O	0
			5	1	4	
7	L	1	Total	Mo	O	0
			5	1	4	

- Molecule 8 is MO(VI)(=O)(OH)₂ CLUSTER (CCD ID: OMO) (formula: H₂MoO₃).

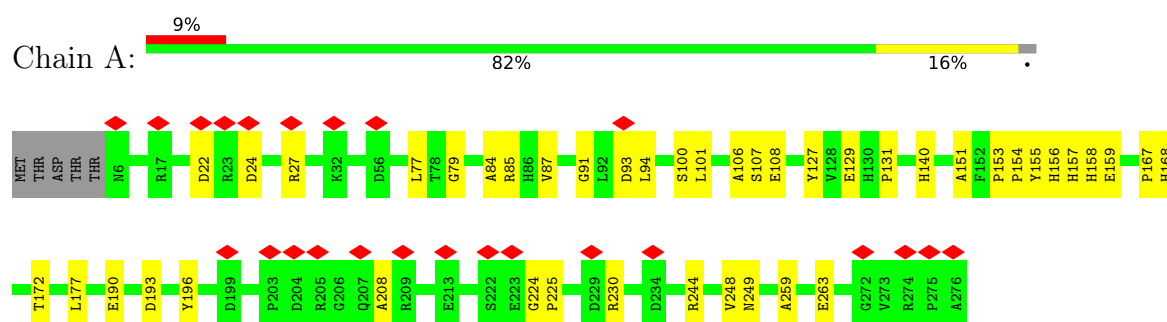


Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	Mo	O	0
			4	1	3	
8	C	1	Total	Mo	O	0
			4	1	3	
8	E	1	Total	Mo	O	0
			4	1	3	
8	G	1	Total	Mo	O	0
			4	1	3	
8	I	1	Total	Mo	O	0
			4	1	3	
8	K	1	Total	Mo	O	0
			4	1	3	

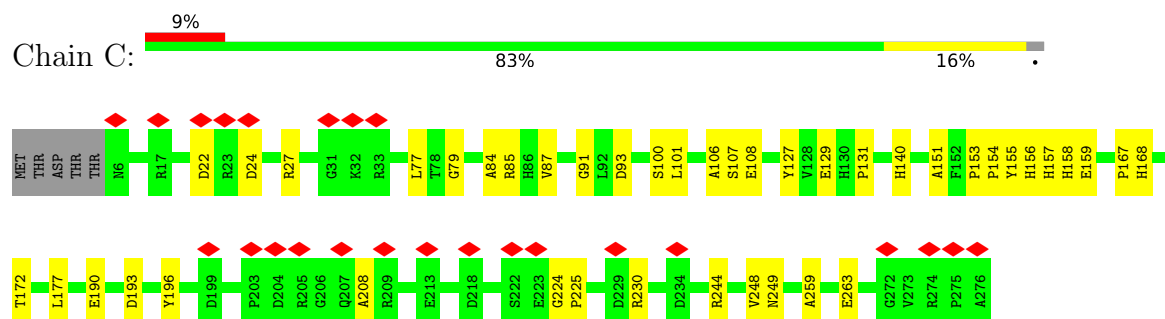
3 Residue-property plots [i](#)

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.

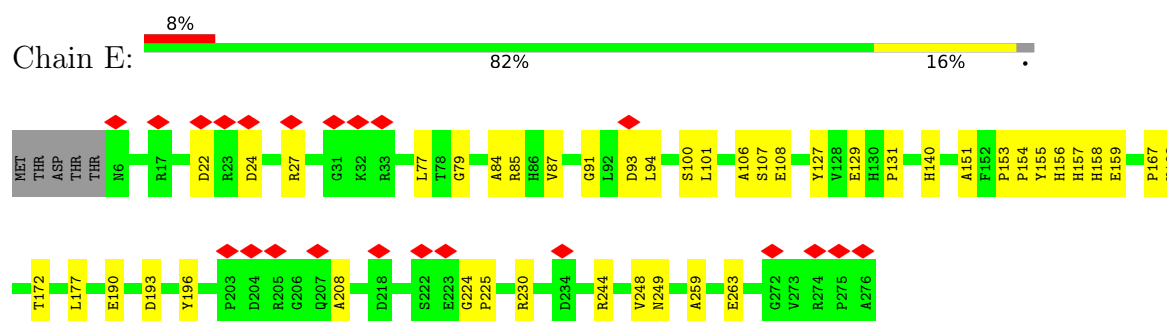
- Molecule 1: Molybdenum storage protein subunit alpha



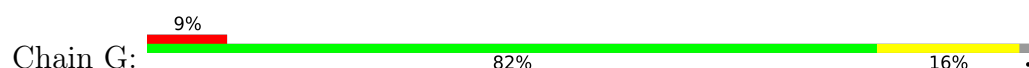
- Molecule 1: Molybdenum storage protein subunit alpha

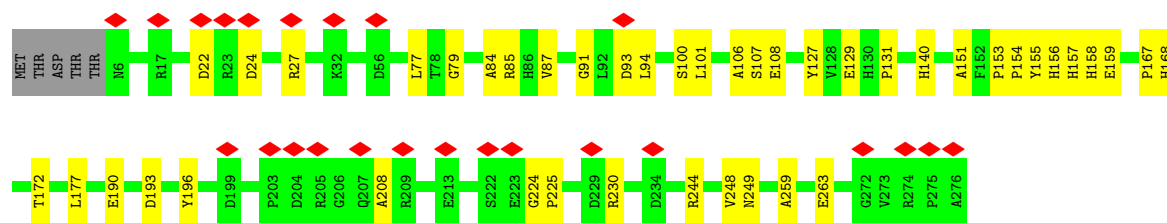


- Molecule 1: Molybdenum storage protein subunit alpha

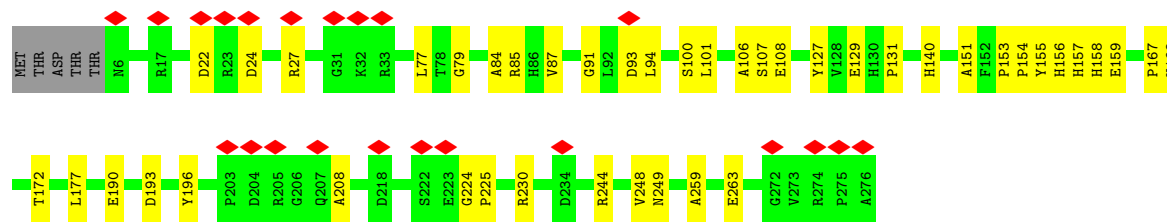
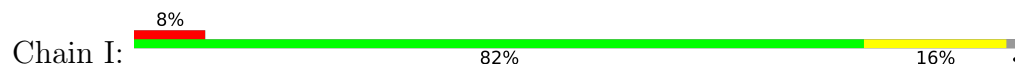


- Molecule 1: Molybdenum storage protein subunit alpha

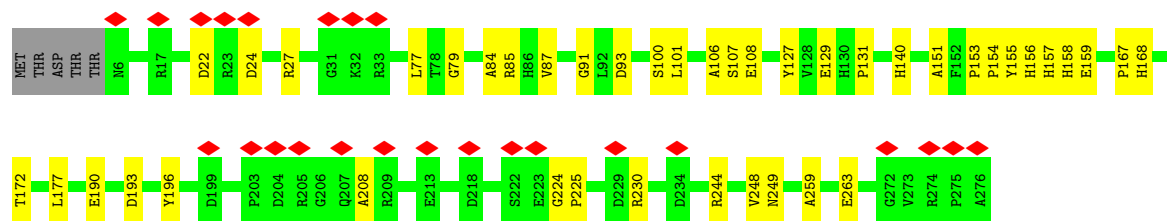
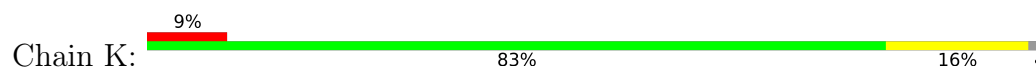




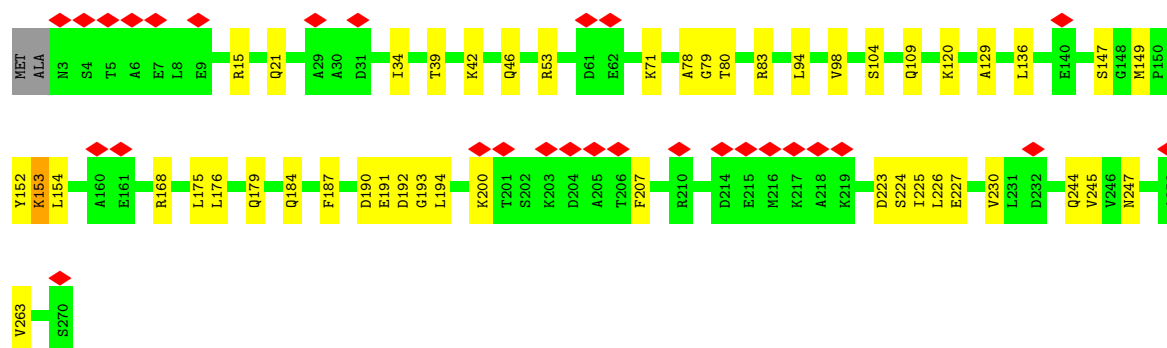
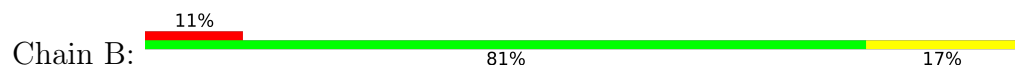
• Molecule 1: Molybdenum storage protein subunit alpha



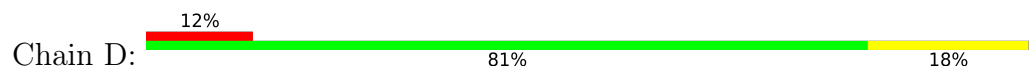
• Molecule 1: Molybdenum storage protein subunit alpha

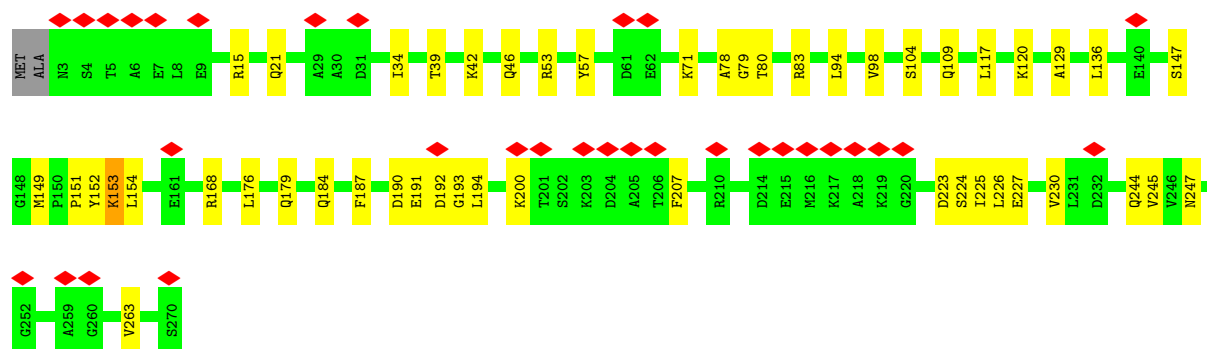


• Molecule 2: Molybdenum storage protein subunit beta



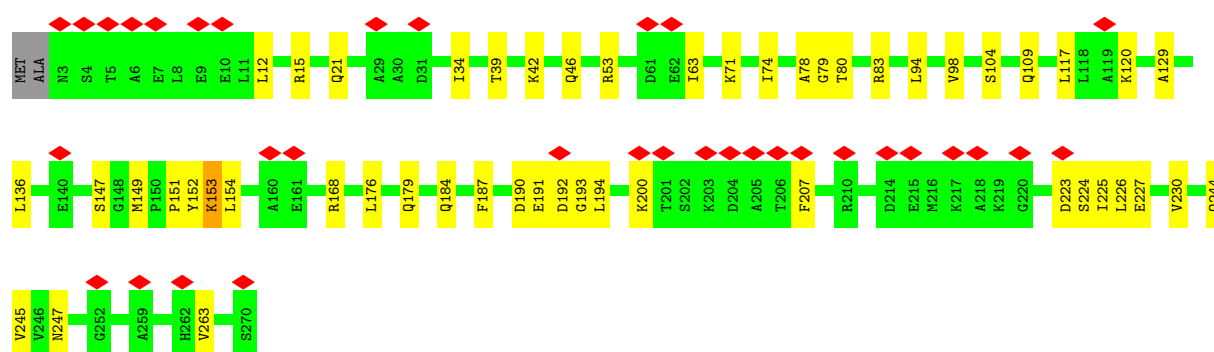
• Molecule 2: Molybdenum storage protein subunit beta





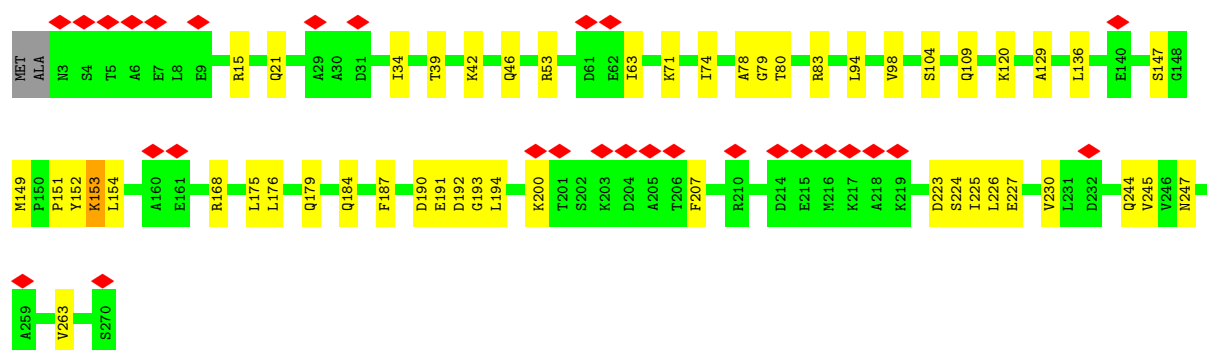
- Molecule 2: Molybdenum storage protein subunit beta

Chain F: 13% 80% 19%



- Molecule 2: Molybdenum storage protein subunit beta

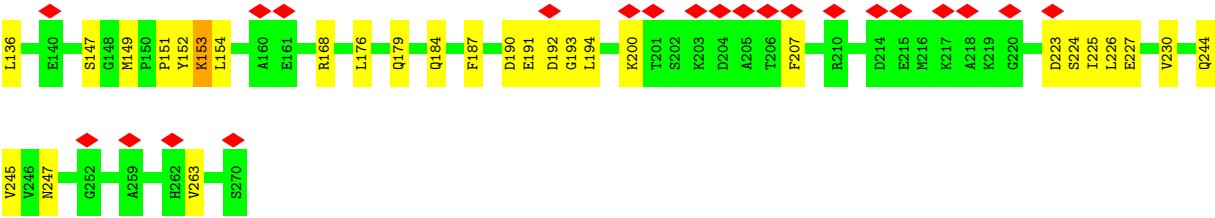
Chain H: 11% 81% 18%



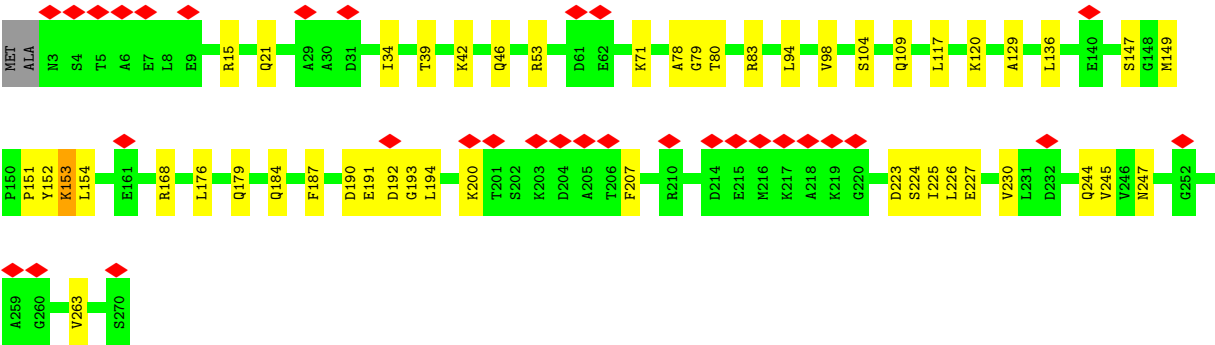
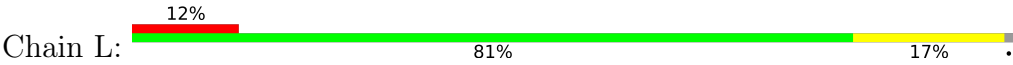
- Molecule 2: Molybdenum storage protein subunit beta

Chain J: 13% 80% 19%





• Molecule 2: Molybdenum storage protein subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	137558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45045	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.618	Depositor
Minimum map value	-0.241	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.068	Depositor
Map size ($\text{\AA}$)	222.0, 222.0, 222.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.11, 1.11, 1.11	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: 8M0, MOO, OMO, MG, ATP, J8E

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	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
1	C	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
1	E	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
1	G	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
1	I	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
1	K	0.56	2/2081 (0.1%)	0.72	2/2836 (0.1%)
2	B	0.38	0/2041	0.60	2/2773 (0.1%)
2	D	0.38	0/2041	0.60	2/2773 (0.1%)
2	F	0.38	0/2041	0.60	2/2773 (0.1%)
2	H	0.38	0/2041	0.60	2/2773 (0.1%)
2	J	0.38	0/2041	0.60	2/2773 (0.1%)
2	L	0.38	0/2041	0.60	2/2773 (0.1%)
All	All	0.48	12/24732 (0.0%)	0.66	24/33654 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	PRO	C-N	12.11	1.51	1.33
1	G	154	PRO	C-N	12.11	1.51	1.33
1	E	154	PRO	C-N	12.10	1.51	1.33
1	I	154	PRO	C-N	12.10	1.51	1.33
1	C	154	PRO	C-N	12.07	1.51	1.33
1	K	154	PRO	C-N	12.07	1.51	1.33
1	A	127	TYR	C-O	-5.52	1.17	1.23
1	G	127	TYR	C-O	-5.52	1.17	1.23
1	E	127	TYR	C-O	-5.50	1.17	1.23
1	I	127	TYR	C-O	-5.50	1.17	1.23
1	C	127	TYR	C-O	-5.50	1.17	1.23
1	K	127	TYR	C-O	-5.50	1.17	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	156	HIS	CB-CA-C	-8.11	107.21	116.54
1	I	156	HIS	CB-CA-C	-8.11	107.21	116.54
1	C	156	HIS	CB-CA-C	-8.11	107.22	116.54
1	K	156	HIS	CB-CA-C	-8.11	107.22	116.54
1	A	156	HIS	CB-CA-C	-8.10	107.23	116.54
1	G	156	HIS	CB-CA-C	-8.10	107.23	116.54
2	D	152	TYR	CA-C-O	-5.87	114.33	120.55
2	L	152	TYR	CA-C-O	-5.87	114.33	120.55
2	B	152	TYR	CA-C-O	-5.86	114.34	120.55
2	H	152	TYR	CA-C-O	-5.86	114.34	120.55
2	F	152	TYR	CA-C-O	-5.83	114.37	120.55
2	J	152	TYR	CA-C-O	-5.83	114.37	120.55
1	E	127	TYR	CA-C-O	-5.44	114.67	120.92
1	I	127	TYR	CA-C-O	-5.44	114.67	120.92
1	C	127	TYR	CA-C-O	-5.41	114.70	120.92
1	K	127	TYR	CA-C-O	-5.41	114.70	120.92
1	A	127	TYR	CA-C-O	-5.41	114.70	120.92
1	G	127	TYR	CA-C-O	-5.41	114.70	120.92
2	B	153	LYS	CB-CA-C	-5.35	110.42	116.63
2	F	153	LYS	CB-CA-C	-5.35	110.42	116.63
2	H	153	LYS	CB-CA-C	-5.35	110.42	116.63
2	J	153	LYS	CB-CA-C	-5.35	110.42	116.63
2	D	153	LYS	CB-CA-C	-5.32	110.46	116.63
2	L	153	LYS	CB-CA-C	-5.32	110.46	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2033	0	2090	43	0
1	C	2033	0	2090	43	0
1	E	2033	0	2090	45	0
1	G	2033	0	2090	43	0
1	I	2033	0	2090	45	0
1	K	2033	0	2090	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1982	0	2024	48	0
2	D	1982	0	2024	50	0
2	F	1982	0	2024	51	0
2	H	1982	0	2024	49	0
2	J	1982	0	2024	51	0
2	L	1982	0	2024	48	0
3	A	31	0	12	5	0
3	B	31	0	12	8	0
3	C	31	0	12	5	0
3	D	31	0	12	8	0
3	E	31	0	12	5	0
3	F	31	0	12	8	0
3	G	31	0	12	5	0
3	H	31	0	12	8	0
3	I	31	0	12	5	0
3	J	31	0	12	8	0
3	K	31	0	12	5	0
3	L	31	0	12	8	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	A	34	0	0	1	0
5	B	36	0	0	8	0
5	C	34	0	0	1	0
5	D	36	0	0	8	0
5	E	34	0	0	2	0
5	F	36	0	0	8	0
5	G	34	0	0	1	0
5	H	36	0	0	8	0
5	I	34	0	0	2	0
5	J	36	0	0	8	0
5	K	34	0	0	1	0
5	L	36	0	0	8	0
6	A	14	0	0	3	0
6	B	14	0	0	0	0
6	C	14	0	0	3	0
6	D	14	0	0	0	0
6	E	14	0	0	3	0
6	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	14	0	0	3	0
6	H	14	0	0	0	0
6	I	14	0	0	3	0
6	J	14	0	0	0	0
6	K	14	0	0	3	0
6	L	14	0	0	0	0
7	A	15	0	0	26	0
7	B	25	0	0	32	0
7	C	10	0	0	17	0
7	D	25	0	0	33	0
7	E	10	0	0	17	0
7	F	20	0	0	26	0
7	G	15	0	0	26	0
7	H	25	0	0	32	0
7	I	15	0	0	26	0
7	J	20	0	0	26	0
7	K	10	0	0	17	0
7	L	20	0	0	25	0
8	A	4	0	0	5	0
8	C	4	0	0	5	0
8	E	4	0	0	5	0
8	G	4	0	0	5	0
8	I	4	0	0	5	0
8	K	4	0	0	5	0
All	All	25290	0	24828	699	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 (699) 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)
7:C:305:MOO:O3	7:C:306:MOO:O1	1.78	1.01
7:K:306:MOO:O3	7:K:307:MOO:O1	1.78	1.01
7:A:305:MOO:O3	7:A:306:MOO:O1	1.78	1.01
7:G:305:MOO:O3	7:G:306:MOO:O1	1.78	1.01
7:E:306:MOO:O3	7:E:307:MOO:O1	1.78	1.00
7:I:306:MOO:O3	7:I:307:MOO:O1	1.78	1.00
7:A:308:MOO:O3	7:E:307:MOO:O1	1.86	0.94
7:G:307:MOO:O3	7:I:307:MOO:O1	1.86	0.94
7:A:308:MOO:O2	7:F:904:MOO:O2	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:307:MOO:O2	7:J:803:MOO:O2	1.85	0.94
7:A:306:MOO:O1	7:B:803:MOO:O3	1.86	0.93
7:I:308:MOO:O2	7:L:904:MOO:O2	1.85	0.93
7:B:803:MOO:O2	7:B:804:MOO:O2	1.85	0.93
7:D:904:MOO:O2	7:D:905:MOO:O2	1.85	0.93
7:H:803:MOO:O2	7:H:804:MOO:O2	1.85	0.93
7:G:306:MOO:O1	7:H:803:MOO:O3	1.86	0.93
7:B:802:MOO:O3	7:B:804:MOO:O1	1.87	0.93
7:H:802:MOO:O3	7:H:804:MOO:O1	1.87	0.93
7:C:306:MOO:O1	7:D:904:MOO:O3	1.86	0.93
7:I:308:MOO:O3	7:K:307:MOO:O1	1.86	0.93
7:D:903:MOO:O3	7:D:905:MOO:O1	1.87	0.92
7:L:903:MOO:O3	7:L:904:MOO:O1	1.87	0.92
7:J:802:MOO:O3	7:J:803:MOO:O1	1.87	0.91
7:F:903:MOO:O3	7:F:904:MOO:O1	1.87	0.91
7:I:308:MOO:O3	7:L:904:MOO:O2	1.92	0.88
7:D:904:MOO:O3	7:D:905:MOO:O2	1.92	0.88
7:B:803:MOO:O3	7:B:804:MOO:O2	1.92	0.88
7:H:803:MOO:O3	7:H:804:MOO:O2	1.92	0.88
7:G:307:MOO:O3	7:J:803:MOO:O2	1.92	0.86
7:A:308:MOO:O3	7:F:904:MOO:O2	1.92	0.86
2:H:168:ARG:HB3	7:H:807:MOO:O4	1.77	0.85
2:B:168:ARG:HB3	7:B:807:MOO:O4	1.77	0.85
2:F:168:ARG:HB3	7:F:907:MOO:O4	1.77	0.84
2:J:168:ARG:HB3	7:J:806:MOO:O4	1.77	0.84
2:D:168:ARG:HB3	7:D:908:MOO:O4	1.77	0.84
2:L:168:ARG:HB3	7:L:907:MOO:O4	1.77	0.84
2:H:190:ASP:OD1	3:H:805:ATP:O3'	1.96	0.83
2:B:190:ASP:OD1	3:B:805:ATP:O3'	1.96	0.83
2:F:190:ASP:OD1	3:F:905:ATP:O3'	1.96	0.83
2:J:190:ASP:OD1	3:J:804:ATP:O3'	1.96	0.83
2:D:190:ASP:OD1	3:D:906:ATP:O3'	1.96	0.82
2:L:190:ASP:OD1	3:L:905:ATP:O3'	1.96	0.82
7:B:801:MOO:O4	5:B:806:8M0:O19	2.00	0.79
7:H:801:MOO:O4	5:H:806:8M0:O19	2.00	0.79
7:F:902:MOO:O4	5:F:906:8M0:O19	2.00	0.79
7:J:801:MOO:O4	5:J:805:8M0:O19	2.00	0.79
7:D:902:MOO:O4	5:D:907:8M0:O19	2.00	0.78
7:L:902:MOO:O4	5:L:906:8M0:O19	2.00	0.78
1:E:190:GLU:OE2	3:E:302:ATP:H5'2	1.84	0.77
1:K:190:GLU:OE2	3:K:302:ATP:H5'2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLU:OE2	3:C:301:ATP:H5'2	1.84	0.77
1:I:190:GLU:OE2	3:I:302:ATP:H5'2	1.84	0.77
1:A:190:GLU:OE2	3:A:301:ATP:H5'2	1.84	0.76
1:G:190:GLU:OE2	3:G:301:ATP:H5'2	1.84	0.76
1:E:129:GLU:HB2	6:E:305:J8E:O45	1.87	0.75
1:I:129:GLU:HB2	6:I:305:J8E:O45	1.87	0.75
1:G:129:GLU:HB2	6:G:304:J8E:O45	1.87	0.74
1:A:129:GLU:HB2	6:A:304:J8E:O45	1.87	0.74
1:C:129:GLU:HB2	6:C:304:J8E:O45	1.87	0.74
1:K:129:GLU:HB2	6:K:305:J8E:O45	1.87	0.74
1:K:190:GLU:OE2	3:K:302:ATP:C5'	2.41	0.69
1:C:190:GLU:OE2	3:C:301:ATP:C5'	2.41	0.69
7:C:306:MOO:O2	7:D:904:MOO:O4	2.10	0.69
1:E:190:GLU:OE2	3:E:302:ATP:C5'	2.41	0.69
1:I:190:GLU:OE2	3:I:302:ATP:C5'	2.41	0.69
7:I:308:MOO:O4	7:K:307:MOO:O2	2.10	0.69
1:G:190:GLU:OE2	3:G:301:ATP:C5'	2.41	0.69
1:A:190:GLU:OE2	3:A:301:ATP:C5'	2.41	0.68
7:G:306:MOO:O2	7:H:803:MOO:O4	2.10	0.68
7:G:307:MOO:O4	7:I:307:MOO:O2	2.10	0.68
7:A:308:MOO:O4	7:E:307:MOO:O2	2.10	0.68
7:A:306:MOO:O2	7:B:803:MOO:O4	2.10	0.68
2:B:78:ALA:HB3	7:B:807:MOO:O2	1.94	0.68
2:F:200:LYS:NZ	3:F:905:ATP:O3'	2.27	0.68
2:D:78:ALA:HB3	7:D:908:MOO:O2	1.94	0.67
2:H:78:ALA:HB3	7:H:807:MOO:O2	1.94	0.67
2:J:200:LYS:NZ	3:J:804:ATP:O3'	2.27	0.67
2:L:78:ALA:HB3	7:L:907:MOO:O2	1.94	0.67
2:B:200:LYS:NZ	3:B:805:ATP:O3'	2.27	0.66
2:D:200:LYS:NZ	3:D:906:ATP:O3'	2.27	0.66
2:H:200:LYS:NZ	3:H:805:ATP:O3'	2.27	0.66
2:L:200:LYS:NZ	3:L:905:ATP:O3'	2.27	0.66
2:F:78:ALA:HB3	7:F:907:MOO:O2	1.94	0.66
2:J:78:ALA:HB3	7:J:806:MOO:O2	1.94	0.66
1:E:131:PRO:HA	7:E:306:MOO:O4	1.98	0.64
1:I:131:PRO:HA	7:I:306:MOO:O4	1.98	0.64
1:C:131:PRO:HA	7:C:305:MOO:O4	1.98	0.64
1:A:131:PRO:HA	7:A:305:MOO:O4	1.98	0.64
1:K:131:PRO:HA	7:K:306:MOO:O4	1.98	0.64
1:G:131:PRO:HA	7:G:305:MOO:O4	1.98	0.64
7:C:306:MOO:O1	7:C:306:MOO:MO	1.69	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:307:MOO:O1	7:K:307:MOO:MO	1.69	0.64
1:A:140:HIS:CE1	8:A:307:OMO:OM2	2.51	0.63
7:B:801:MOO:O1	7:B:801:MOO:MO	1.69	0.63
1:C:140:HIS:CE1	8:C:307:OMO:OM2	2.51	0.63
1:G:140:HIS:CE1	8:G:308:OMO:OM2	2.51	0.63
1:K:140:HIS:CE1	8:K:301:OMO:OM2	2.51	0.63
1:E:140:HIS:CE1	8:E:301:OMO:OM2	2.51	0.63
2:F:191:GLU:HG3	3:F:905:ATP:H2'	1.81	0.63
7:H:801:MOO:MO	7:H:801:MOO:O1	1.69	0.63
2:J:191:GLU:HG3	3:J:804:ATP:H2'	1.81	0.63
7:C:305:MOO:MO	7:C:305:MOO:O1	1.69	0.63
7:G:305:MOO:O1	7:G:305:MOO:MO	1.69	0.63
1:I:140:HIS:CE1	8:I:301:OMO:OM2	2.51	0.63
7:A:305:MOO:O3	7:A:305:MOO:MO	1.70	0.63
7:A:305:MOO:MO	7:A:305:MOO:O1	1.69	0.63
7:A:306:MOO:MO	7:A:306:MOO:O3	1.70	0.63
7:B:803:MOO:MO	7:B:803:MOO:O1	1.69	0.63
7:G:306:MOO:O3	7:G:306:MOO:MO	1.70	0.63
7:H:801:MOO:MO	7:H:801:MOO:O3	1.70	0.63
7:K:306:MOO:O1	7:K:306:MOO:MO	1.69	0.63
1:A:153:PRO:HB2	1:A:155:TYR:CD1	2.34	0.63
7:B:801:MOO:MO	7:B:801:MOO:O3	1.70	0.63
7:D:903:MOO:MO	7:D:903:MOO:O1	1.69	0.63
1:G:153:PRO:HB2	1:G:155:TYR:CD1	2.34	0.63
7:G:305:MOO:O3	7:G:305:MOO:MO	1.70	0.63
7:H:803:MOO:MO	7:H:803:MOO:O1	1.69	0.63
7:H:807:MOO:MO	7:H:807:MOO:O3	1.70	0.63
7:L:903:MOO:MO	7:L:903:MOO:O1	1.69	0.63
7:A:308:MOO:MO	7:A:308:MOO:O1	1.70	0.63
7:B:807:MOO:O3	7:B:807:MOO:MO	1.70	0.63
7:G:307:MOO:MO	7:G:307:MOO:O1	1.70	0.63
7:L:903:MOO:O3	7:L:903:MOO:MO	1.70	0.63
7:B:804:MOO:MO	7:B:804:MOO:O3	1.70	0.63
7:D:903:MOO:O3	7:D:903:MOO:MO	1.70	0.63
7:H:804:MOO:O3	7:H:804:MOO:MO	1.70	0.63
1:I:153:PRO:HB2	1:I:155:TYR:CD1	2.34	0.63
1:E:106:ALA:C	5:E:304:8M0:O6	2.42	0.62
1:E:153:PRO:HB2	1:E:155:TYR:CD1	2.34	0.62
7:E:306:MOO:MO	7:E:306:MOO:O1	1.69	0.62
1:I:106:ALA:C	5:I:304:8M0:O6	2.42	0.62
7:I:306:MOO:MO	7:I:306:MOO:O1	1.69	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:803:MOO:MO	7:J:803:MOO:O3	1.70	0.62
7:J:806:MOO:O3	7:J:806:MOO:MO	1.70	0.62
7:L:904:MOO:MO	7:L:904:MOO:O3	1.70	0.62
2:B:191:GLU:HG3	3:B:805:ATP:H2'	1.81	0.62
7:C:306:MOO:MO	7:C:306:MOO:O3	1.70	0.62
7:D:908:MOO:O3	7:D:908:MOO:MO	1.70	0.62
2:H:191:GLU:HG3	3:H:805:ATP:H2'	1.81	0.62
7:H:803:MOO:O3	7:H:803:MOO:MO	1.70	0.62
7:J:801:MOO:MO	7:J:801:MOO:O1	1.69	0.62
7:K:306:MOO:O3	7:K:306:MOO:MO	1.70	0.62
7:K:307:MOO:MO	7:K:307:MOO:O3	1.70	0.62
7:L:907:MOO:O3	7:L:907:MOO:MO	1.70	0.62
8:A:307:OMO:MO	8:E:301:OMO:OR1	1.70	0.62
7:A:308:MOO:O3	7:A:308:MOO:MO	1.70	0.62
7:B:803:MOO:O3	7:B:803:MOO:MO	1.70	0.62
7:C:305:MOO:O3	7:C:305:MOO:MO	1.70	0.62
7:D:902:MOO:O3	7:D:902:MOO:MO	1.70	0.62
7:D:904:MOO:O3	7:D:904:MOO:MO	1.70	0.62
7:D:905:MOO:MO	7:D:905:MOO:O3	1.70	0.62
7:F:902:MOO:MO	7:F:902:MOO:O1	1.69	0.62
7:F:904:MOO:O3	7:F:904:MOO:MO	1.70	0.62
7:F:907:MOO:MO	7:F:907:MOO:O3	1.70	0.62
7:G:307:MOO:O3	7:G:307:MOO:MO	1.70	0.62
7:L:902:MOO:MO	7:L:902:MOO:O3	1.70	0.62
8:C:307:OMO:OR1	8:E:301:OMO:MO	1.70	0.62
7:G:306:MOO:O1	7:G:306:MOO:MO	1.69	0.62
8:G:308:OMO:MO	8:I:301:OMO:OR1	1.70	0.62
8:G:308:OMO:OR1	8:K:301:OMO:MO	1.70	0.62
8:I:301:OMO:MO	8:K:301:OMO:OR1	1.70	0.62
8:A:307:OMO:OR1	8:C:307:OMO:MO	1.70	0.62
7:E:307:MOO:O1	7:E:307:MOO:MO	1.69	0.62
7:I:308:MOO:O3	7:I:308:MOO:MO	1.70	0.62
7:A:306:MOO:O1	7:A:306:MOO:MO	1.69	0.62
2:B:129:ALA:CB	5:B:806:8M0:O23	2.48	0.62
1:C:153:PRO:HB2	1:C:155:TYR:CD1	2.34	0.62
7:F:904:MOO:O1	7:F:904:MOO:MO	1.69	0.62
2:H:129:ALA:CB	5:H:806:8M0:O23	2.48	0.62
7:I:307:MOO:O1	7:I:307:MOO:MO	1.69	0.62
1:K:153:PRO:HB2	1:K:155:TYR:CD1	2.34	0.62
7:L:904:MOO:O1	7:L:904:MOO:MO	1.70	0.62
7:J:803:MOO:O1	7:J:803:MOO:MO	1.69	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:902:MOO:MO	7:D:902:MOO:O1	1.69	0.62
2:H:200:LYS:NZ	3:H:805:ATP:O2'	2.28	0.62
7:D:905:MOO:O1	7:D:905:MOO:MO	1.70	0.61
1:G:106:ALA:C	5:G:303:8M0:O6	2.42	0.61
7:L:902:MOO:MO	7:L:902:MOO:O1	1.69	0.61
1:A:106:ALA:C	5:A:303:8M0:O6	2.42	0.61
7:A:305:MOO:O4	7:A:305:MOO:MO	1.71	0.61
7:B:803:MOO:O4	7:B:803:MOO:MO	1.72	0.61
1:C:106:ALA:C	5:C:303:8M0:O6	2.42	0.61
7:E:306:MOO:O3	7:E:306:MOO:MO	1.70	0.61
7:G:306:MOO:MO	7:G:306:MOO:O4	1.71	0.61
7:J:801:MOO:MO	7:J:801:MOO:O3	1.70	0.61
1:K:106:ALA:C	5:K:304:8M0:O6	2.42	0.61
7:A:306:MOO:MO	7:A:306:MOO:O4	1.71	0.61
7:B:804:MOO:O2	7:B:804:MOO:MO	1.72	0.61
2:D:129:ALA:CB	5:D:907:8M0:O23	2.48	0.61
2:D:191:GLU:HG3	3:D:906:ATP:H2'	1.81	0.61
7:D:905:MOO:MO	7:D:905:MOO:O4	1.71	0.61
7:F:907:MOO:O2	7:F:907:MOO:MO	1.72	0.61
7:G:305:MOO:O4	7:G:305:MOO:MO	1.71	0.61
7:H:802:MOO:MO	7:H:802:MOO:O1	1.69	0.61
7:H:803:MOO:O4	7:H:803:MOO:MO	1.72	0.61
7:J:806:MOO:O2	7:J:806:MOO:MO	1.72	0.61
2:L:129:ALA:CB	5:L:906:8M0:O23	2.48	0.61
2:L:168:ARG:NE	7:L:907:MOO:O3	2.33	0.61
2:D:168:ARG:NE	7:D:908:MOO:O3	2.33	0.61
2:F:129:ALA:CB	5:F:906:8M0:O23	2.48	0.61
7:F:904:MOO:MO	7:F:904:MOO:O4	1.71	0.61
7:H:804:MOO:O2	7:H:804:MOO:MO	1.72	0.61
7:I:308:MOO:O2	7:I:308:MOO:MO	1.72	0.61
2:L:191:GLU:HG3	3:L:905:ATP:H2'	1.81	0.61
7:L:902:MOO:O4	7:L:902:MOO:MO	1.71	0.61
7:L:904:MOO:MO	7:L:904:MOO:O4	1.71	0.61
7:B:802:MOO:MO	7:B:802:MOO:O1	1.69	0.61
7:D:902:MOO:O4	7:D:902:MOO:MO	1.71	0.61
7:D:902:MOO:MO	7:D:902:MOO:O2	1.72	0.61
7:D:904:MOO:O2	7:D:904:MOO:MO	1.72	0.61
7:F:902:MOO:MO	7:F:902:MOO:O3	1.70	0.61
7:I:306:MOO:O3	7:I:306:MOO:MO	1.70	0.61
2:J:129:ALA:CB	5:J:805:8M0:O23	2.48	0.61
7:L:902:MOO:MO	7:L:902:MOO:O2	1.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:306:MOO:O2	7:C:306:MOO:MO	1.72	0.61
7:E:307:MOO:MO	7:E:307:MOO:O3	1.70	0.61
7:I:306:MOO:MO	7:I:306:MOO:O2	1.72	0.61
7:J:803:MOO:MO	7:J:803:MOO:O4	1.71	0.61
7:K:307:MOO:O2	7:K:307:MOO:MO	1.72	0.61
7:B:801:MOO:MO	7:B:801:MOO:O2	1.72	0.61
7:B:802:MOO:O3	7:B:802:MOO:MO	1.70	0.61
7:E:306:MOO:MO	7:E:306:MOO:O2	1.72	0.61
7:H:801:MOO:MO	7:H:801:MOO:O2	1.72	0.61
7:H:802:MOO:O3	7:H:802:MOO:MO	1.70	0.61
7:H:804:MOO:O1	7:H:804:MOO:MO	1.70	0.61
7:H:804:MOO:MO	7:H:804:MOO:O4	1.71	0.61
7:I:307:MOO:MO	7:I:307:MOO:O3	1.70	0.61
7:B:803:MOO:O2	7:B:803:MOO:MO	1.72	0.61
7:B:804:MOO:MO	7:B:804:MOO:O4	1.71	0.61
7:J:802:MOO:O3	7:J:802:MOO:MO	1.70	0.61
7:A:308:MOO:O4	7:A:308:MOO:MO	1.72	0.61
2:B:168:ARG:NE	7:B:807:MOO:O3	2.33	0.61
2:H:168:ARG:NE	7:H:807:MOO:O3	2.33	0.61
7:I:308:MOO:MO	7:I:308:MOO:O1	1.69	0.61
7:L:907:MOO:O4	7:L:907:MOO:MO	1.72	0.61
7:B:804:MOO:O1	7:B:804:MOO:MO	1.70	0.61
7:D:904:MOO:MO	7:D:904:MOO:O1	1.69	0.61
7:D:908:MOO:O4	7:D:908:MOO:MO	1.72	0.61
7:F:903:MOO:O3	7:F:903:MOO:MO	1.70	0.61
7:F:903:MOO:MO	7:F:903:MOO:O1	1.69	0.61
7:H:801:MOO:O4	7:H:801:MOO:MO	1.71	0.61
7:H:803:MOO:O2	7:H:803:MOO:MO	1.72	0.61
7:A:306:MOO:O2	7:A:306:MOO:MO	1.72	0.60
7:D:904:MOO:O4	7:D:904:MOO:MO	1.72	0.60
7:G:306:MOO:O2	7:G:306:MOO:MO	1.72	0.60
7:G:307:MOO:O4	7:G:307:MOO:MO	1.72	0.60
2:J:168:ARG:NE	7:J:806:MOO:O3	2.33	0.60
7:L:907:MOO:O2	7:L:907:MOO:MO	1.72	0.60
7:B:801:MOO:O4	7:B:801:MOO:MO	1.71	0.60
2:F:168:ARG:NE	7:F:907:MOO:O3	2.33	0.60
7:G:305:MOO:MO	7:G:305:MOO:O2	1.72	0.60
8:I:301:OMO:MO	8:I:301:OMO:OM1	1.72	0.60
7:J:801:MOO:MO	7:J:801:MOO:O2	1.72	0.60
7:J:802:MOO:MO	7:J:802:MOO:O1	1.69	0.60
7:A:305:MOO:MO	7:A:305:MOO:O2	1.72	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:307:OMO:MO	8:A:307:OMO:OM1	1.72	0.60
7:D:908:MOO:O2	7:D:908:MOO:MO	1.72	0.60
8:E:301:OMO:MO	8:E:301:OMO:OM1	1.72	0.60
7:I:307:MOO:MO	7:I:307:MOO:O4	1.71	0.60
7:I:308:MOO:O4	7:I:308:MOO:MO	1.72	0.60
7:K:307:MOO:MO	7:K:307:MOO:O4	1.71	0.60
7:F:902:MOO:MO	7:F:902:MOO:O2	1.72	0.60
7:K:306:MOO:MO	7:K:306:MOO:O2	1.72	0.60
7:L:904:MOO:O2	7:L:904:MOO:MO	1.72	0.60
7:C:305:MOO:MO	7:C:305:MOO:O2	1.72	0.60
7:C:306:MOO:MO	7:C:306:MOO:O4	1.71	0.60
7:E:307:MOO:MO	7:E:307:MOO:O4	1.71	0.60
7:F:902:MOO:O4	7:F:902:MOO:MO	1.71	0.60
8:G:308:OMO:MO	8:G:308:OMO:OM1	1.72	0.60
7:D:905:MOO:O2	7:D:905:MOO:MO	1.72	0.60
1:E:168:HIS:HD2	1:E:172:THR:HG21	1.67	0.60
2:B:200:LYS:NZ	3:B:805:ATP:O2'	2.28	0.60
1:I:168:HIS:HD2	1:I:172:THR:HG21	1.67	0.60
7:F:904:MOO:O2	7:F:904:MOO:MO	1.72	0.60
7:I:306:MOO:O4	7:I:306:MOO:MO	1.71	0.60
7:J:801:MOO:O4	7:J:801:MOO:MO	1.71	0.60
2:B:151:PRO:HB3	5:B:806:8M0:O4	2.02	0.60
7:B:807:MOO:O2	7:B:807:MOO:MO	1.72	0.60
7:E:306:MOO:O4	7:E:306:MOO:MO	1.71	0.60
2:L:151:PRO:HB3	5:L:906:8M0:O4	2.02	0.60
2:D:151:PRO:HB3	5:D:907:8M0:O4	2.02	0.60
7:H:807:MOO:O2	7:H:807:MOO:MO	1.72	0.60
7:J:803:MOO:O2	7:J:803:MOO:MO	1.72	0.60
8:C:307:OMO:MO	8:C:307:OMO:OM1	1.72	0.59
2:H:151:PRO:HB3	5:H:806:8M0:O4	2.02	0.59
7:C:305:MOO:O4	7:C:305:MOO:MO	1.71	0.59
8:K:301:OMO:MO	8:K:301:OMO:OM1	1.72	0.59
2:D:154:LEU:O	2:D:154:LEU:HG	2.02	0.59
7:K:306:MOO:O4	7:K:306:MOO:MO	1.71	0.59
2:B:154:LEU:O	2:B:154:LEU:HG	2.02	0.59
7:B:807:MOO:O4	7:B:807:MOO:MO	1.72	0.59
2:F:154:LEU:HG	2:F:154:LEU:O	2.02	0.59
2:H:154:LEU:HG	2:H:154:LEU:O	2.02	0.59
2:L:154:LEU:O	2:L:154:LEU:HG	2.02	0.59
7:A:308:MOO:O2	7:A:308:MOO:MO	1.72	0.59
7:H:807:MOO:O4	7:H:807:MOO:MO	1.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:307:MOO:O2	7:E:307:MOO:MO	1.72	0.59
7:G:307:MOO:O2	7:G:307:MOO:MO	1.72	0.59
2:J:151:PRO:HB3	5:J:805:8M0:O4	2.02	0.59
2:J:154:LEU:O	2:J:154:LEU:HG	2.02	0.59
7:J:806:MOO:O4	7:J:806:MOO:MO	1.71	0.59
1:C:168:HIS:HD2	1:C:172:THR:HG21	1.67	0.59
2:F:151:PRO:HB3	5:F:906:8M0:O4	2.02	0.59
7:I:307:MOO:O2	7:I:307:MOO:MO	1.72	0.59
2:B:53:ARG:N	1:C:93:ASP:OD2	2.36	0.59
7:F:907:MOO:O4	7:F:907:MOO:MO	1.71	0.59
2:H:53:ARG:N	1:K:93:ASP:OD2	2.36	0.59
1:A:168:HIS:HD2	1:A:172:THR:HG21	1.67	0.58
1:K:168:HIS:HD2	1:K:172:THR:HG21	1.67	0.58
1:A:93:ASP:OD2	2:F:53:ARG:N	2.36	0.58
2:D:53:ARG:N	1:E:93:ASP:OD2	2.36	0.58
1:G:93:ASP:OD2	2:J:53:ARG:N	2.36	0.58
1:G:168:HIS:HD2	1:G:172:THR:HG21	1.67	0.58
2:H:71:LYS:NZ	2:H:136:LEU:O	2.36	0.58
1:I:93:ASP:OD2	2:L:53:ARG:N	2.36	0.58
2:B:71:LYS:NZ	2:B:136:LEU:O	2.36	0.58
2:D:200:LYS:NZ	3:D:906:ATP:O2'	2.28	0.58
1:E:158:HIS:ND1	5:F:906:8M0:O8	2.37	0.58
2:L:200:LYS:NZ	3:L:905:ATP:O2'	2.28	0.58
2:D:129:ALA:HB2	5:D:907:8M0:O23	2.04	0.58
1:I:158:HIS:ND1	5:J:805:8M0:O8	2.37	0.58
2:L:104:SER:HB3	7:L:902:MOO:O2	2.04	0.58
2:D:104:SER:HB3	7:D:902:MOO:O2	2.04	0.57
2:F:104:SER:HB3	7:F:902:MOO:O2	2.04	0.57
2:J:104:SER:HB3	7:J:801:MOO:O2	2.04	0.57
2:L:129:ALA:HB2	5:L:906:8M0:O23	2.04	0.57
1:G:79:GLY:HA3	3:G:301:ATP:O1G	2.04	0.57
7:G:305:MOO:O2	7:G:306:MOO:O1	2.22	0.57
1:A:79:GLY:HA3	3:A:301:ATP:O1G	2.04	0.57
7:A:305:MOO:O2	7:A:306:MOO:O1	2.22	0.57
1:C:79:GLY:HA3	3:C:301:ATP:O1G	2.04	0.57
1:K:79:GLY:HA3	3:K:302:ATP:O1G	2.04	0.57
1:A:158:HIS:ND1	5:B:806:8M0:O8	2.37	0.57
1:E:131:PRO:HB3	7:E:306:MOO:O4	2.05	0.57
2:F:200:LYS:NZ	3:F:905:ATP:O2'	2.28	0.57
1:I:131:PRO:HB3	7:I:306:MOO:O4	2.05	0.57
1:G:158:HIS:ND1	5:H:806:8M0:O8	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:306:MOO:O2	7:E:307:MOO:O1	2.22	0.56
2:F:129:ALA:HB2	5:F:906:8M0:O23	2.04	0.56
2:H:104:SER:HB3	7:H:801:MOO:O2	2.04	0.56
1:A:131:PRO:HB3	7:A:305:MOO:O4	2.04	0.56
2:B:129:ALA:HB2	5:B:806:8M0:O23	2.04	0.56
1:C:131:PRO:HB3	7:C:305:MOO:O4	2.05	0.56
7:C:305:MOO:O2	7:C:306:MOO:O1	2.22	0.56
7:I:306:MOO:O2	7:I:307:MOO:O1	2.22	0.56
1:K:131:PRO:CB	7:K:306:MOO:O4	2.53	0.56
7:K:306:MOO:O2	7:K:307:MOO:O1	2.22	0.56
2:B:104:SER:HB3	7:B:801:MOO:O2	2.04	0.56
1:C:131:PRO:CB	7:C:305:MOO:O4	2.53	0.56
1:G:131:PRO:HB3	7:G:305:MOO:O4	2.04	0.56
2:H:129:ALA:HB2	5:H:806:8M0:O23	2.04	0.56
2:J:129:ALA:HB2	5:J:805:8M0:O23	2.04	0.56
2:J:200:LYS:NZ	3:J:804:ATP:O2'	2.28	0.56
1:K:131:PRO:HB3	7:K:306:MOO:O4	2.05	0.56
1:E:131:PRO:CB	7:E:306:MOO:O4	2.53	0.56
1:A:131:PRO:CB	7:A:305:MOO:O4	2.53	0.56
2:F:191:GLU:HG3	3:F:905:ATP:C2'	2.36	0.56
7:G:307:MOO:O4	7:I:306:MOO:O2	2.23	0.56
1:I:131:PRO:CB	7:I:306:MOO:O4	2.53	0.56
7:A:308:MOO:O4	7:E:306:MOO:O2	2.23	0.56
7:I:308:MOO:O4	7:K:306:MOO:O2	2.23	0.56
2:J:191:GLU:HG3	3:J:804:ATP:C2'	2.36	0.56
7:C:305:MOO:O2	7:D:904:MOO:O4	2.23	0.56
1:G:131:PRO:CB	7:G:305:MOO:O4	2.53	0.56
2:D:46:GLN:HB2	2:D:79:GLY:HA2	1.88	0.56
1:E:157:HIS:HD2	5:F:906:8M0:O15	1.89	0.56
1:I:157:HIS:HD2	5:J:805:8M0:O15	1.89	0.56
2:L:46:GLN:HB2	2:L:79:GLY:HA2	1.88	0.56
7:A:305:MOO:O2	7:B:803:MOO:O4	2.23	0.56
2:B:46:GLN:HB2	2:B:79:GLY:HA2	1.88	0.56
7:G:305:MOO:O2	7:H:803:MOO:O4	2.23	0.56
1:I:79:GLY:HA3	3:I:302:ATP:O1G	2.04	0.56
1:A:157:HIS:HD2	5:B:806:8M0:O15	1.89	0.55
1:E:79:GLY:HA3	3:E:302:ATP:O1G	2.04	0.55
2:H:46:GLN:HB2	2:H:79:GLY:HA2	1.88	0.55
1:G:157:HIS:HD2	5:H:806:8M0:O15	1.89	0.55
2:H:191:GLU:HG3	3:H:805:ATP:C2'	2.36	0.55
2:B:191:GLU:HG3	3:B:805:ATP:C2'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:SER:HA	2:F:149:MET:HG3	1.89	0.55
2:J:104:SER:HA	2:J:149:MET:HG3	1.89	0.55
2:D:191:GLU:HG3	3:D:906:ATP:C2'	2.36	0.55
2:D:104:SER:HA	2:D:149:MET:HG3	1.89	0.55
1:K:157:HIS:HD2	5:L:906:8M0:O15	1.89	0.55
1:C:157:HIS:HD2	5:D:907:8M0:O15	1.89	0.55
2:L:104:SER:HA	2:L:149:MET:HG3	1.89	0.55
2:L:191:GLU:HG3	3:L:905:ATP:C2'	2.36	0.55
2:B:168:ARG:CB	7:B:807:MOO:O4	2.52	0.55
2:D:168:ARG:CB	7:D:908:MOO:O4	2.52	0.55
2:F:71:LYS:NZ	2:F:136:LEU:O	2.36	0.55
2:F:168:ARG:CB	7:F:907:MOO:O4	2.52	0.54
1:I:85:ARG:NH1	2:J:15:ARG:O	2.40	0.54
2:J:46:GLN:HB2	2:J:79:GLY:HA2	1.88	0.54
2:J:71:LYS:NZ	2:J:136:LEU:O	2.36	0.54
1:E:85:ARG:NH1	2:F:15:ARG:O	2.40	0.54
2:H:168:ARG:CB	7:H:807:MOO:O4	2.52	0.54
2:F:46:GLN:HB2	2:F:79:GLY:HA2	1.88	0.54
2:J:168:ARG:CB	7:J:806:MOO:O4	2.52	0.54
2:L:168:ARG:CB	7:L:907:MOO:O4	2.52	0.54
1:A:85:ARG:NH1	2:B:15:ARG:O	2.40	0.54
2:B:104:SER:HA	2:B:149:MET:HG3	1.89	0.54
1:C:85:ARG:NH1	2:D:15:ARG:O	2.40	0.54
2:H:104:SER:HA	2:H:149:MET:HG3	1.89	0.54
1:K:85:ARG:NH1	2:L:15:ARG:O	2.40	0.54
1:G:85:ARG:NH1	2:H:15:ARG:O	2.40	0.54
2:L:71:LYS:NZ	2:L:136:LEU:O	2.36	0.54
1:A:244:ARG:HH12	1:I:263:GLU:HG2	1.73	0.53
1:A:108:GLU:OE2	2:F:109:GLN:NE2	2.41	0.53
1:E:263:GLU:HG2	1:G:244:ARG:HH12	1.73	0.53
1:G:108:GLU:OE2	2:J:109:GLN:NE2	2.41	0.53
2:D:71:LYS:NZ	2:D:136:LEU:O	2.36	0.53
1:A:263:GLU:HG2	1:I:244:ARG:HH12	1.73	0.53
1:E:244:ARG:HH12	1:G:263:GLU:HG2	1.73	0.53
2:D:109:GLN:NE2	1:E:108:GLU:OE2	2.41	0.53
2:F:168:ARG:HD2	7:F:907:MOO:O4	2.09	0.53
1:I:108:GLU:OE2	2:L:109:GLN:NE2	2.41	0.53
2:J:15:ARG:NH1	2:J:21:GLN:OE1	2.38	0.53
2:J:168:ARG:HD2	7:J:806:MOO:O4	2.09	0.53
1:E:131:PRO:CA	7:E:306:MOO:O4	2.57	0.53
1:I:131:PRO:CA	7:I:306:MOO:O4	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:168:ARG:HD2	7:L:907:MOO:O4	2.09	0.53
2:D:168:ARG:HD2	7:D:908:MOO:O4	2.09	0.52
2:F:15:ARG:NH1	2:F:21:GLN:OE1	2.38	0.52
1:C:131:PRO:CA	7:C:305:MOO:O4	2.57	0.52
1:C:244:ARG:HH12	1:K:263:GLU:HG2	1.73	0.52
1:C:263:GLU:HG2	1:K:244:ARG:HH12	1.73	0.52
2:L:244:GLN:NE2	2:L:263:VAL:O	2.37	0.52
1:K:131:PRO:CA	7:K:306:MOO:O4	2.57	0.52
2:B:168:ARG:HD2	7:B:807:MOO:O4	2.09	0.52
2:H:168:ARG:HD2	7:H:807:MOO:O4	2.09	0.52
2:D:244:GLN:NE2	2:D:263:VAL:O	2.37	0.52
1:A:225:PRO:HB2	3:A:301:ATP:N7	2.25	0.52
1:G:225:PRO:HB2	3:G:301:ATP:N7	2.25	0.52
2:L:15:ARG:NH1	2:L:21:GLN:OE1	2.38	0.52
1:A:131:PRO:CA	7:A:305:MOO:O4	2.57	0.52
1:C:225:PRO:HB2	3:C:301:ATP:N7	2.25	0.51
1:G:131:PRO:CA	7:G:305:MOO:O4	2.57	0.51
2:D:15:ARG:NH1	2:D:21:GLN:OE1	2.38	0.51
2:H:15:ARG:NH1	2:H:21:GLN:OE1	2.38	0.51
1:K:225:PRO:HB2	3:K:302:ATP:N7	2.25	0.51
2:B:15:ARG:NH1	2:B:21:GLN:OE1	2.38	0.51
1:I:225:PRO:HB2	3:I:302:ATP:N7	2.25	0.51
1:E:225:PRO:HB2	3:E:302:ATP:N7	2.25	0.51
1:K:24:ASP:OD1	1:K:27:ARG:NH2	2.38	0.51
1:C:24:ASP:OD1	1:C:27:ARG:NH2	2.38	0.51
1:C:158:HIS:ND1	5:D:907:8M0:O8	2.37	0.51
1:K:158:HIS:ND1	5:L:906:8M0:O8	2.37	0.50
1:I:107[B]:SER:HB2	2:L:109:GLN:HE21	1.77	0.50
2:L:147:SER:OG	7:L:902:MOO:O4	2.30	0.50
2:D:109:GLN:HE21	1:E:107[B]:SER:HB2	1.77	0.50
2:D:147:SER:OG	7:D:902:MOO:O4	2.30	0.50
1:A:107[A]:SER:HB2	2:F:109:GLN:HE21	1.77	0.50
1:A:107[B]:SER:HB2	2:F:109:GLN:HE21	1.77	0.50
1:G:107[A]:SER:HB2	2:J:109:GLN:HE21	1.77	0.50
1:G:107[B]:SER:HB2	2:J:109:GLN:HE21	1.77	0.50
2:H:109:GLN:HE21	1:K:107[B]:SER:HB2	1.77	0.50
2:H:109:GLN:HE21	1:K:107[A]:SER:HB2	1.77	0.50
1:I:129:GLU:CB	6:I:305:J8E:O45	2.59	0.50
2:B:109:GLN:HE21	1:C:107[B]:SER:HB2	1.77	0.49
2:B:109:GLN:HE21	1:C:107[A]:SER:HB2	1.77	0.49
2:B:147:SER:OG	7:B:801:MOO:O4	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:GLU:CB	6:E:305:J8E:O45	2.59	0.49
2:H:147:SER:OG	7:H:801:MOO:O4	2.30	0.49
2:B:224:SER:OG	2:B:226:LEU:O	2.29	0.49
2:H:224:SER:OG	2:H:226:LEU:O	2.29	0.49
1:K:129:GLU:CB	6:K:305:J8E:O45	2.59	0.49
1:C:129:GLU:CB	6:C:304:J8E:O45	2.59	0.49
2:J:147:SER:OG	7:J:801:MOO:O4	2.30	0.49
2:B:109:GLN:NE2	1:C:108:GLU:OE2	2.41	0.48
2:D:193:GLY:HA3	2:D:207:PHE:HE1	1.78	0.48
2:F:147:SER:OG	7:F:902:MOO:O4	2.30	0.48
2:L:193:GLY:HA3	2:L:207:PHE:HE1	1.78	0.48
1:G:129:GLU:CB	6:G:304:J8E:O45	2.59	0.48
1:A:129:GLU:CB	6:A:304:J8E:O45	2.59	0.48
2:H:109:GLN:NE2	1:K:108:GLU:OE2	2.41	0.48
1:I:91:GLY:HA3	1:I:101:LEU:HD21	1.95	0.48
2:B:193:GLY:HA3	2:B:207:PHE:HE1	1.78	0.48
2:B:244:GLN:NE2	2:B:263:VAL:O	2.36	0.48
1:E:91:GLY:HA3	1:E:101:LEU:HD21	1.95	0.48
2:H:244:GLN:NE2	2:H:263:VAL:O	2.36	0.48
2:H:193:GLY:HA3	2:H:207:PHE:HE1	1.78	0.48
1:A:91:GLY:HA3	1:A:101:LEU:HD21	1.95	0.48
2:D:168:ARG:CD	7:D:908:MOO:O4	2.62	0.48
1:G:91:GLY:HA3	1:G:101:LEU:HD21	1.95	0.48
1:G:193:ASP:HA	1:G:249:ASN:HB2	1.96	0.48
1:A:193:ASP:HA	1:A:249:ASN:HB2	1.96	0.48
2:D:109:GLN:HE21	1:E:107[A]:SER:HB2	1.77	0.48
2:L:168:ARG:CD	7:L:907:MOO:O4	2.62	0.48
1:C:91:GLY:HA3	1:C:101:LEU:HD21	1.95	0.48
2:F:94:LEU:HD13	2:F:98:VAL:HG11	1.95	0.48
2:D:94:LEU:HD13	2:D:98:VAL:HG11	1.95	0.48
2:H:191:GLU:HG2	3:H:805:ATP:O3'	2.14	0.48
1:I:107[A]:SER:HB2	2:L:109:GLN:HE21	1.77	0.48
2:J:94:LEU:HD13	2:J:98:VAL:HG11	1.95	0.48
1:K:91:GLY:HA3	1:K:101:LEU:HD21	1.95	0.48
2:B:191:GLU:HG2	3:B:805:ATP:O3'	2.14	0.47
2:L:94:LEU:HD13	2:L:98:VAL:HG11	1.95	0.47
1:E:193:ASP:HA	1:E:249:ASN:HB2	1.96	0.47
1:I:193:ASP:HA	1:I:249:ASN:HB2	1.96	0.47
2:F:168:ARG:CD	7:F:907:MOO:O4	2.62	0.47
1:K:193:ASP:HA	1:K:249:ASN:HB2	1.96	0.47
2:H:94:LEU:HD13	2:H:98:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:HA	1:C:249:ASN:HB2	1.96	0.47
2:H:168:ARG:CD	7:H:807:MOO:O4	2.62	0.47
2:J:168:ARG:CD	7:J:806:MOO:O4	2.62	0.47
1:A:248:VAL:HG11	1:A:259:ALA:HB2	1.96	0.47
2:B:94:LEU:HD13	2:B:98:VAL:HG11	1.95	0.47
2:B:168:ARG:CD	7:B:807:MOO:O4	2.62	0.47
1:C:190:GLU:OE2	3:C:301:ATP:H5'1	2.14	0.47
1:C:248:VAL:HG11	1:C:259:ALA:HB2	1.96	0.47
2:D:224:SER:OG	2:D:226:LEU:O	2.29	0.47
1:G:248:VAL:HG11	1:G:259:ALA:HB2	1.96	0.47
1:I:24:ASP:OD1	1:I:27:ARG:NH2	2.38	0.47
1:K:248:VAL:HG11	1:K:259:ALA:HB2	1.96	0.47
2:L:224:SER:OG	2:L:226:LEU:O	2.29	0.47
1:C:196:TYR:HD2	1:C:208:ALA:HB1	1.80	0.47
2:F:193:GLY:HA3	2:F:207:PHE:HE1	1.78	0.47
1:K:190:GLU:OE2	3:K:302:ATP:H5'1	2.14	0.47
1:K:196:TYR:HD2	1:K:208:ALA:HB1	1.80	0.47
1:E:24:ASP:OD1	1:E:27:ARG:NH2	2.38	0.47
2:J:193:GLY:HA3	2:J:207:PHE:HE1	1.78	0.47
1:I:248:VAL:HG11	1:I:259:ALA:HB2	1.96	0.47
2:J:191:GLU:HG2	3:J:804:ATP:O3'	2.14	0.47
1:E:248:VAL:HG11	1:E:259:ALA:HB2	1.96	0.46
2:F:191:GLU:HG2	3:F:905:ATP:O3'	2.14	0.46
1:G:196:TYR:HD2	1:G:208:ALA:HB1	1.80	0.46
1:A:196:TYR:HD2	1:A:208:ALA:HB1	1.80	0.46
2:D:191:GLU:HG2	3:D:906:ATP:O3'	2.14	0.46
2:F:80:THR:HA	2:F:83:ARG:HD3	1.97	0.46
2:J:244:GLN:NE2	2:J:263:VAL:O	2.36	0.46
2:J:80:THR:HA	2:J:83:ARG:HD3	1.97	0.46
2:L:191:GLU:HG2	3:L:905:ATP:O3'	2.14	0.46
1:A:263:GLU:HG2	1:I:244:ARG:NH1	2.31	0.46
2:B:187:PHE:HB2	2:B:245:VAL:HG22	1.98	0.46
2:F:244:GLN:NE2	2:F:263:VAL:O	2.36	0.46
2:H:80:THR:HA	2:H:83:ARG:HD3	1.97	0.46
2:H:187:PHE:HB2	2:H:245:VAL:HG22	1.98	0.46
2:J:224:SER:OG	2:J:226:LEU:O	2.29	0.46
2:B:80:THR:HA	2:B:83:ARG:HD3	1.97	0.46
1:E:244:ARG:NH1	1:G:263:GLU:HG2	2.31	0.46
2:F:224:SER:OG	2:F:226:LEU:O	2.29	0.46
2:J:225:ILE:HG13	3:J:804:ATP:H5'2	1.98	0.46
2:D:147:SER:OG	7:D:902:MOO:O3	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:ILE:HG13	3:F:905:ATP:H5'2	1.98	0.46
1:G:24:ASP:OD1	1:G:27:ARG:NH2	2.38	0.46
2:L:80:THR:HA	2:L:83:ARG:HD3	1.97	0.46
1:A:190:GLU:OE2	3:A:301:ATP:H5'1	2.14	0.46
2:D:80:THR:HA	2:D:83:ARG:HD3	1.97	0.46
1:G:190:GLU:OE2	3:G:301:ATP:H5'1	2.14	0.46
1:I:196:TYR:HD2	1:I:208:ALA:HB1	1.80	0.46
2:J:129:ALA:HB3	5:J:805:8M0:O23	2.16	0.46
1:E:77:LEU:HB3	1:E:151:ALA:HB2	1.98	0.45
1:E:196:TYR:HD2	1:E:208:ALA:HB1	1.80	0.45
2:F:129:ALA:HB3	5:F:906:8M0:O23	2.16	0.45
1:I:77:LEU:HB3	1:I:151:ALA:HB2	1.98	0.45
1:K:224:GLY:O	1:K:230:ARG:NH2	2.49	0.45
1:A:24:ASP:OD1	1:A:27:ARG:NH2	2.38	0.45
1:C:224:GLY:O	1:C:230:ARG:NH2	2.49	0.45
2:B:129:ALA:HB3	5:B:806:8M0:O23	2.16	0.45
1:C:263:GLU:HG2	1:K:244:ARG:NH1	2.31	0.45
1:E:177:LEU:HD23	2:F:154:LEU:CD2	2.46	0.45
1:A:129:GLU:CG	6:A:304:J8E:O45	2.65	0.45
1:C:22:ASP:HB2	2:D:223:ASP:HB3	1.99	0.45
1:C:244:ARG:NH1	1:K:263:GLU:HG2	2.31	0.45
1:G:129:GLU:CG	6:G:304:J8E:O45	2.65	0.45
1:I:177:LEU:HD23	2:J:154:LEU:CD2	2.46	0.45
1:A:22:ASP:HB2	2:B:223:ASP:HB3	1.99	0.45
1:A:177:LEU:HD23	2:B:154:LEU:CD2	2.46	0.45
1:A:224:GLY:O	1:A:230:ARG:NH2	2.49	0.45
2:D:225:ILE:HG13	3:D:906:ATP:H5'2	1.98	0.45
1:G:22:ASP:HB2	2:H:223:ASP:HB3	1.99	0.45
1:G:177:LEU:HD23	2:H:154:LEU:CD2	2.46	0.45
1:G:224:GLY:O	1:G:230:ARG:NH2	2.49	0.45
2:H:129:ALA:HB3	5:H:806:8M0:O23	2.16	0.45
1:K:22:ASP:HB2	2:L:223:ASP:HB3	1.99	0.45
1:K:129:GLU:CG	6:K:305:J8E:O45	2.65	0.45
2:L:187:PHE:HB2	2:L:245:VAL:HG22	1.98	0.45
1:C:129:GLU:CG	6:C:304:J8E:O45	2.65	0.45
2:D:187:PHE:HB2	2:D:245:VAL:HG22	1.98	0.45
1:E:224:GLY:O	1:E:230:ARG:NH2	2.49	0.45
2:L:225:ILE:HG13	3:L:905:ATP:H5'2	1.98	0.45
1:I:224:GLY:O	1:I:230:ARG:NH2	2.49	0.45
1:I:129:GLU:CG	6:I:305:J8E:O45	2.65	0.45
2:J:187:PHE:HB2	2:J:245:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ASP:HB2	2:F:223:ASP:HB3	1.99	0.44
1:E:129:GLU:CG	6:E:305:J8E:O45	2.65	0.44
1:E:263:GLU:HG2	1:G:244:ARG:NH1	2.31	0.44
1:I:22:ASP:HB2	2:J:223:ASP:HB3	1.99	0.44
1:A:244:ARG:NH1	1:I:263:GLU:HG2	2.31	0.44
2:B:225:ILE:HG13	3:B:805:ATP:H5'2	1.98	0.44
2:F:187:PHE:HB2	2:F:245:VAL:HG22	1.98	0.44
2:H:225:ILE:HG13	3:H:805:ATP:H5'2	1.98	0.44
1:C:177:LEU:HD23	2:D:154:LEU:HD21	2.00	0.44
1:E:190:GLU:OE2	3:E:302:ATP:H5'1	2.15	0.44
2:B:42:LYS:NZ	3:B:805:ATP:O1B	2.51	0.44
1:C:77:LEU:HB3	1:C:151:ALA:HB2	1.98	0.44
2:H:42:LYS:NZ	3:H:805:ATP:O1B	2.51	0.44
1:I:84:ALA:HA	1:I:87:VAL:HG12	2.00	0.44
1:I:190:GLU:OE2	3:I:302:ATP:H5'1	2.15	0.44
1:K:177:LEU:HD23	2:L:154:LEU:HD21	2.00	0.44
1:E:84:ALA:HA	1:E:87:VAL:HG12	2.00	0.44
8:G:308:OMO:OR1	1:K:140:HIS:CE1	2.71	0.44
1:K:77:LEU:HB3	1:K:151:ALA:HB2	1.98	0.44
1:A:140:HIS:CE1	8:E:301:OMO:OR1	2.71	0.44
8:A:307:OMO:OR1	1:C:140:HIS:CE1	2.71	0.44
1:K:177:LEU:HD23	2:L:154:LEU:CD2	2.46	0.44
1:C:177:LEU:HD23	2:D:154:LEU:CD2	2.46	0.44
1:G:140:HIS:CE1	8:I:301:OMO:OR1	2.71	0.44
1:A:77:LEU:HB3	1:A:151:ALA:HB2	1.98	0.44
1:A:159:GLU:OE2	1:A:167:PRO:HD2	2.18	0.44
1:C:159:GLU:OE2	1:C:167:PRO:HD2	2.18	0.44
8:C:307:OMO:OR1	1:E:140:HIS:CE1	2.71	0.44
1:G:84:ALA:HA	1:G:87:VAL:HG12	2.00	0.44
1:K:159:GLU:OE2	1:K:167:PRO:HD2	2.18	0.44
1:A:84:ALA:HA	1:A:87:VAL:HG12	2.00	0.44
1:G:77:LEU:HB3	1:G:151:ALA:HB2	1.98	0.44
1:G:159:GLU:OE2	1:G:167:PRO:HD2	2.18	0.44
1:I:140:HIS:CE1	8:K:301:OMO:OR1	2.71	0.44
2:L:42:LYS:NZ	3:L:905:ATP:O1B	2.51	0.44
2:D:42:LYS:NZ	3:D:906:ATP:O1B	2.51	0.43
2:J:42:LYS:NZ	3:J:804:ATP:O1B	2.51	0.43
2:F:42:LYS:NZ	3:F:905:ATP:O1B	2.51	0.43
2:F:192:ASP:HA	2:F:247:ASN:HB2	2.00	0.43
1:G:177:LEU:HD23	2:H:154:LEU:HD21	2.00	0.43
1:A:177:LEU:HD23	2:B:154:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:HIS:CE1	5:F:906:8M0:O7	2.71	0.43
1:I:158:HIS:CE1	5:J:805:8M0:O7	2.71	0.43
2:J:192:ASP:HA	2:J:247:ASN:HB2	2.00	0.43
2:B:192:ASP:HA	2:B:247:ASN:HB2	2.00	0.43
2:H:192:ASP:HA	2:H:247:ASN:HB2	2.00	0.43
1:K:84:ALA:HA	1:K:87:VAL:HG12	2.00	0.43
1:C:84:ALA:HA	1:C:87:VAL:HG12	2.00	0.43
1:E:177:LEU:HD23	2:F:154:LEU:HD21	2.00	0.43
1:I:177:LEU:HD23	2:J:154:LEU:HD21	2.00	0.43
1:K:158:HIS:CE1	5:L:906:8M0:O7	2.71	0.43
1:C:153:PRO:HB2	1:C:155:TYR:HD1	1.82	0.43
1:C:158:HIS:CE1	5:D:907:8M0:O7	2.71	0.43
1:G:158:HIS:CE1	5:H:806:8M0:O7	2.71	0.43
2:L:129:ALA:HB3	5:L:906:8M0:O23	2.16	0.43
1:A:158:HIS:CE1	5:B:806:8M0:O7	2.71	0.43
2:D:129:ALA:HB3	5:D:907:8M0:O23	2.16	0.43
1:I:159:GLU:OE2	1:I:167:PRO:HD2	2.18	0.43
1:E:159:GLU:OE2	1:E:167:PRO:HD2	2.18	0.42
1:K:153:PRO:HB2	1:K:155:TYR:HD1	1.82	0.42
1:E:153:PRO:HB2	1:E:155:TYR:HD1	1.82	0.42
1:I:153:PRO:HB2	1:I:155:TYR:HD1	1.82	0.42
2:D:192:ASP:HA	2:D:247:ASN:HB2	2.00	0.42
2:J:39:THR:HG23	2:J:184:GLN:HB3	2.02	0.42
2:J:227:GLU:HB2	2:J:230:VAL:HG23	2.02	0.42
2:D:39:THR:HG23	2:D:184:GLN:HB3	2.02	0.42
2:F:39:THR:HG23	2:F:184:GLN:HB3	2.02	0.42
2:F:227:GLU:HB2	2:F:230:VAL:HG23	2.02	0.42
2:L:192:ASP:HA	2:L:247:ASN:HB2	2.00	0.42
2:D:227:GLU:HB2	2:D:230:VAL:HG23	2.02	0.42
2:L:39:THR:HG23	2:L:184:GLN:HB3	2.02	0.42
2:L:227:GLU:HB2	2:L:230:VAL:HG23	2.02	0.42
2:F:194:LEU:HD13	2:F:225:ILE:HG22	2.02	0.42
2:J:194:LEU:HD13	2:J:225:ILE:HG22	2.02	0.42
2:B:227:GLU:HB2	2:B:230:VAL:HG23	2.02	0.42
1:A:100:SER:OG	2:B:179:GLN:NE2	2.53	0.41
2:D:194:LEU:HD13	2:D:225:ILE:HG22	2.02	0.41
1:G:100:SER:OG	2:H:179:GLN:NE2	2.53	0.41
2:H:227:GLU:HB2	2:H:230:VAL:HG23	2.02	0.41
2:L:194:LEU:HD13	2:L:225:ILE:HG22	2.02	0.41
2:F:147:SER:OG	7:F:902:MOO:O3	2.34	0.41
2:B:34:ILE:O	2:F:120:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:LYS:HB3	2:D:34:ILE:O	2.21	0.41
2:D:120:LYS:HB3	2:F:34:ILE:O	2.21	0.41
2:H:34:ILE:O	2:J:120:LYS:HB3	2.21	0.41
2:J:34:ILE:O	2:L:120:LYS:HB3	2.21	0.41
2:J:147:SER:OG	7:J:801:MOO:O3	2.34	0.41
2:H:120:LYS:HB3	2:L:34:ILE:O	2.21	0.41
1:I:85:ARG:NH1	2:J:12:LEU:O	2.43	0.41
1:I:94:LEU:HD13	2:L:117:LEU:HD11	2.03	0.41
2:D:117:LEU:HD11	1:E:94:LEU:HD13	2.03	0.41
2:B:39:THR:HG23	2:B:184:GLN:HB3	2.02	0.41
1:E:100:SER:OG	2:F:179:GLN:NE2	2.53	0.41
2:J:63:ILE:HD13	2:J:74:ILE:HD13	2.03	0.41
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.89	0.41
1:C:100:SER:OG	2:D:179:GLN:NE2	2.54	0.41
2:F:63:ILE:HD13	2:F:74:ILE:HD13	2.03	0.41
2:H:175:LEU:HA	2:H:175:LEU:HD23	1.89	0.41
1:I:100:SER:OG	2:J:179:GLN:NE2	2.53	0.41
1:K:100:SER:OG	2:L:179:GLN:NE2	2.54	0.41
1:E:85:ARG:NH1	2:F:12:LEU:O	2.43	0.40
2:H:39:THR:HG23	2:H:184:GLN:HB3	2.02	0.40
1:A:94:LEU:HD13	2:F:117:LEU:HD11	2.03	0.40
1:G:94:LEU:HD13	2:J:117:LEU:HD11	2.03	0.40
2:B:194:LEU:HD13	2:B:225:ILE:HG22	2.02	0.40
2:H:194:LEU:HD13	2:H:225:ILE:HG22	2.02	0.40
2:D:57:TYR:HE1	2:D:117:LEU:HD22	1.86	0.40
2:H:63:ILE:HD13	2:H:74:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	252/276 (91%)	244 (97%)	8 (3%)	0	100	100
1	C	270/276 (98%)	261 (97%)	9 (3%)	0	100	100
1	E	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	G	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	I	270/276 (98%)	262 (97%)	8 (3%)	0	100	100
1	K	270/276 (98%)	261 (97%)	9 (3%)	0	100	100
2	B	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	D	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	F	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	H	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	J	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
2	L	269/270 (100%)	261 (97%)	8 (3%)	0	100	100
All	All	3216/3276 (98%)	3118 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	212/216 (98%)	212 (100%)	0	100	100
1	C	212/216 (98%)	212 (100%)	0	100	100
1	E	212/216 (98%)	212 (100%)	0	100	100
1	G	212/216 (98%)	212 (100%)	0	100	100
1	I	212/216 (98%)	212 (100%)	0	100	100
1	K	212/216 (98%)	212 (100%)	0	100	100
2	B	208/206 (101%)	207 (100%)	1 (0%)	81	85
2	D	208/206 (101%)	207 (100%)	1 (0%)	81	85
2	F	208/206 (101%)	207 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	208/206 (101%)	207 (100%)	1 (0%)	81	85
2	J	208/206 (101%)	207 (100%)	1 (0%)	81	85
2	L	208/206 (101%)	207 (100%)	1 (0%)	81	85
All	All	2520/2532 (100%)	2514 (100%)	6 (0%)	85	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	153	LYS
2	D	153	LYS
2	F	153	LYS
2	H	153	LYS
2	J	153	LYS
2	L	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	72	HIS
1	A	86	HIS
1	A	111	GLN
2	B	121	HIS
2	B	142	ASN
2	B	179	GLN
1	C	21	GLN
1	C	72	HIS
1	C	86	HIS
1	C	111	GLN
2	D	121	HIS
2	D	142	ASN
2	D	179	GLN
1	E	21	GLN
1	E	72	HIS
1	E	86	HIS
1	E	111	GLN
2	F	101	GLN
2	F	121	HIS
2	F	142	ASN
2	F	179	GLN

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Mol	Chain	Res	Type
1	G	21	GLN
1	G	72	HIS
1	G	86	HIS
1	G	111	GLN
2	H	121	HIS
2	H	142	ASN
2	H	179	GLN
1	I	21	GLN
1	I	72	HIS
1	I	86	HIS
1	I	111	GLN
1	I	246	GLN
2	J	121	HIS
2	J	142	ASN
2	J	179	GLN
1	K	21	GLN
1	K	72	HIS
1	K	86	HIS
1	K	111	GLN
2	L	121	HIS
2	L	142	ASN
2	L	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 6 are monoatomic - leaving 84 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	$\# Z > 2$
7	MOO	H	804	-	2,4,4	2.00	1 (50%)	-		
8	OMO	A	307	-	0,3,3	-	-	-		
6	J8E	D	901	-	0,14,14	-	-	-		
8	OMO	I	301	-	0,3,3	-	-	-		
8	OMO	E	301	-	0,3,3	-	-	-		
7	MOO	D	902	-	2,4,4	2.01	1 (50%)	-		
3	ATP	J	804	7	32,33,33	0.52	0	48,52,52	0.69	0
3	ATP	C	301	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
7	MOO	H	802	-	2,4,4	2.01	1 (50%)	-		
7	MOO	L	902	-	2,4,4	2.01	1 (50%)	-		
5	8M0	C	303	-	21,46,48	2.06	5 (23%)	-		
7	MOO	D	904	-	2,4,4	1.99	1 (50%)	-		
6	J8E	L	901	-	0,14,14	-	-	-		
3	ATP	F	905	7	32,33,33	0.52	0	48,52,52	0.69	0
5	8M0	J	805	-	34,48,48	2.48	10 (29%)	-		
7	MOO	L	907	3	2,4,4	2.01	1 (50%)	-		
7	MOO	F	904	-	2,4,4	2.01	1 (50%)	-		
7	MOO	B	803	-	2,4,4	2.02	1 (50%)	-		
5	8M0	L	906	-	34,48,48	2.49	10 (29%)	-		
7	MOO	H	801	-	2,4,4	2.01	1 (50%)	-		
7	MOO	F	907	3	2,4,4	2.01	1 (50%)	-		
5	8M0	G	303	-	21,46,48	2.06	5 (23%)	-		
7	MOO	B	801	-	2,4,4	2.01	1 (50%)	-		
5	8M0	F	906	-	34,48,48	2.48	10 (29%)	-		
7	MOO	A	306	-	2,4,4	2.01	1 (50%)	-		
6	J8E	E	305	-	0,14,14	-	-	-		
7	MOO	J	802	-	2,4,4	2.01	1 (50%)	-		
6	J8E	G	304	-	0,14,14	-	-	-		
7	MOO	G	307	-	2,4,4	1.99	1 (50%)	-		
7	MOO	I	307	-	2,4,4	2.01	1 (50%)	-		
6	J8E	J	807	-	0,14,14	-	-	-		
7	MOO	B	807	3	2,4,4	2.00	1 (50%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	8M0	A	303	-	21,46,48	2.06	5 (23%)	-		
7	MOO	L	903	-	2,4,4	2.00	1 (50%)	-		
7	MOO	E	306	-	2,4,4	2.00	1 (50%)	-		
5	8M0	H	806	-	34,48,48	2.49	10 (29%)	-		
7	MOO	G	306	-	2,4,4	2.01	1 (50%)	-		
7	MOO	I	306	-	2,4,4	2.00	1 (50%)	-		
7	MOO	H	807	3	2,4,4	2.00	1 (50%)	-		
7	MOO	H	803	-	2,4,4	2.02	1 (50%)	-		
7	MOO	J	801	-	2,4,4	2.02	1 (50%)	-		
7	MOO	G	305	-	2,4,4	2.00	1 (50%)	-		
6	J8E	H	808	-	0,14,14	-	-	-		
3	ATP	D	906	7	32,33,33	0.52	0	48,52,52	0.69	0
6	J8E	B	808	-	0,14,14	-	-	-		
7	MOO	J	806	3	2,4,4	2.01	1 (50%)	-		
7	MOO	A	305	-	2,4,4	2.00	1 (50%)	-		
6	J8E	A	304	-	0,14,14	-	-	-		
5	8M0	D	907	-	34,48,48	2.49	10 (29%)	-		
7	MOO	E	307	-	2,4,4	2.01	1 (50%)	-		
6	J8E	I	305	-	0,14,14	-	-	-		
7	MOO	C	305	-	2,4,4	2.00	1 (50%)	-		
3	ATP	I	302	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
5	8M0	E	304	-	21,46,48	2.06	5 (23%)	-		
3	ATP	B	805	7	32,33,33	0.52	0	48,52,52	0.69	0
6	J8E	F	901	-	0,14,14	-	-	-		
6	J8E	C	304	-	0,14,14	-	-	-		
8	OMO	C	307	-	0,3,3	-	-	-		
5	8M0	K	304	-	21,46,48	2.06	5 (23%)	-		
3	ATP	K	302	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
6	J8E	K	305	-	0,14,14	-	-	-		
7	MOO	I	308	-	2,4,4	1.99	1 (50%)	-		
7	MOO	D	908	3	2,4,4	2.01	1 (50%)	-		
3	ATP	L	905	7	32,33,33	0.52	0	48,52,52	0.69	0
7	MOO	L	904	-	2,4,4	2.00	1 (50%)	-		
8	OMO	K	301	-	0,3,3	-	-	-		
3	ATP	E	302	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
3	ATP	H	805	7	32,33,33	0.52	0	48,52,52	0.69	0
7	MOO	D	905	-	2,4,4	2.00	1 (50%)	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	8M0	B	806	-	34,48,48	2.49	10 (29%)	-		
7	MOO	K	306	-	2,4,4	2.00	1 (50%)	-		
7	MOO	F	903	-	2,4,4	2.01	1 (50%)	-		
7	MOO	B	804	-	2,4,4	2.00	1 (50%)	-		
7	MOO	A	308	-	2,4,4	1.99	1 (50%)	-		
3	ATP	A	301	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
7	MOO	C	306	-	2,4,4	2.00	1 (50%)	-		
5	8M0	I	304	-	21,46,48	2.06	5 (23%)	-		
7	MOO	F	902	-	2,4,4	2.02	1 (50%)	-		
7	MOO	D	903	-	2,4,4	2.00	1 (50%)	-		
7	MOO	K	307	-	2,4,4	2.00	1 (50%)	-		
8	OMO	G	308	-	0,3,3	-	-	-		
3	ATP	G	301	4	32,33,33	1.34	4 (12%)	48,52,52	1.92	11 (22%)
7	MOO	B	802	-	2,4,4	2.01	1 (50%)	-		
7	MOO	J	803	-	2,4,4	2.01	1 (50%)	-		

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
3	ATP	E	302	4	-	3/22/38/38	0/3/3/3
3	ATP	H	805	7	-	3/22/38/38	0/3/3/3
6	J8E	A	304	-	-	-	0/1/1/1
6	J8E	D	901	-	-	-	0/1/1/1
6	J8E	E	305	-	-	-	0/1/1/1
6	J8E	G	304	-	-	-	0/1/1/1
6	J8E	I	305	-	-	-	0/1/1/1
6	J8E	J	807	-	-	-	0/1/1/1
3	ATP	I	302	4	-	3/22/38/38	0/3/3/3
3	ATP	B	805	7	-	3/22/38/38	0/3/3/3
6	J8E	F	901	-	-	-	0/1/1/1
6	J8E	C	304	-	-	-	0/1/1/1
3	ATP	A	301	4	-	3/22/38/38	0/3/3/3
3	ATP	J	804	7	-	3/22/38/38	0/3/3/3
3	ATP	C	301	4	-	3/22/38/38	0/3/3/3
3	ATP	K	302	4	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	J8E	K	305	-	-	-	0/1/1/1
6	J8E	L	901	-	-	-	0/1/1/1
3	ATP	F	905	7	-	3/22/38/38	0/3/3/3
6	J8E	H	808	-	-	-	0/1/1/1
3	ATP	D	906	7	-	3/22/38/38	0/3/3/3
3	ATP	L	905	7	-	3/22/38/38	0/3/3/3
3	ATP	G	301	4	-	3/22/38/38	0/3/3/3
6	J8E	B	808	-	-	-	0/1/1/1

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	906	8M0	O23-MO7	7.80	1.88	1.71
5	J	805	8M0	O23-MO7	7.80	1.88	1.71
5	D	907	8M0	O23-MO7	7.80	1.88	1.71
5	L	906	8M0	O23-MO7	7.80	1.88	1.71
5	B	806	8M0	O23-MO7	7.80	1.88	1.71
5	H	806	8M0	O23-MO7	7.80	1.88	1.71
5	F	906	8M0	O1-MO1	7.02	1.86	1.71
5	J	805	8M0	O1-MO1	7.02	1.86	1.71
5	D	907	8M0	O1-MO1	7.02	1.86	1.71
5	L	906	8M0	O1-MO1	7.02	1.86	1.71
5	B	806	8M0	O1-MO1	7.02	1.86	1.71
5	H	806	8M0	O1-MO1	7.02	1.86	1.71
5	E	304	8M0	O18-MO6	4.86	1.81	1.71
5	I	304	8M0	O18-MO6	4.86	1.81	1.71
5	C	303	8M0	O18-MO6	4.85	1.81	1.71
5	K	304	8M0	O18-MO6	4.85	1.81	1.71
5	A	303	8M0	O18-MO6	4.84	1.81	1.71
5	G	303	8M0	O18-MO6	4.84	1.81	1.71
5	A	303	8M0	O23-MO7	4.72	1.81	1.71
5	G	303	8M0	O23-MO7	4.72	1.81	1.71
5	E	304	8M0	O23-MO7	4.71	1.81	1.71
5	I	304	8M0	O23-MO7	4.71	1.81	1.71
5	C	303	8M0	O23-MO7	4.71	1.81	1.71
5	K	304	8M0	O23-MO7	4.71	1.81	1.71
5	B	806	8M0	O18-MO6	4.34	1.80	1.71
5	H	806	8M0	O18-MO6	4.34	1.80	1.71
5	D	907	8M0	O18-MO6	4.33	1.80	1.71
5	L	906	8M0	O18-MO6	4.33	1.80	1.71
5	F	906	8M0	O18-MO6	4.30	1.80	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	805	8M0	O18-MO6	4.30	1.80	1.71
3	E	302	ATP	C5-C4	4.21	1.46	1.39
3	I	302	ATP	C5-C4	4.21	1.46	1.39
3	A	301	ATP	C5-C4	4.21	1.46	1.39
3	G	301	ATP	C5-C4	4.21	1.46	1.39
3	C	301	ATP	C5-C4	4.20	1.46	1.39
3	K	302	ATP	C5-C4	4.20	1.46	1.39
5	A	303	8M0	O20-MO6	4.11	2.28	1.89
5	G	303	8M0	O20-MO6	4.11	2.28	1.89
5	C	303	8M0	O20-MO6	4.11	2.28	1.89
5	E	304	8M0	O20-MO6	4.11	2.28	1.89
5	I	304	8M0	O20-MO6	4.11	2.28	1.89
5	K	304	8M0	O20-MO6	4.11	2.28	1.89
5	D	907	8M0	O27-MO3	-3.99	1.76	2.34
5	L	906	8M0	O27-MO3	-3.99	1.76	2.34
5	F	906	8M0	O27-MO3	-3.99	1.76	2.34
5	J	805	8M0	O27-MO3	-3.99	1.76	2.34
5	B	806	8M0	O27-MO3	-3.99	1.76	2.34
5	H	806	8M0	O27-MO3	-3.99	1.76	2.34
5	D	907	8M0	O20-MO6	3.35	2.21	1.89
5	L	906	8M0	O20-MO6	3.35	2.21	1.89
5	B	806	8M0	O20-MO6	3.35	2.21	1.89
5	H	806	8M0	O20-MO6	3.35	2.21	1.89
5	F	906	8M0	O20-MO6	3.35	2.21	1.89
5	J	805	8M0	O20-MO6	3.35	2.21	1.89
5	D	907	8M0	O7-MO2	2.93	2.17	1.89
5	L	906	8M0	O7-MO2	2.93	2.17	1.89
5	F	906	8M0	O7-MO2	2.93	2.17	1.89
5	J	805	8M0	O7-MO2	2.93	2.17	1.89
5	B	806	8M0	O7-MO2	2.93	2.17	1.89
5	H	806	8M0	O7-MO2	2.93	2.17	1.89
5	C	303	8M0	O7-MO2	2.63	2.14	1.89
5	K	304	8M0	O7-MO2	2.63	2.14	1.89
5	A	303	8M0	O7-MO2	2.63	2.14	1.89
5	G	303	8M0	O7-MO2	2.63	2.14	1.89
5	F	906	8M0	O3-MO3	2.63	2.02	1.93
5	J	805	8M0	O3-MO3	2.63	2.02	1.93
5	E	304	8M0	O7-MO2	2.63	2.14	1.89
5	I	304	8M0	O7-MO2	2.63	2.14	1.89
5	B	806	8M0	O3-MO3	2.63	2.02	1.93
5	H	806	8M0	O3-MO3	2.63	2.02	1.93
5	D	907	8M0	O3-MO3	2.63	2.02	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	906	8M0	O3-MO3	2.63	2.02	1.93
5	F	906	8M0	O15-MO5	-2.60	1.96	2.34
5	J	805	8M0	O15-MO5	-2.60	1.96	2.34
5	D	907	8M0	O15-MO5	-2.60	1.96	2.34
5	L	906	8M0	O15-MO5	-2.60	1.96	2.34
5	B	806	8M0	O15-MO5	-2.60	1.96	2.34
5	H	806	8M0	O15-MO5	-2.60	1.96	2.34
5	B	806	8M0	O26-MO6	-2.57	1.99	2.24
5	H	806	8M0	O26-MO6	-2.57	1.99	2.24
5	F	906	8M0	O26-MO6	-2.57	1.99	2.24
5	J	805	8M0	O26-MO6	-2.57	1.99	2.24
5	D	907	8M0	O26-MO6	-2.57	1.99	2.24
5	L	906	8M0	O26-MO6	-2.57	1.99	2.24
7	F	902	MOO	O1-MO	-2.47	1.69	1.75
7	J	801	MOO	O1-MO	-2.47	1.69	1.75
7	E	307	MOO	O1-MO	-2.47	1.69	1.75
7	I	307	MOO	O1-MO	-2.47	1.69	1.75
7	C	306	MOO	O1-MO	-2.46	1.69	1.75
7	K	307	MOO	O1-MO	-2.46	1.69	1.75
7	A	306	MOO	O1-MO	-2.46	1.69	1.75
7	G	306	MOO	O1-MO	-2.46	1.69	1.75
7	B	802	MOO	O1-MO	-2.46	1.69	1.75
7	H	802	MOO	O1-MO	-2.46	1.69	1.75
7	B	803	MOO	O1-MO	-2.46	1.69	1.75
7	H	803	MOO	O1-MO	-2.46	1.69	1.75
7	B	807	MOO	O1-MO	-2.46	1.69	1.75
7	H	807	MOO	O1-MO	-2.46	1.69	1.75
7	D	902	MOO	O1-MO	-2.45	1.69	1.75
7	L	902	MOO	O1-MO	-2.45	1.69	1.75
7	D	908	MOO	O1-MO	-2.45	1.69	1.75
7	L	907	MOO	O1-MO	-2.45	1.69	1.75
7	A	305	MOO	O1-MO	-2.45	1.69	1.75
7	F	907	MOO	O1-MO	-2.45	1.69	1.75
7	G	305	MOO	O1-MO	-2.45	1.69	1.75
7	J	806	MOO	O1-MO	-2.45	1.69	1.75
7	E	306	MOO	O1-MO	-2.44	1.69	1.75
7	I	306	MOO	O1-MO	-2.44	1.69	1.75
7	B	801	MOO	O1-MO	-2.44	1.69	1.75
7	H	801	MOO	O1-MO	-2.44	1.69	1.75
7	F	904	MOO	O1-MO	-2.44	1.69	1.75
7	J	803	MOO	O1-MO	-2.44	1.69	1.75
7	C	305	MOO	O1-MO	-2.44	1.69	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	306	MOO	O1-MO	-2.44	1.69	1.75
7	D	903	MOO	O1-MO	-2.44	1.69	1.75
7	L	903	MOO	O1-MO	-2.44	1.69	1.75
7	F	903	MOO	O1-MO	-2.44	1.69	1.75
7	J	802	MOO	O1-MO	-2.44	1.69	1.75
7	D	904	MOO	O1-MO	-2.43	1.69	1.75
7	I	308	MOO	O1-MO	-2.43	1.69	1.75
7	D	905	MOO	O1-MO	-2.43	1.70	1.75
7	L	904	MOO	O1-MO	-2.43	1.70	1.75
7	B	804	MOO	O1-MO	-2.43	1.70	1.75
7	H	804	MOO	O1-MO	-2.43	1.70	1.75
7	A	308	MOO	O1-MO	-2.42	1.70	1.75
7	G	307	MOO	O1-MO	-2.42	1.70	1.75
3	A	301	ATP	C5-C6	2.33	1.47	1.41
3	G	301	ATP	C5-C6	2.33	1.47	1.41
3	C	301	ATP	C5-C6	2.33	1.47	1.41
3	K	302	ATP	C5-C6	2.33	1.47	1.41
3	E	302	ATP	C5-C6	2.33	1.47	1.41
3	I	302	ATP	C5-C6	2.33	1.47	1.41
5	B	806	8M0	O25-MO2	-2.18	2.02	2.24
5	H	806	8M0	O25-MO2	-2.18	2.02	2.24
5	F	906	8M0	O25-MO2	-2.18	2.02	2.24
5	J	805	8M0	O25-MO2	-2.18	2.02	2.24
5	D	907	8M0	O25-MO2	-2.18	2.02	2.24
5	L	906	8M0	O25-MO2	-2.18	2.02	2.24
3	A	301	ATP	PG-O3G	-2.18	1.46	1.54
3	G	301	ATP	PG-O3G	-2.18	1.46	1.54
3	C	301	ATP	PG-O3G	-2.17	1.46	1.54
3	K	302	ATP	PG-O3G	-2.17	1.46	1.54
3	E	302	ATP	PG-O3G	-2.16	1.46	1.54
3	I	302	ATP	PG-O3G	-2.16	1.46	1.54
3	A	301	ATP	C2-N3	2.16	1.37	1.33
3	G	301	ATP	C2-N3	2.16	1.37	1.33
3	C	301	ATP	C2-N3	2.12	1.37	1.33
3	K	302	ATP	C2-N3	2.12	1.37	1.33
3	E	302	ATP	C2-N3	2.12	1.37	1.33
3	I	302	ATP	C2-N3	2.12	1.37	1.33
5	E	304	8M0	O3-MO3	2.04	1.94	1.86
5	I	304	8M0	O3-MO3	2.04	1.94	1.86
5	A	303	8M0	O3-MO3	2.03	1.94	1.86
5	G	303	8M0	O3-MO3	2.03	1.94	1.86
5	C	303	8M0	O3-MO3	2.03	1.94	1.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	304	8M0	O3-MO3	2.03	1.94	1.86

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	ATP	N3-C2-N1	-5.06	120.92	128.58
3	K	302	ATP	N3-C2-N1	-5.06	120.92	128.58
3	E	302	ATP	N3-C2-N1	-5.06	120.93	128.58
3	I	302	ATP	N3-C2-N1	-5.06	120.93	128.58
3	A	301	ATP	N3-C2-N1	-5.05	120.94	128.58
3	G	301	ATP	N3-C2-N1	-5.05	120.94	128.58
3	A	301	ATP	C4-N9-C8	4.48	110.44	105.74
3	G	301	ATP	C4-N9-C8	4.48	110.44	105.74
3	C	301	ATP	C4-N9-C8	4.47	110.43	105.74
3	K	302	ATP	C4-N9-C8	4.47	110.43	105.74
3	E	302	ATP	C4-N9-C8	4.46	110.42	105.74
3	I	302	ATP	C4-N9-C8	4.46	110.42	105.74
3	C	301	ATP	N3-C4-N9	4.05	134.06	127.17
3	K	302	ATP	N3-C4-N9	4.05	134.06	127.17
3	E	302	ATP	N3-C4-N9	4.04	134.04	127.17
3	I	302	ATP	N3-C4-N9	4.04	134.04	127.17
3	A	301	ATP	N3-C4-N9	4.03	134.02	127.17
3	G	301	ATP	N3-C4-N9	4.03	134.02	127.17
3	E	302	ATP	O4'-C1'-N9	3.49	114.80	108.09
3	I	302	ATP	O4'-C1'-N9	3.49	114.80	108.09
3	C	301	ATP	C5-C4-N3	-3.49	121.91	126.72
3	K	302	ATP	C5-C4-N3	-3.49	121.91	126.72
3	A	301	ATP	O4'-C1'-N9	3.49	114.79	108.09
3	G	301	ATP	O4'-C1'-N9	3.49	114.79	108.09
3	E	302	ATP	C5-C4-N3	-3.48	121.92	126.72
3	I	302	ATP	C5-C4-N3	-3.48	121.92	126.72
3	C	301	ATP	O4'-C1'-N9	3.47	114.75	108.09
3	K	302	ATP	O4'-C1'-N9	3.47	114.75	108.09
3	A	301	ATP	C5-C4-N3	-3.47	121.94	126.72
3	G	301	ATP	C5-C4-N3	-3.47	121.94	126.72
3	A	301	ATP	C2-N1-C6	3.22	124.02	118.73
3	G	301	ATP	C2-N1-C6	3.22	124.02	118.73
3	C	301	ATP	C2-N1-C6	3.20	123.99	118.73
3	K	302	ATP	C2-N1-C6	3.20	123.99	118.73
3	E	302	ATP	C2-N1-C6	3.20	123.98	118.73
3	I	302	ATP	C2-N1-C6	3.20	123.98	118.73
3	C	301	ATP	C2-N3-C4	3.09	119.38	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	302	ATP	C2-N3-C4	3.09	119.38	111.83
3	E	302	ATP	C2-N3-C4	3.09	119.37	111.83
3	I	302	ATP	C2-N3-C4	3.09	119.37	111.83
3	A	301	ATP	C2-N3-C4	3.07	119.32	111.83
3	G	301	ATP	C2-N3-C4	3.07	119.32	111.83
3	C	301	ATP	O3A-PB-O1B	-2.87	102.07	110.70
3	K	302	ATP	O3A-PB-O1B	-2.87	102.07	110.70
3	A	301	ATP	O3A-PB-O1B	-2.87	102.08	110.70
3	G	301	ATP	O3A-PB-O1B	-2.87	102.08	110.70
3	E	302	ATP	O3A-PB-O1B	-2.86	102.10	110.70
3	I	302	ATP	O3A-PB-O1B	-2.86	102.10	110.70
3	A	301	ATP	N9-C8-N7	-2.35	110.60	113.94
3	G	301	ATP	N9-C8-N7	-2.35	110.60	113.94
3	E	302	ATP	N9-C8-N7	-2.34	110.61	113.94
3	I	302	ATP	N9-C8-N7	-2.34	110.61	113.94
3	C	301	ATP	N9-C8-N7	-2.34	110.62	113.94
3	K	302	ATP	N9-C8-N7	-2.34	110.62	113.94
3	C	301	ATP	O5'-C5'-C4'	-2.31	101.13	108.99
3	K	302	ATP	O5'-C5'-C4'	-2.31	101.13	108.99
3	E	302	ATP	O5'-C5'-C4'	-2.30	101.15	108.99
3	I	302	ATP	O5'-C5'-C4'	-2.30	101.15	108.99
3	A	301	ATP	O5'-C5'-C4'	-2.30	101.16	108.99
3	G	301	ATP	O5'-C5'-C4'	-2.30	101.16	108.99
3	C	301	ATP	C4'-O4'-C1'	-2.19	104.64	109.47
3	K	302	ATP	C4'-O4'-C1'	-2.19	104.64	109.47
3	E	302	ATP	C4'-O4'-C1'	-2.18	104.64	109.47
3	I	302	ATP	C4'-O4'-C1'	-2.18	104.64	109.47
3	A	301	ATP	C4'-O4'-C1'	-2.17	104.66	109.47
3	G	301	ATP	C4'-O4'-C1'	-2.17	104.66	109.47

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	805	ATP	C2'-C1'-N9-C4
3	D	906	ATP	C2'-C1'-N9-C4
3	F	905	ATP	C2'-C1'-N9-C4
3	H	805	ATP	C2'-C1'-N9-C4
3	J	804	ATP	C2'-C1'-N9-C4
3	L	905	ATP	C2'-C1'-N9-C4
3	B	805	ATP	C2'-C1'-N9-C8
3	D	906	ATP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	F	905	ATP	C2'-C1'-N9-C8
3	H	805	ATP	C2'-C1'-N9-C8
3	J	804	ATP	C2'-C1'-N9-C8
3	L	905	ATP	C2'-C1'-N9-C8
3	B	805	ATP	C4'-C5'-O5'-PA
3	D	906	ATP	C4'-C5'-O5'-PA
3	F	905	ATP	C4'-C5'-O5'-PA
3	H	805	ATP	C4'-C5'-O5'-PA
3	J	804	ATP	C4'-C5'-O5'-PA
3	L	905	ATP	C4'-C5'-O5'-PA
3	A	301	ATP	O4'-C1'-N9-C8
3	C	301	ATP	O4'-C1'-N9-C8
3	E	302	ATP	O4'-C1'-N9-C8
3	G	301	ATP	O4'-C1'-N9-C8
3	I	302	ATP	O4'-C1'-N9-C8
3	K	302	ATP	O4'-C1'-N9-C8
3	A	301	ATP	PG-O3B-PB-O1B
3	C	301	ATP	PG-O3B-PB-O1B
3	E	302	ATP	PG-O3B-PB-O1B
3	G	301	ATP	PG-O3B-PB-O1B
3	I	302	ATP	PG-O3B-PB-O1B
3	K	302	ATP	PG-O3B-PB-O1B
3	A	301	ATP	C2'-C1'-N9-C8
3	C	301	ATP	C2'-C1'-N9-C8
3	E	302	ATP	C2'-C1'-N9-C8
3	G	301	ATP	C2'-C1'-N9-C8
3	I	302	ATP	C2'-C1'-N9-C8
3	K	302	ATP	C2'-C1'-N9-C8

There are no ring outliers.

78 monomers are involved in 449 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	804	MOO	7	0
8	A	307	OMO	5	0
8	I	301	OMO	5	0
8	E	301	OMO	5	0
7	D	902	MOO	8	0
3	J	804	ATP	8	0
3	C	301	ATP	5	0
7	H	802	MOO	3	0
7	L	902	MOO	7	0

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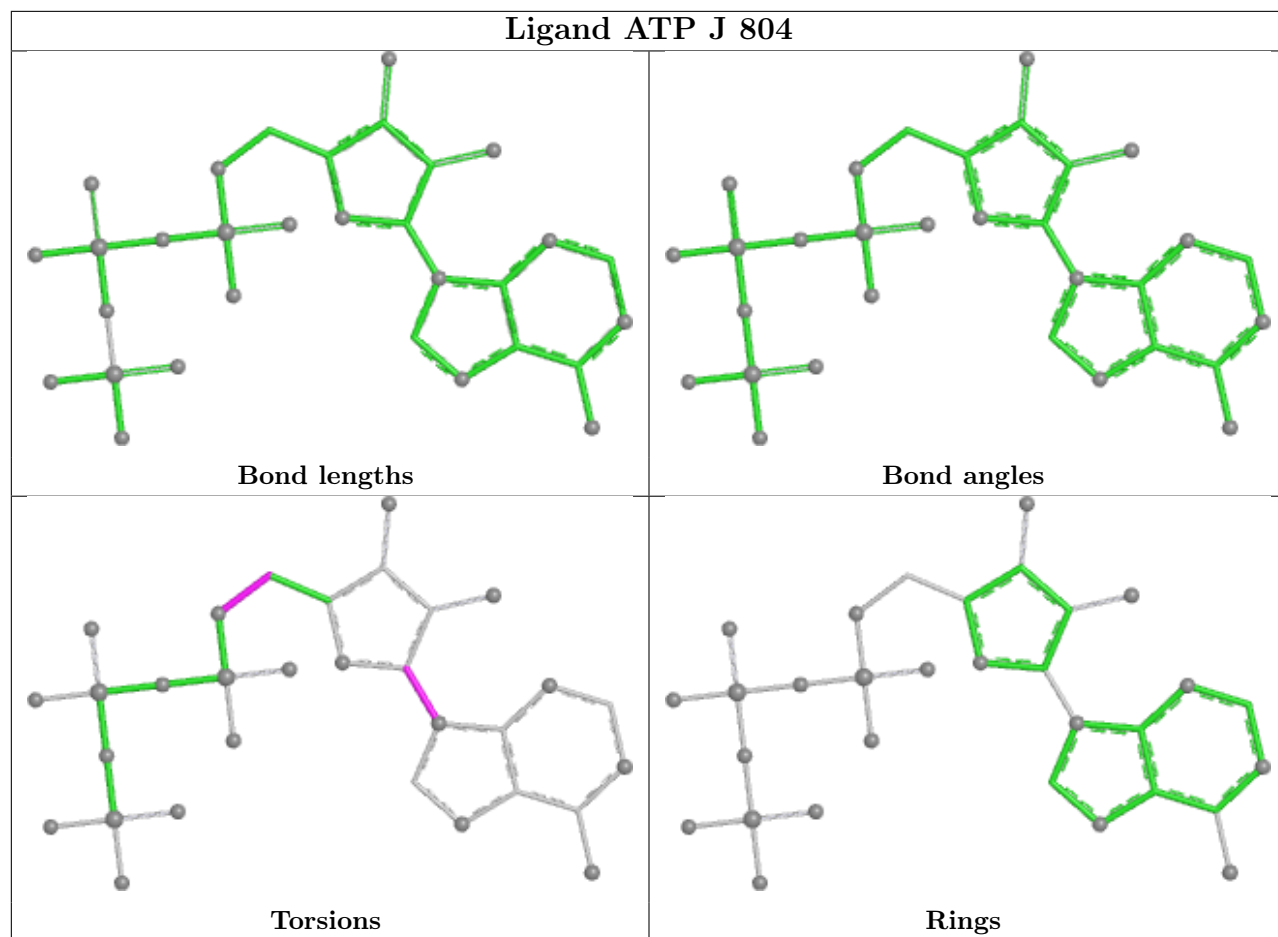
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	303	8M0	1	0
7	D	904	MOO	9	0
3	F	905	ATP	8	0
5	J	805	8M0	8	0
7	L	907	MOO	9	0
7	F	904	MOO	7	0
7	B	803	MOO	9	0
5	L	906	8M0	8	0
7	H	801	MOO	7	0
7	F	907	MOO	9	0
5	G	303	8M0	1	0
7	B	801	MOO	7	0
5	F	906	8M0	8	0
7	A	306	MOO	8	0
6	E	305	J8E	3	0
7	J	802	MOO	3	0
6	G	304	J8E	3	0
7	G	307	MOO	9	0
7	I	307	MOO	8	0
7	B	807	MOO	9	0
5	A	303	8M0	1	0
7	L	903	MOO	3	0
7	E	306	MOO	11	0
5	H	806	8M0	8	0
7	G	306	MOO	8	0
7	I	306	MOO	11	0
7	H	807	MOO	9	0
7	H	803	MOO	9	0
7	J	801	MOO	8	0
7	G	305	MOO	11	0
3	D	906	ATP	8	0
7	J	806	MOO	9	0
7	A	305	MOO	11	0
6	A	304	J8E	3	0
5	D	907	8M0	8	0
7	E	307	MOO	8	0
6	I	305	J8E	3	0
7	C	305	MOO	11	0
3	I	302	ATP	5	0
5	E	304	8M0	2	0
3	B	805	ATP	8	0
6	C	304	J8E	3	0

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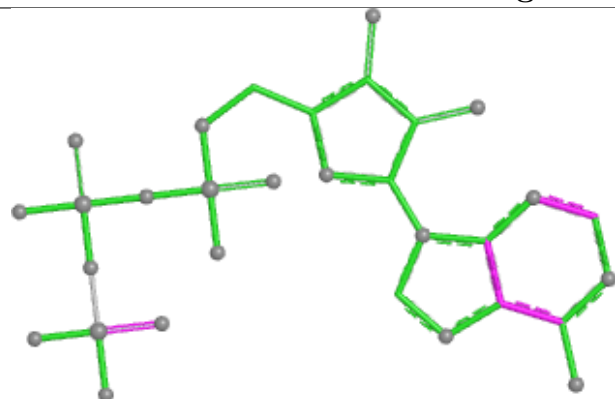
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	307	OMO	5	0
5	K	304	8M0	1	0
3	K	302	ATP	5	0
6	K	305	J8E	3	0
7	I	308	MOO	9	0
7	D	908	MOO	9	0
3	L	905	ATP	8	0
7	L	904	MOO	7	0
8	K	301	OMO	5	0
3	E	302	ATP	5	0
3	H	805	ATP	8	0
7	D	905	MOO	7	0
5	B	806	8M0	8	0
7	K	306	MOO	11	0
7	F	903	MOO	3	0
7	B	804	MOO	7	0
7	A	308	MOO	9	0
3	A	301	ATP	5	0
7	C	306	MOO	8	0
5	I	304	8M0	2	0
7	F	902	MOO	8	0
7	D	903	MOO	3	0
7	K	307	MOO	8	0
8	G	308	OMO	5	0
3	G	301	ATP	5	0
7	B	802	MOO	3	0
7	J	803	MOO	7	0

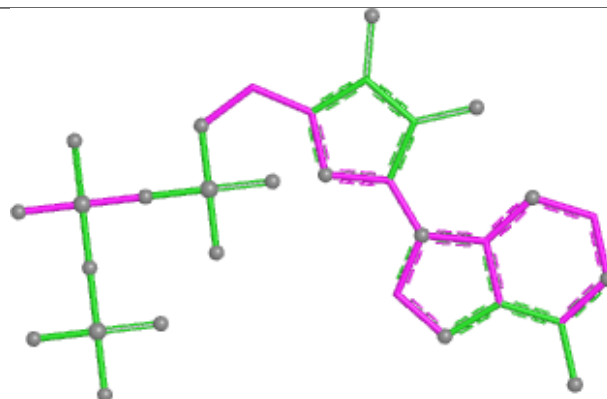
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



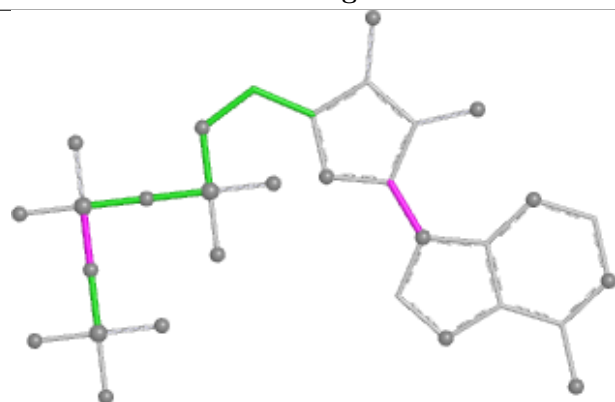
Ligand ATP C 301



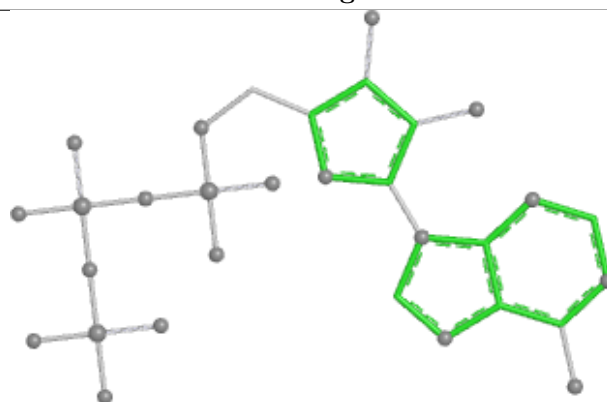
Bond lengths



Bond angles

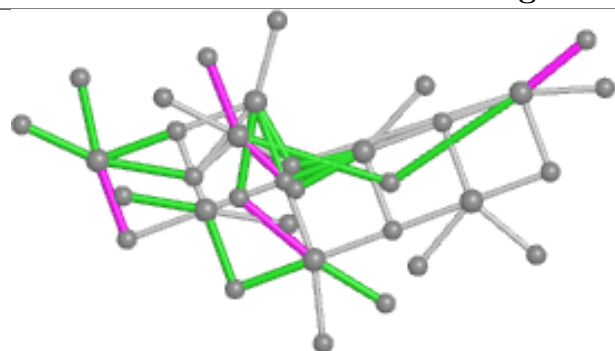


Torsions

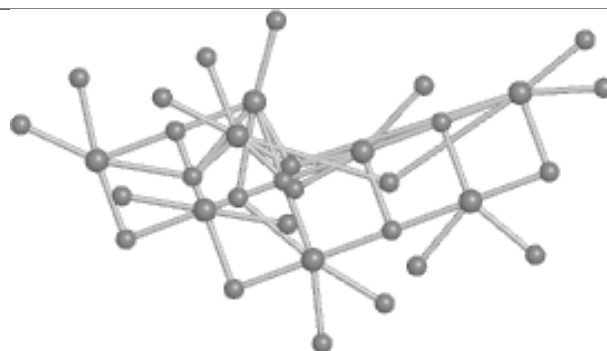


Rings

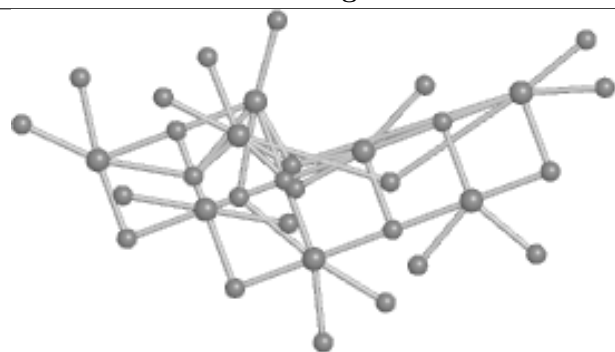
Ligand 8M0 C 303



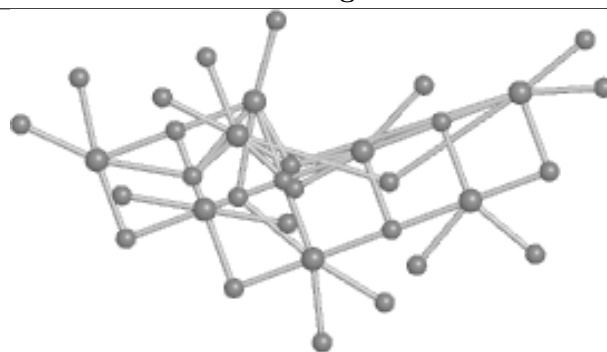
Bond lengths



Bond angles

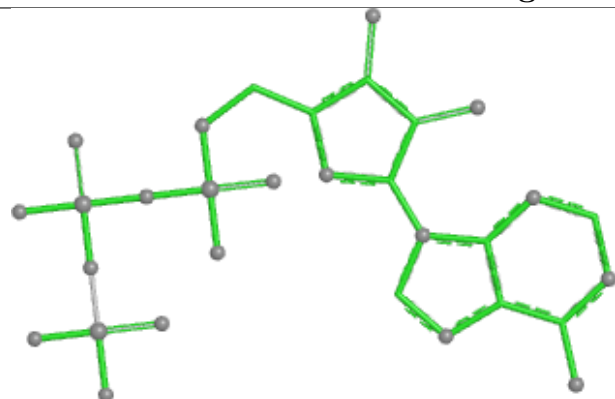


Torsions

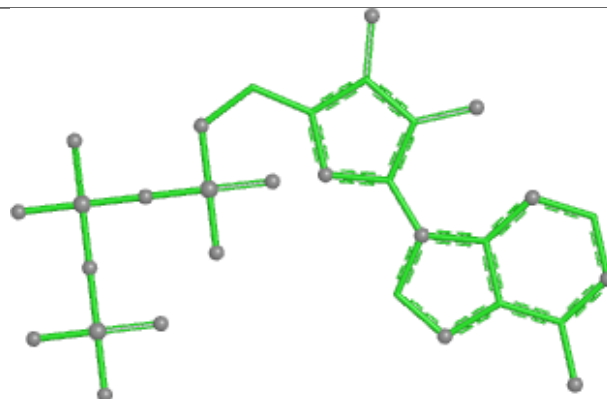


Rings

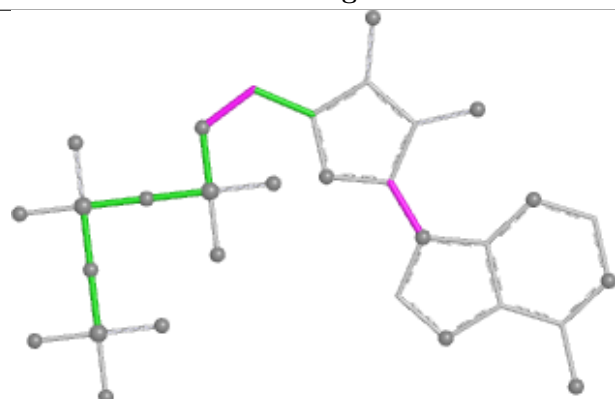
Ligand ATP F 905



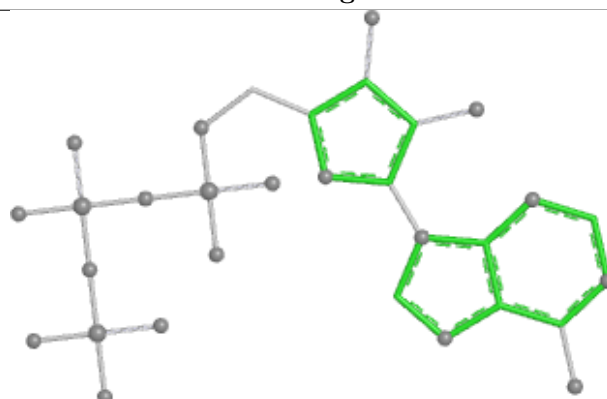
Bond lengths



Bond angles

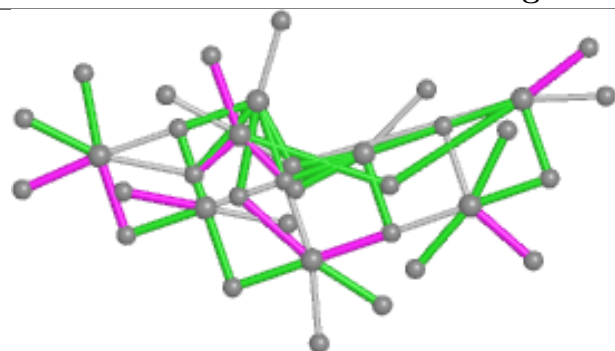


Torsions

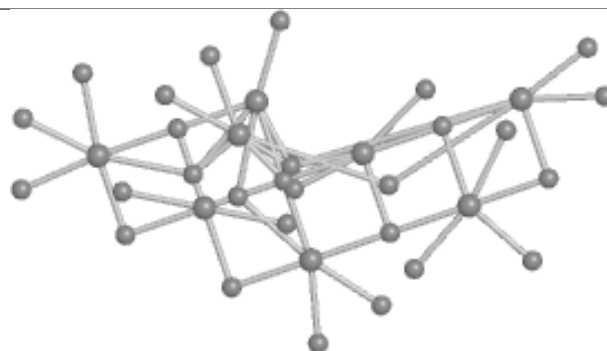


Rings

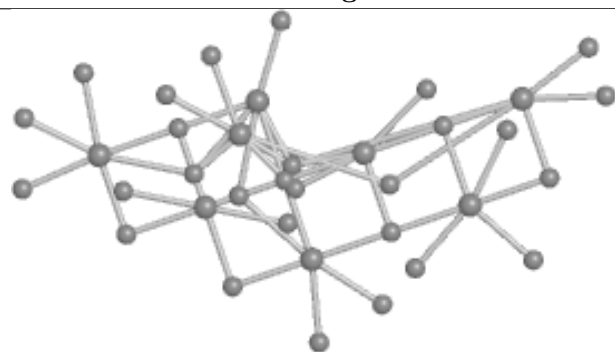
Ligand 8M0 J 805



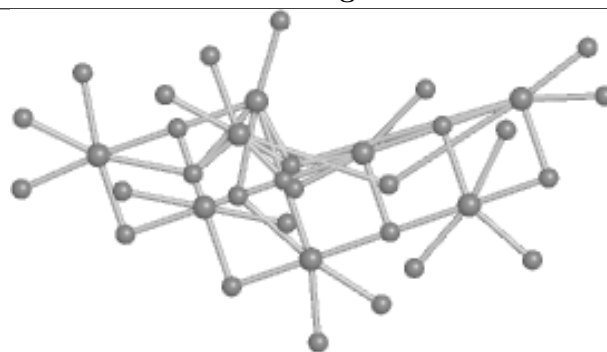
Bond lengths



Bond angles

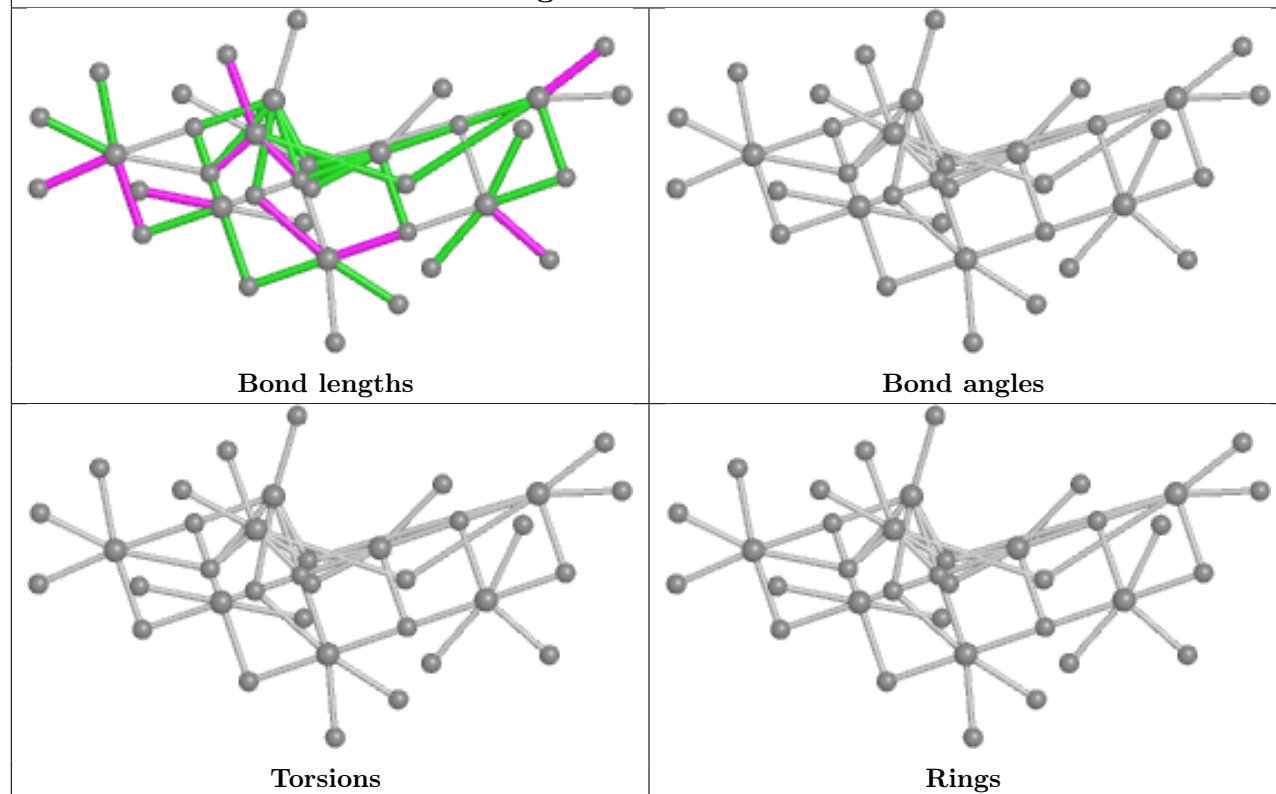


Torsions

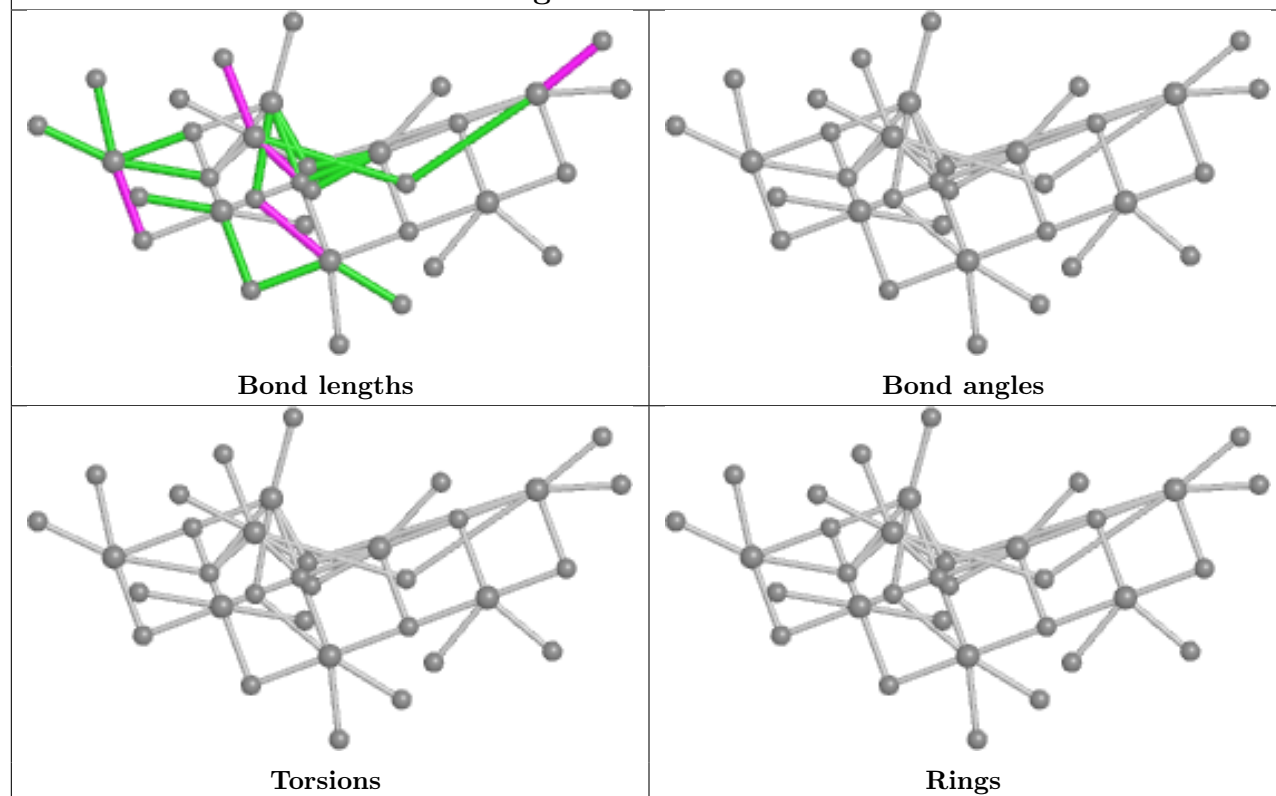


Rings

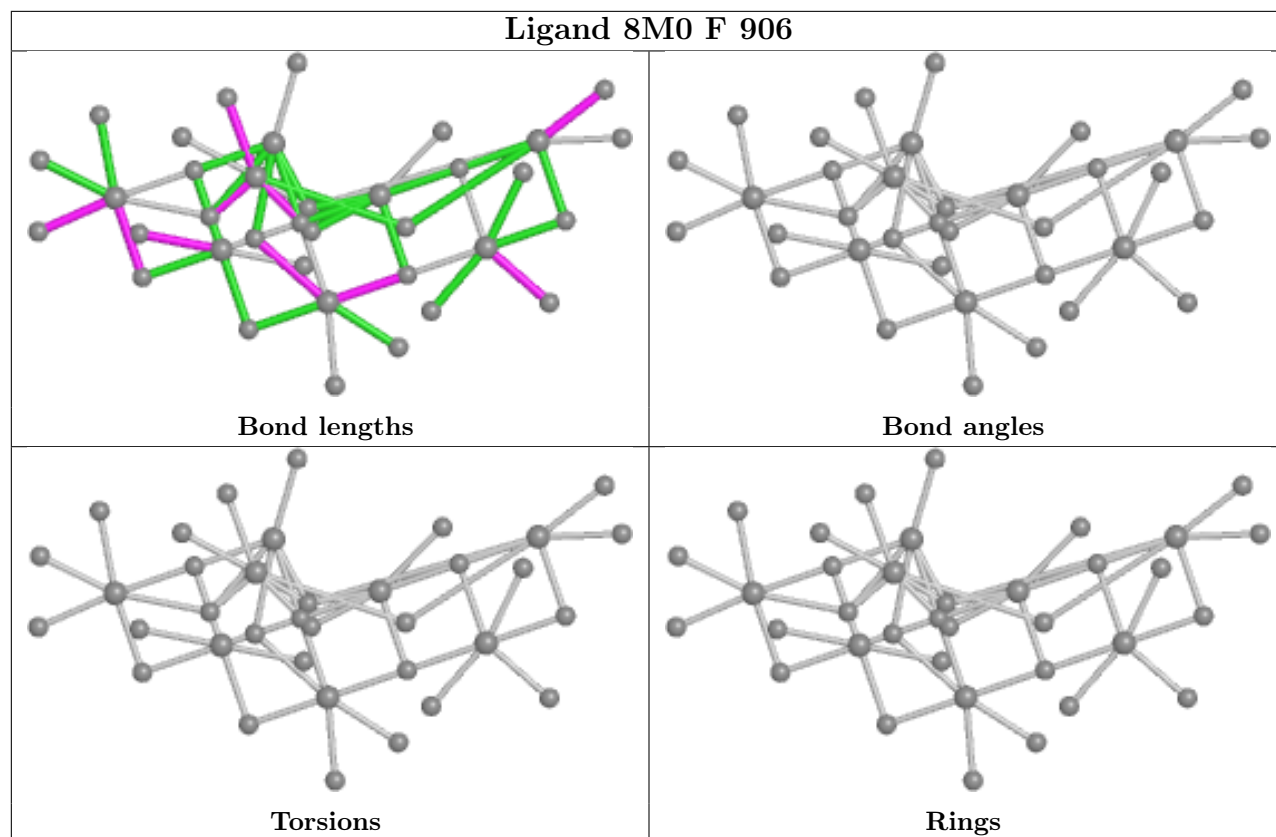
Ligand 8M0 L 906



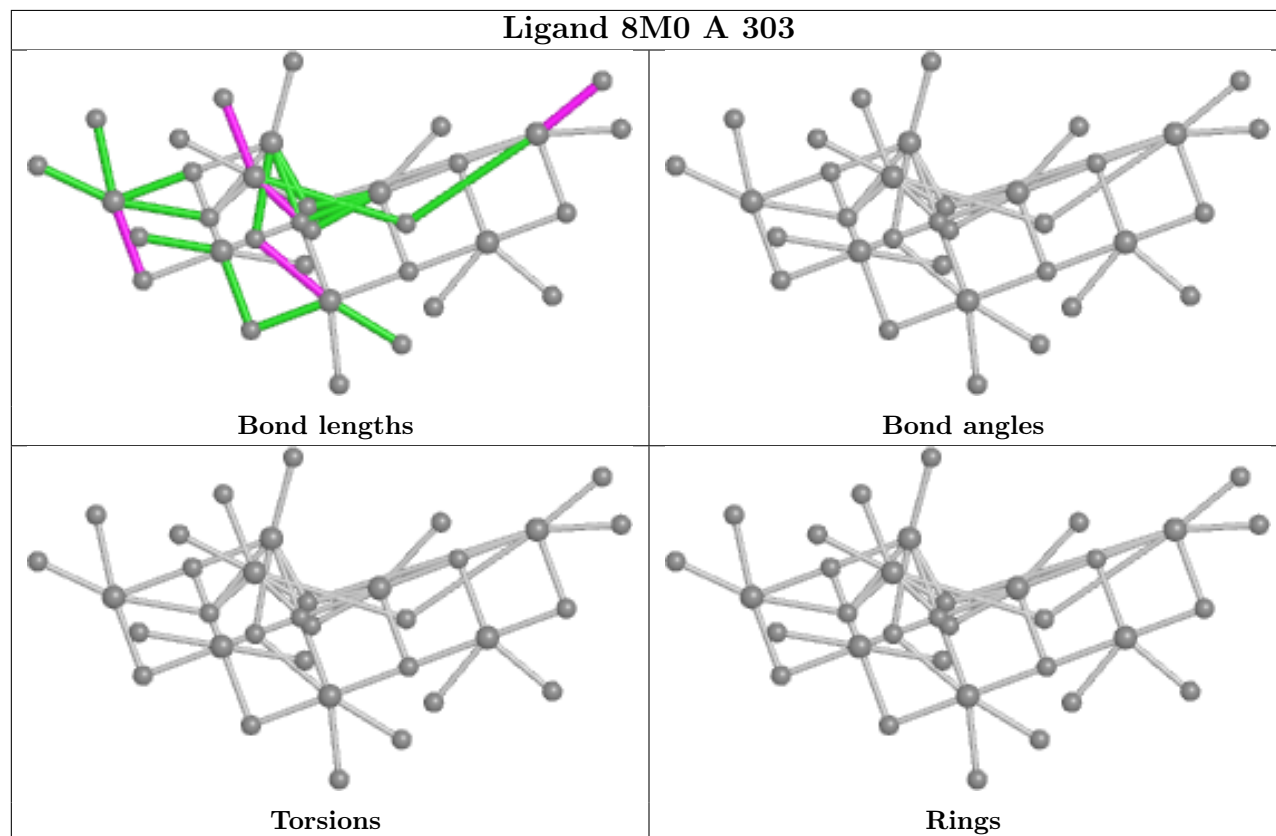
Ligand 8M0 G 303



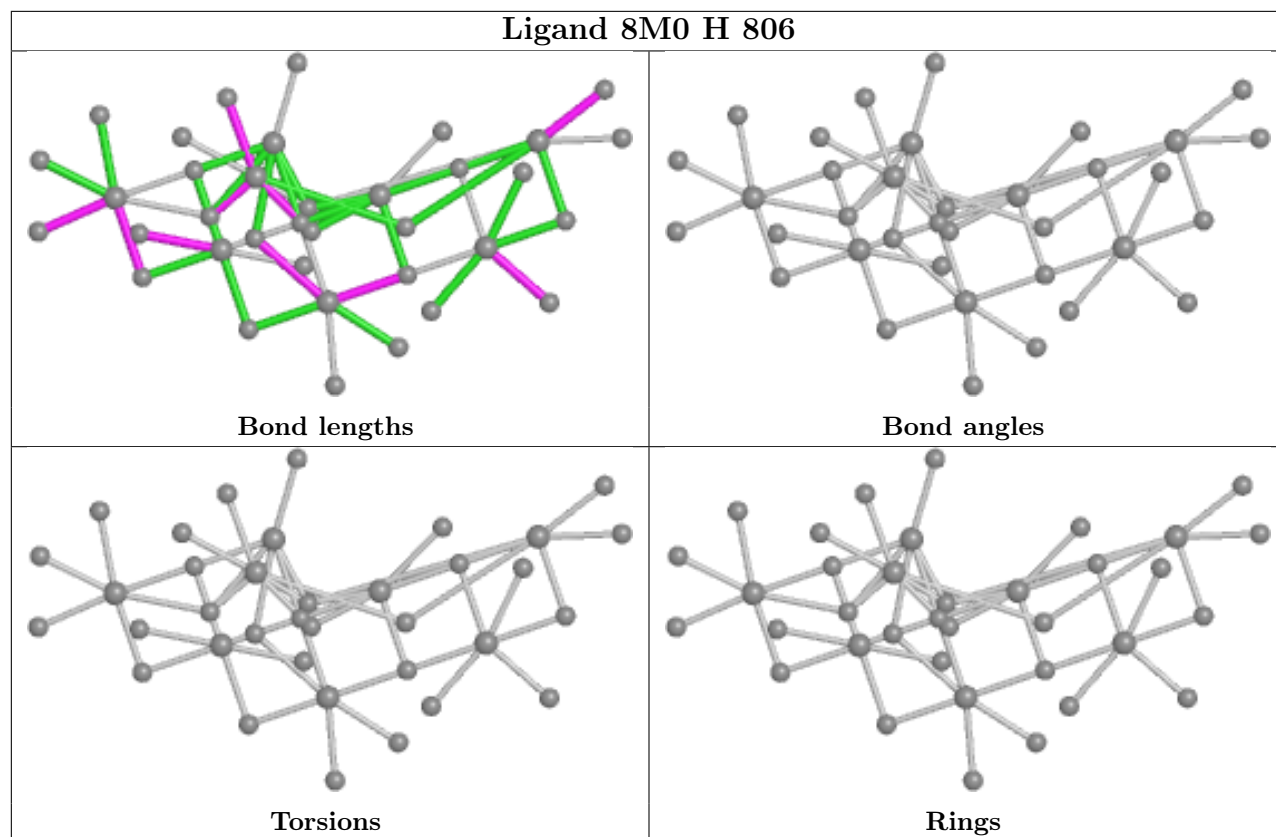
Ligand 8M0 F 906



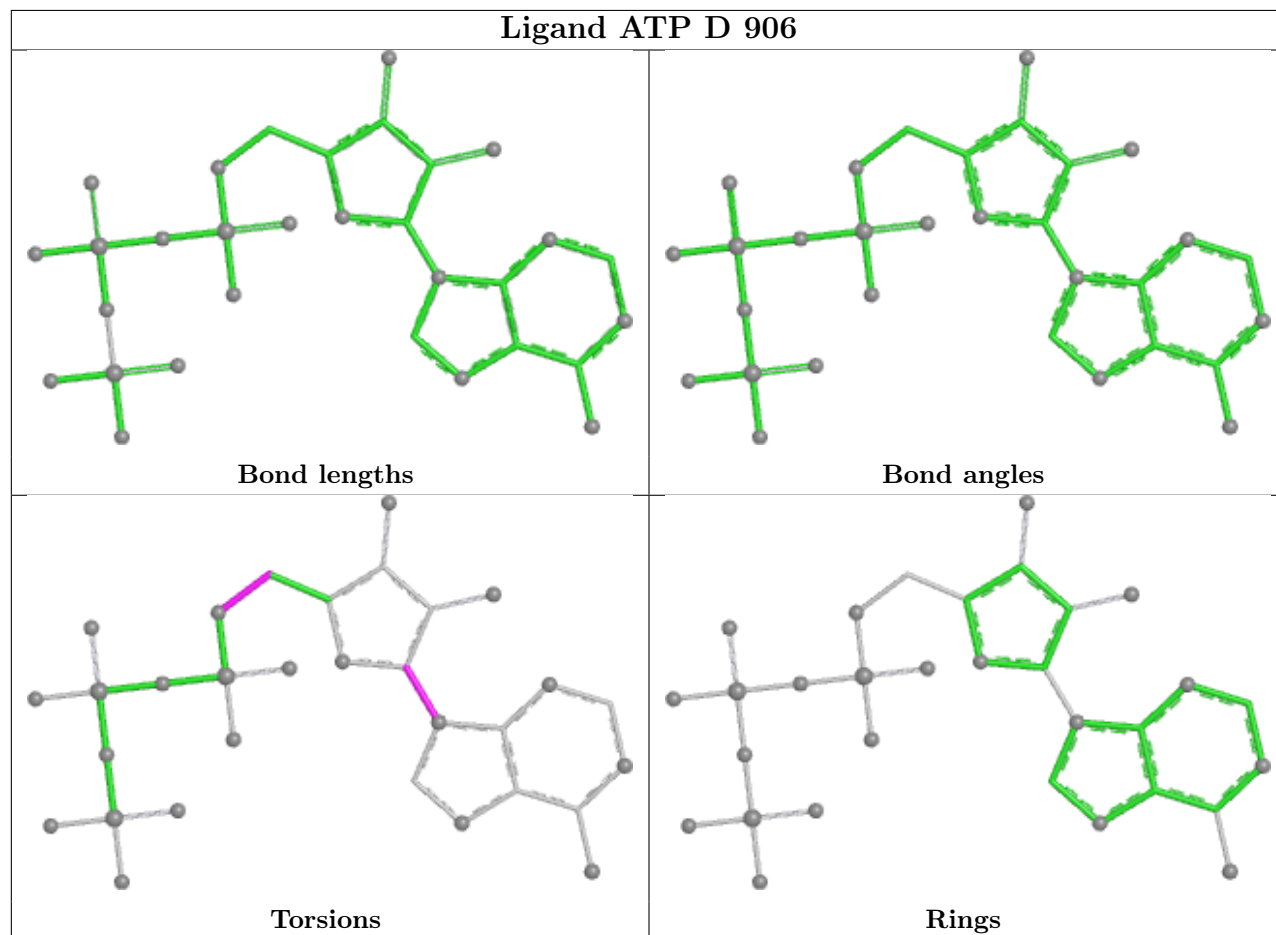
Ligand 8M0 A 303



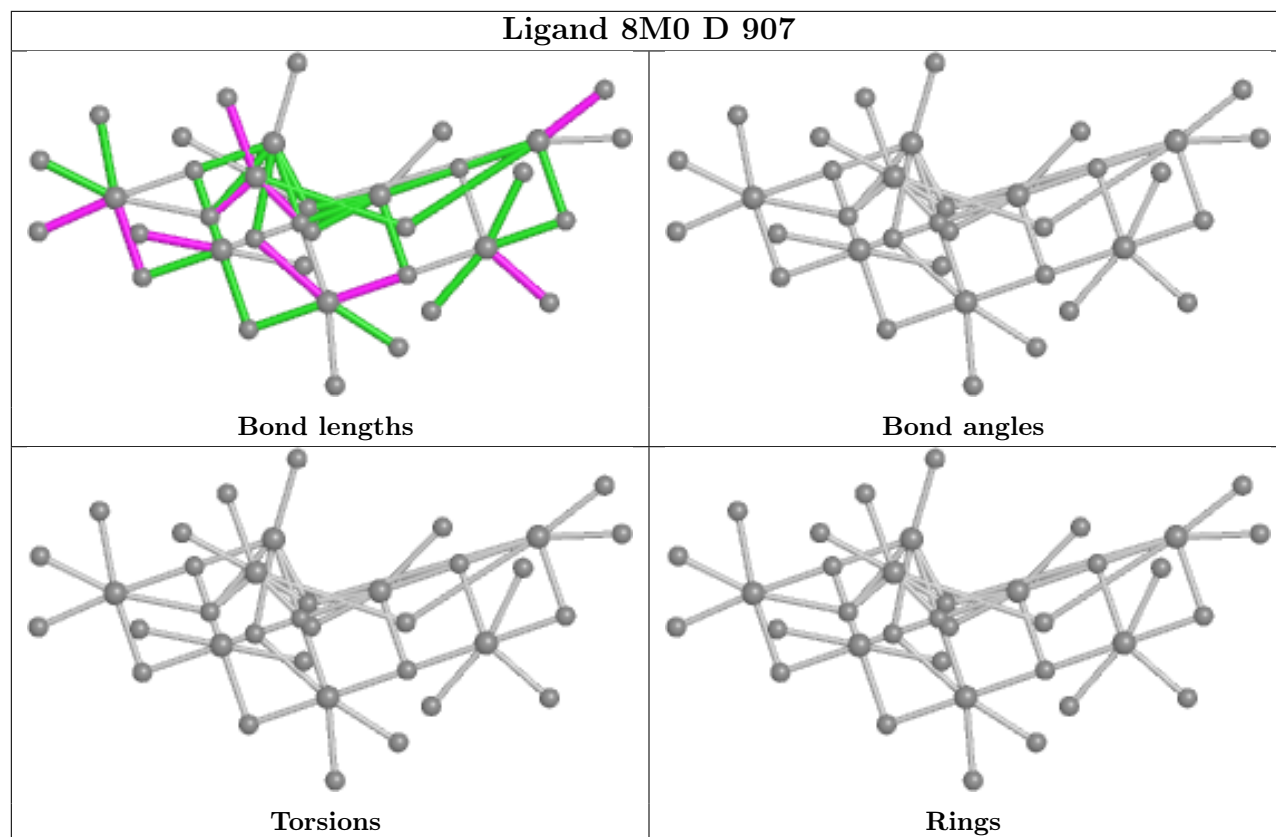
Ligand 8M0 H 806



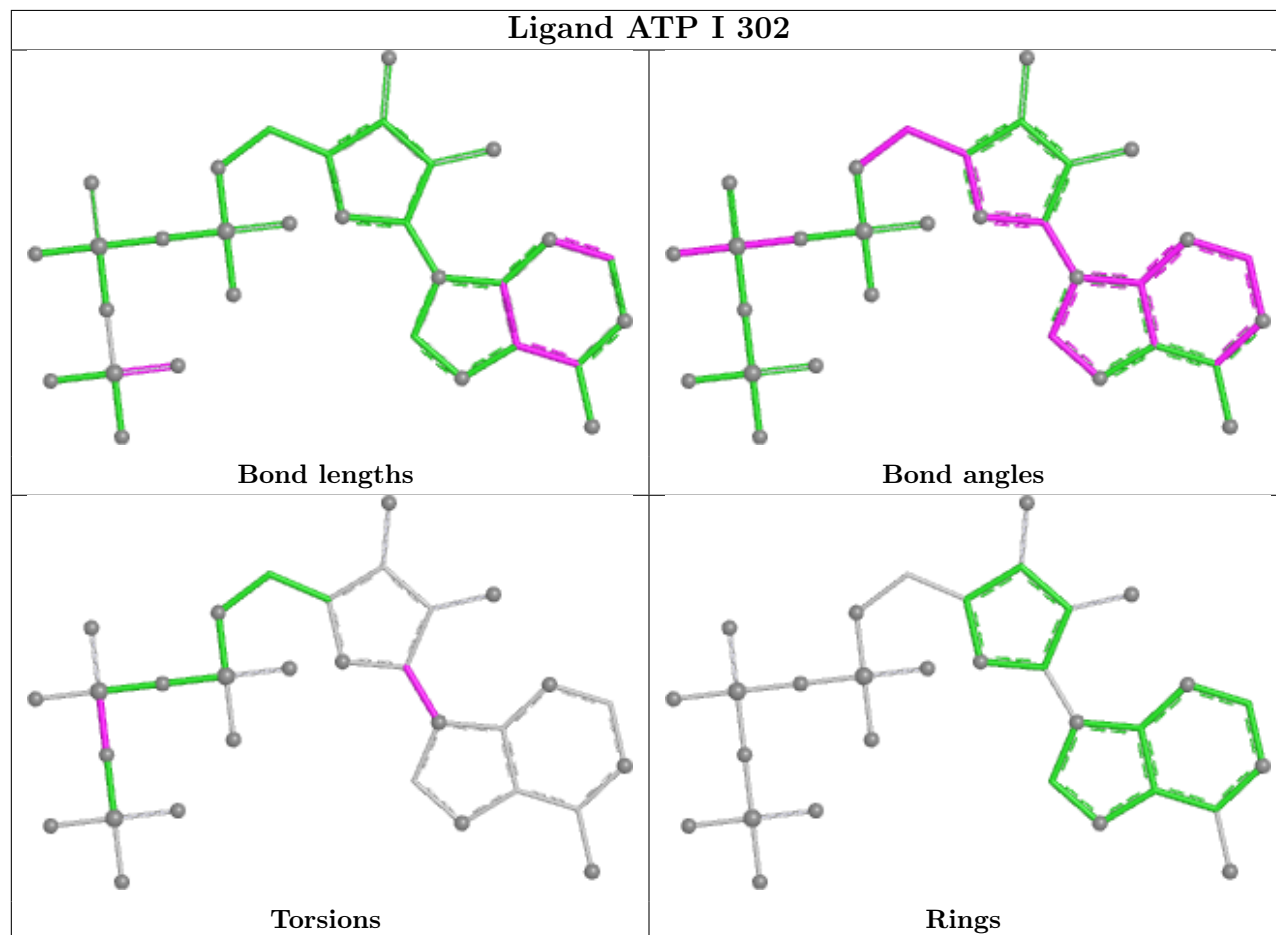
Ligand ATP D 906



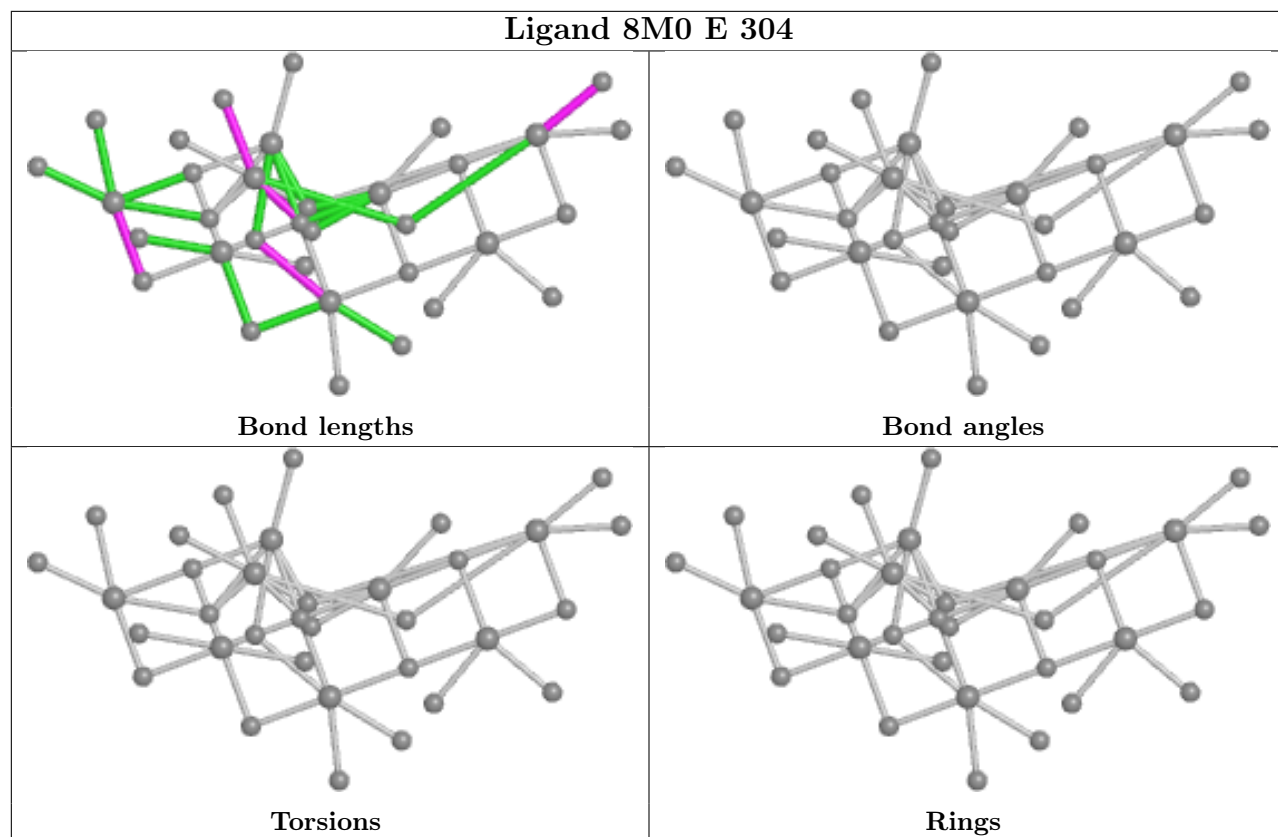
Ligand 8M0 D 907



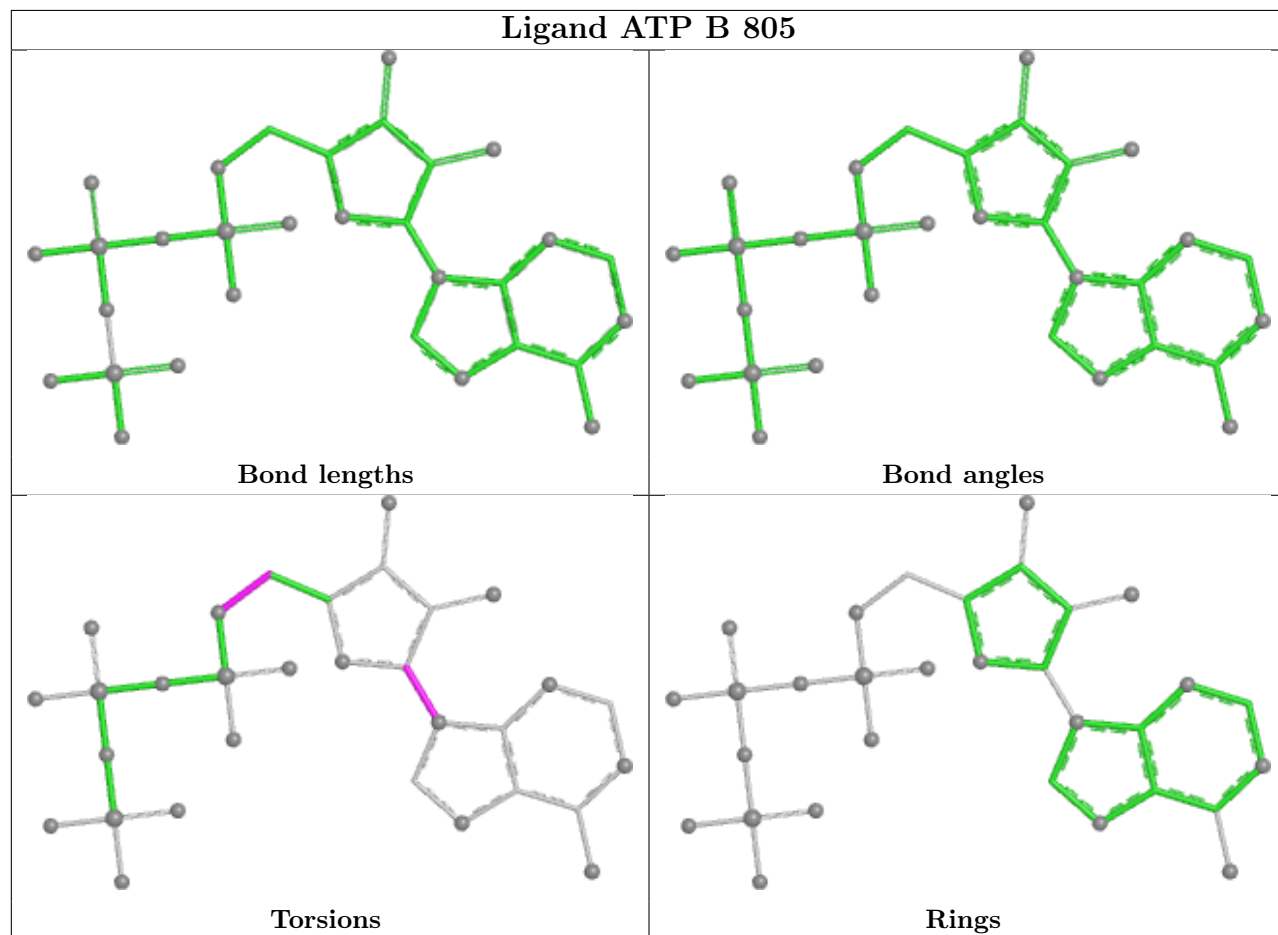
Ligand ATP I 302



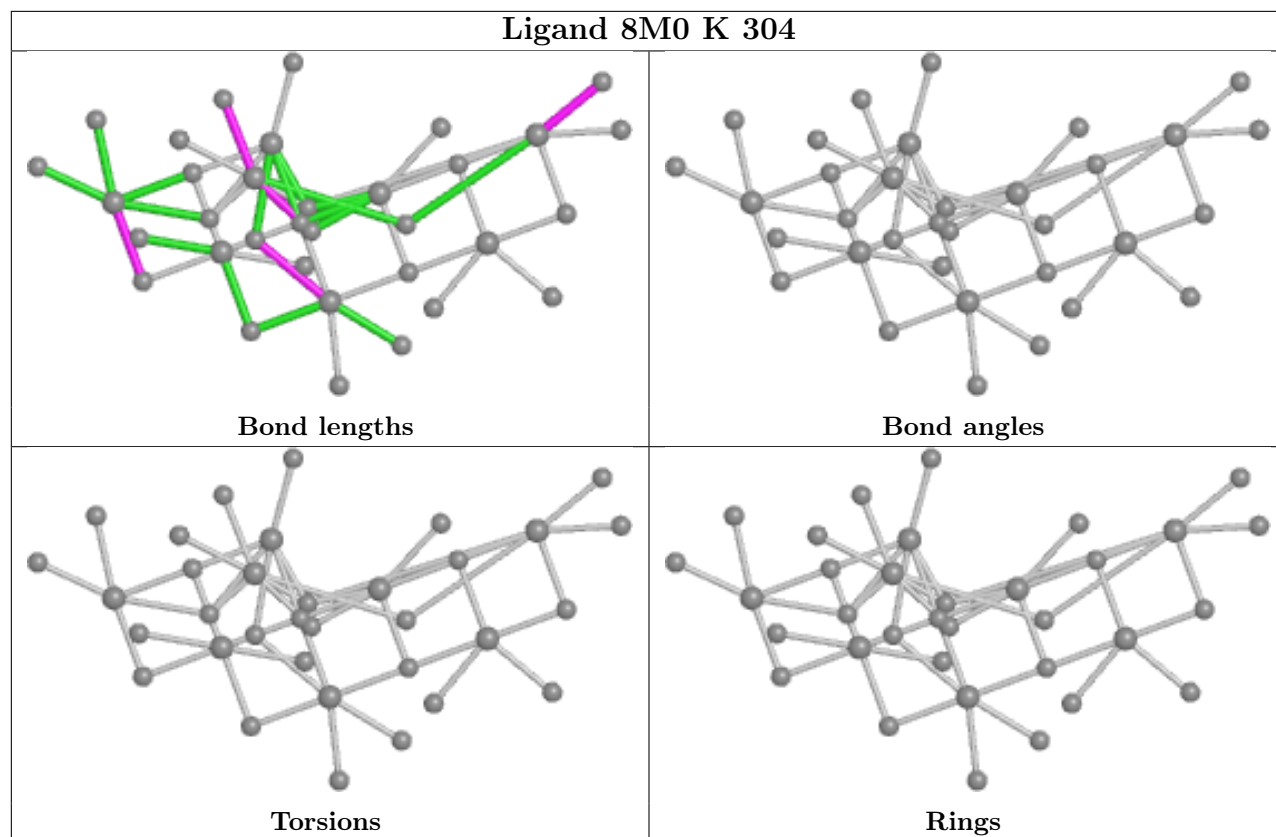
Ligand 8M0 E 304



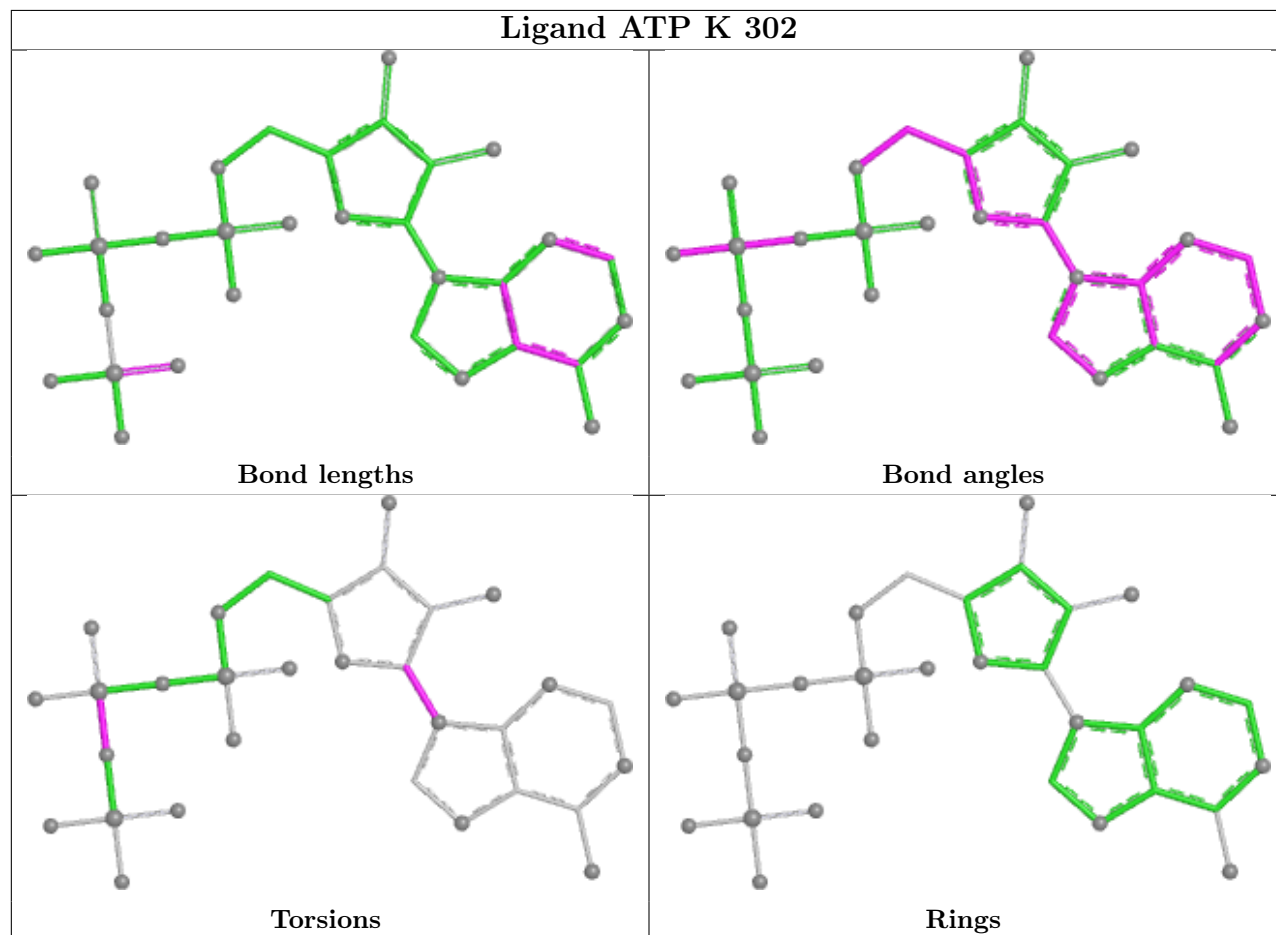
Ligand ATP B 805

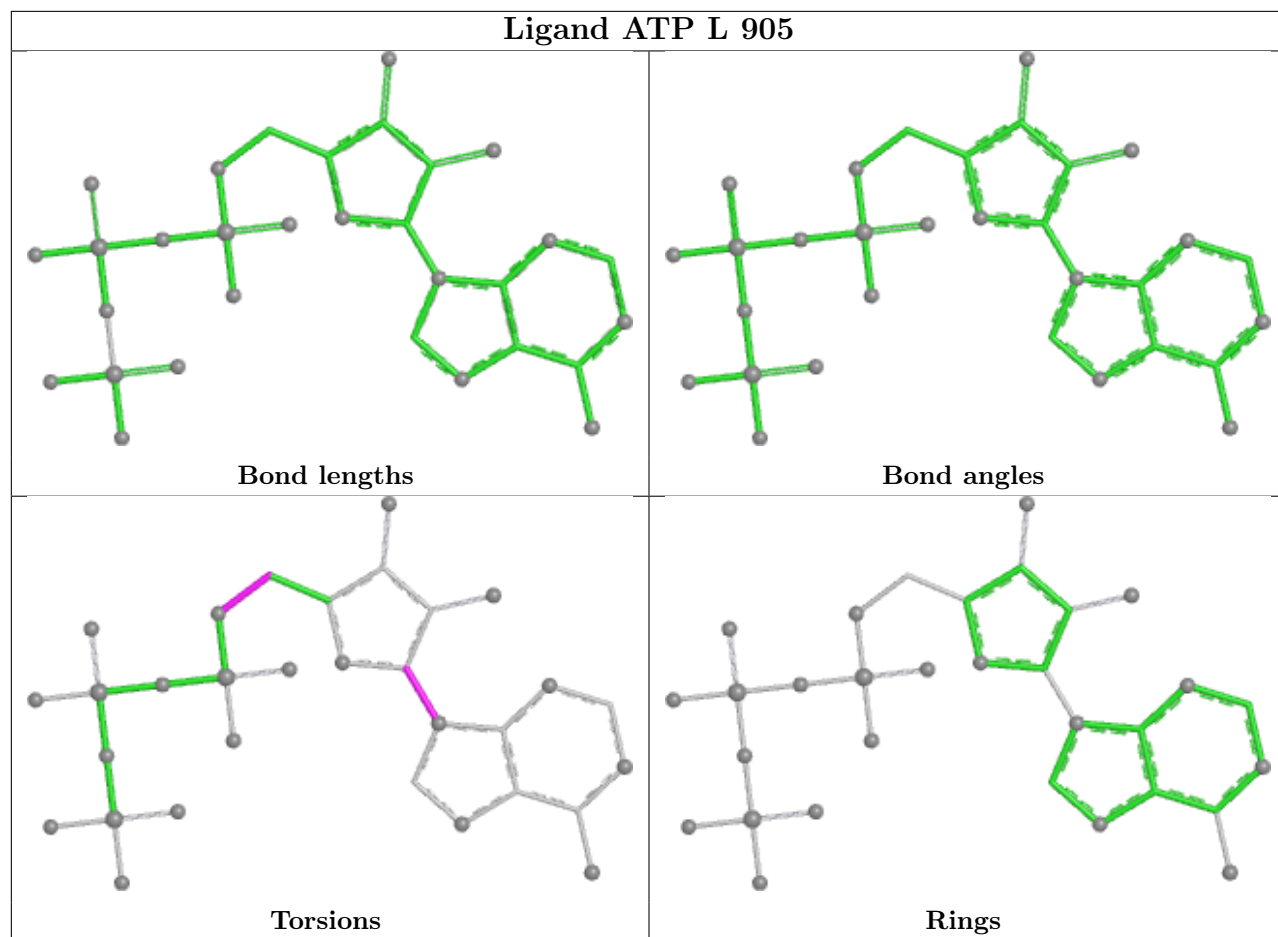


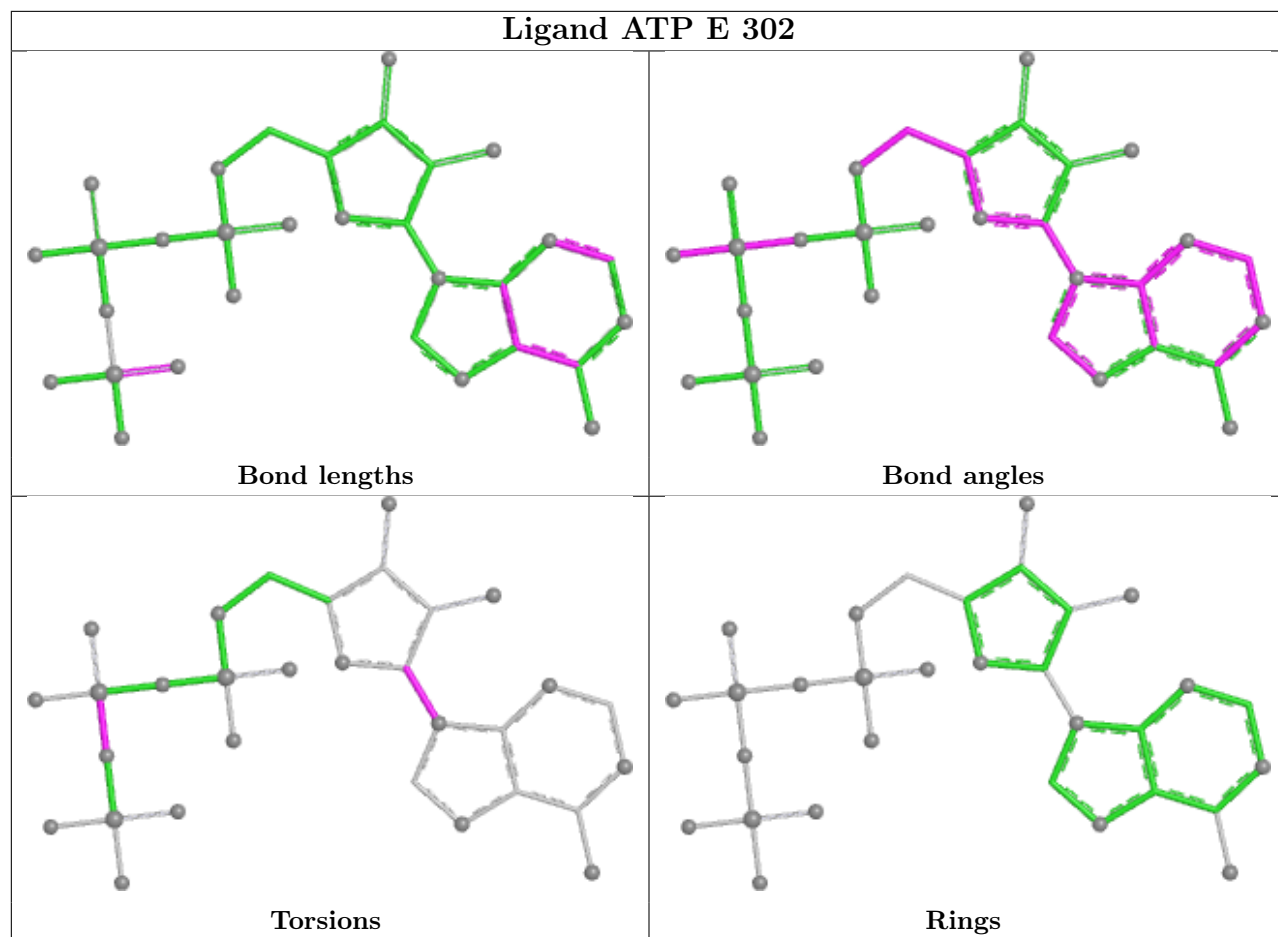
Ligand 8M0 K 304



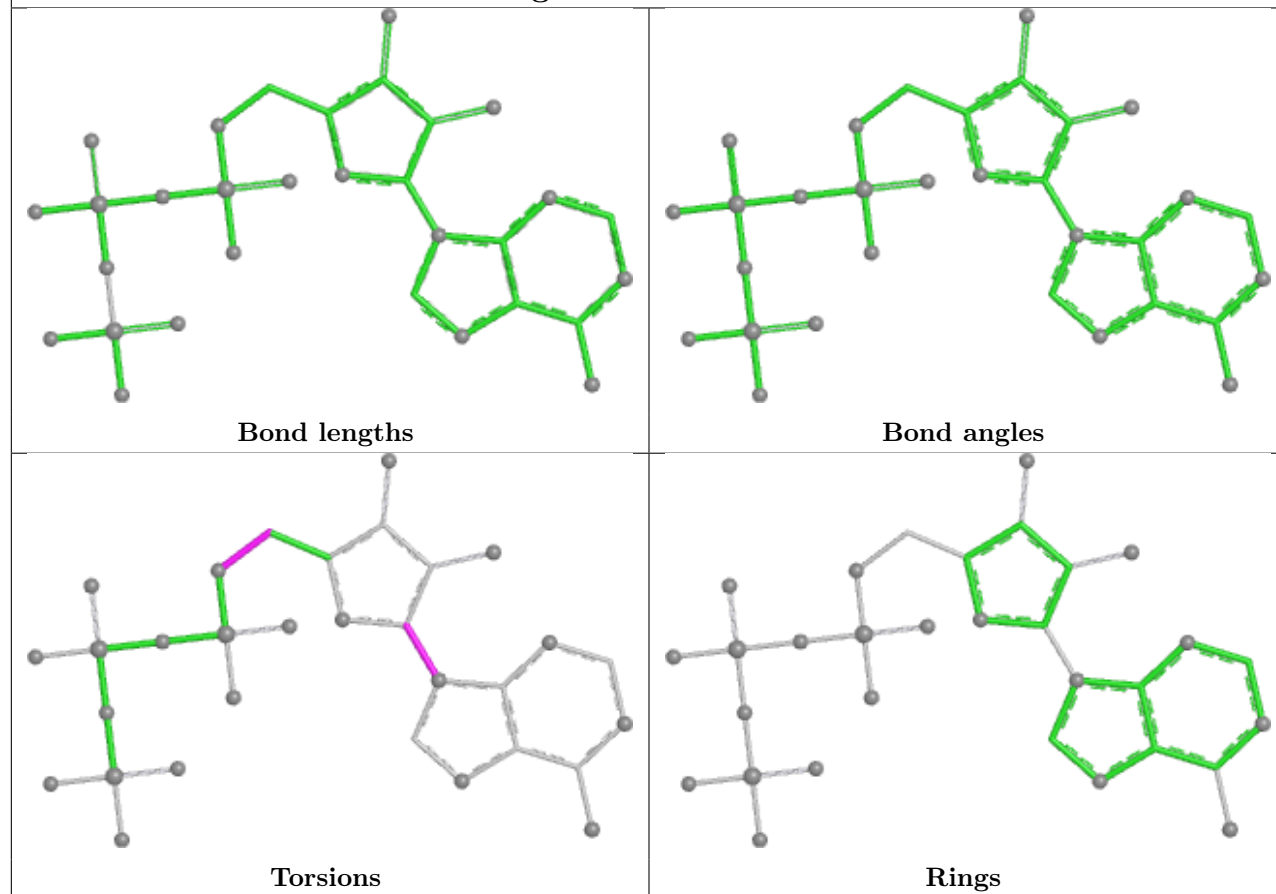
Ligand ATP K 302



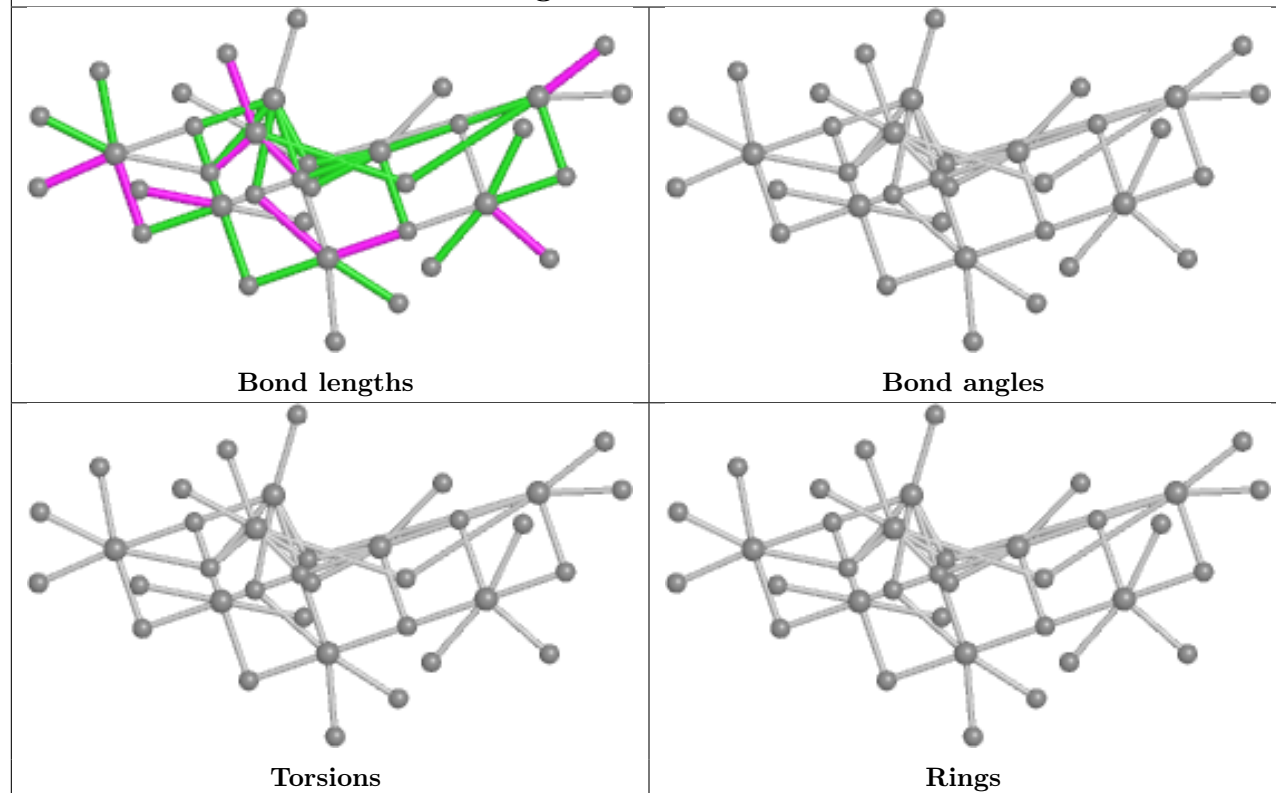




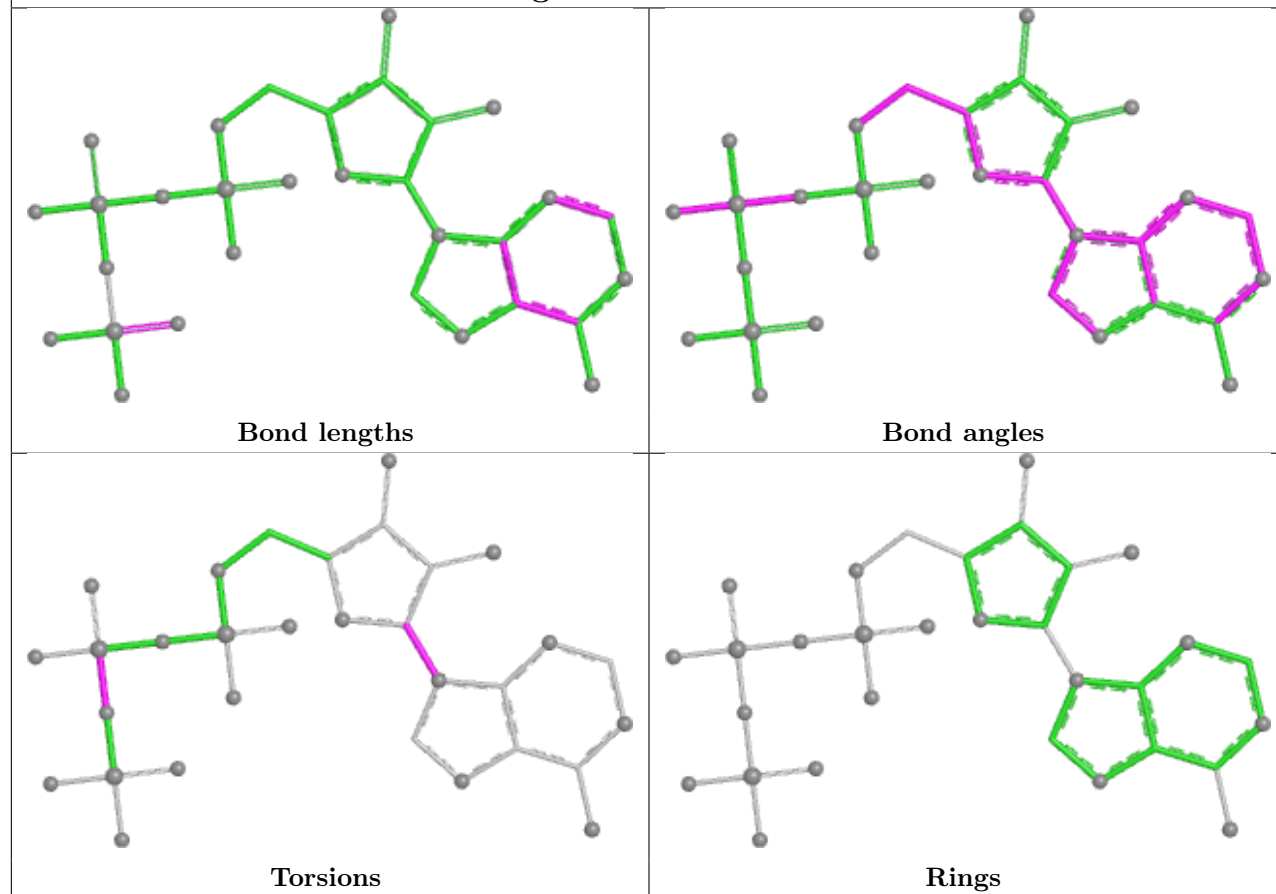
Ligand ATP H 805



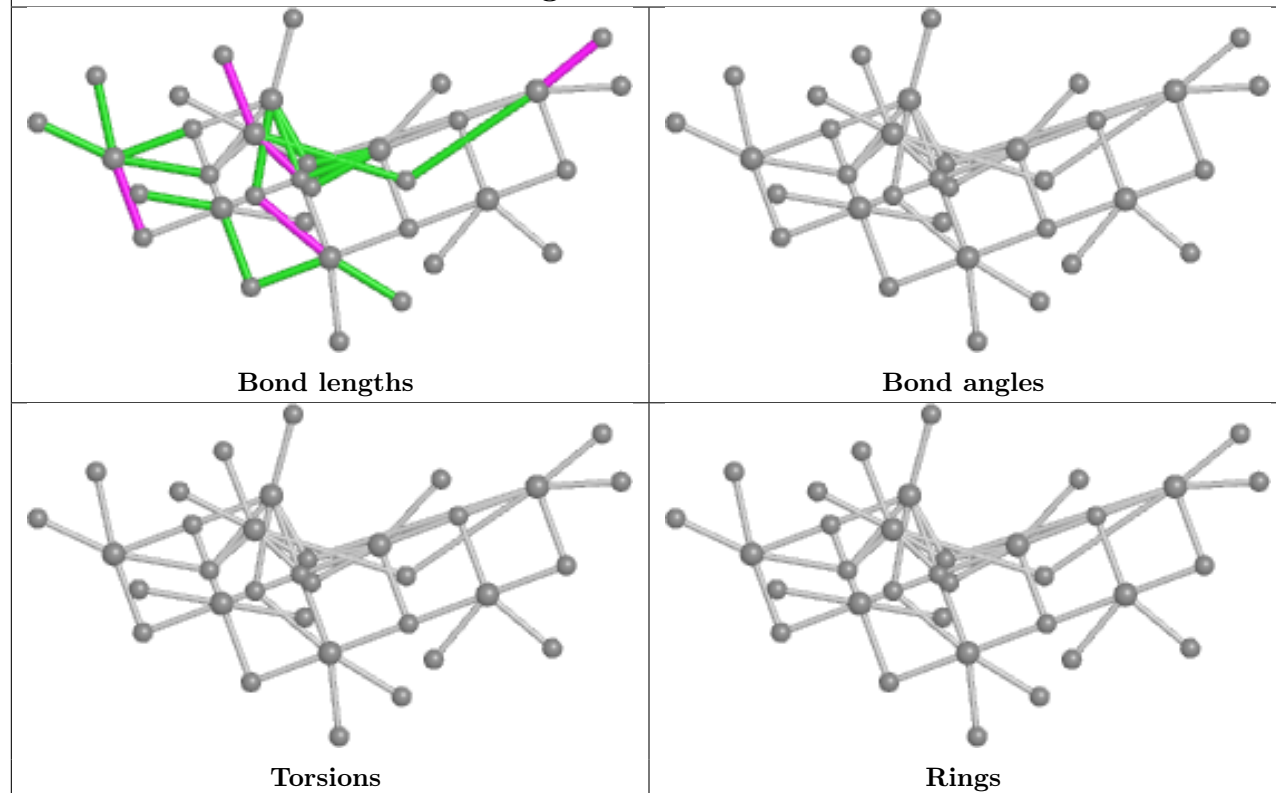
Ligand 8M0 B 806

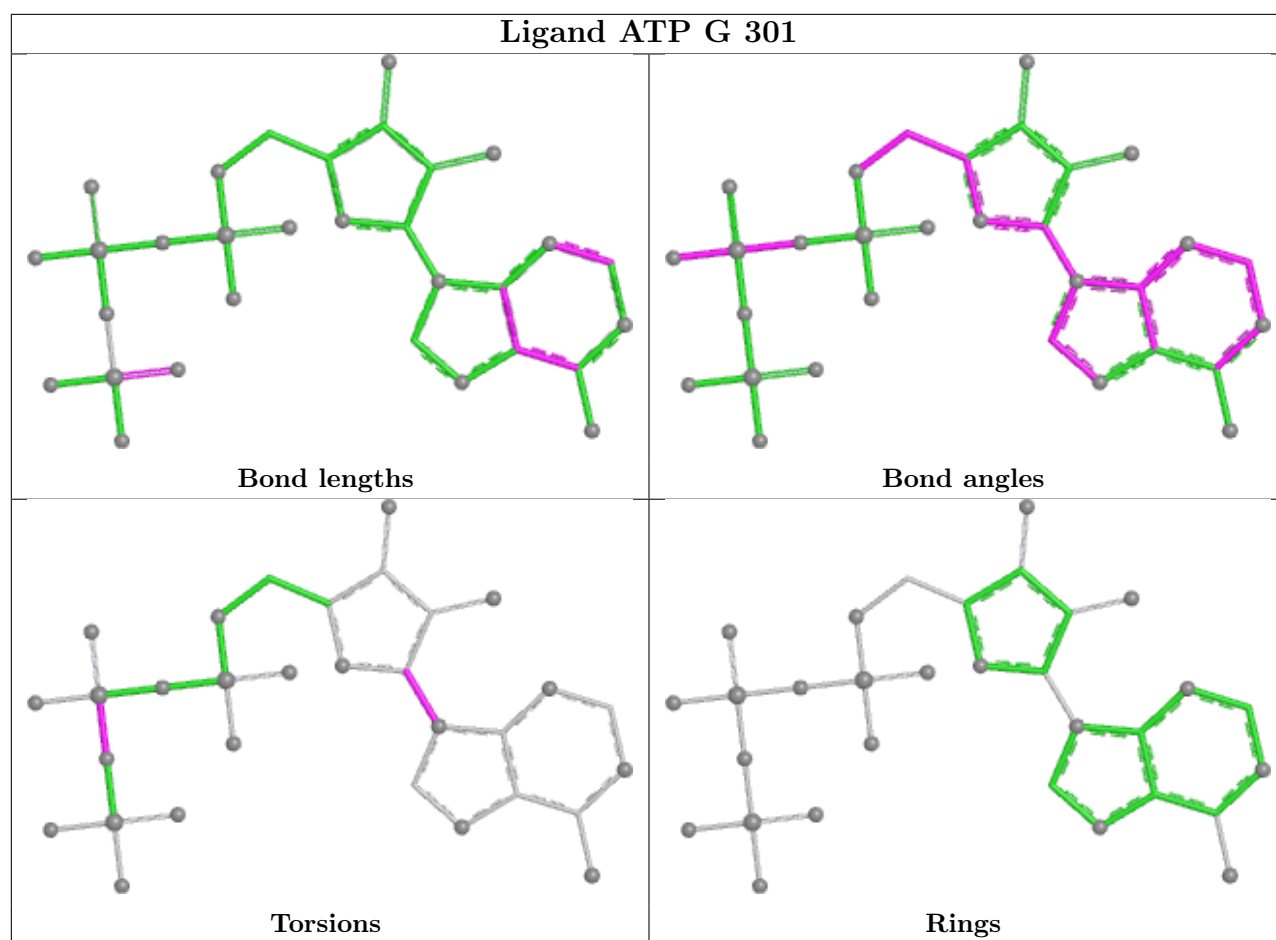


Ligand ATP A 301



Ligand 8M0 I 304





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

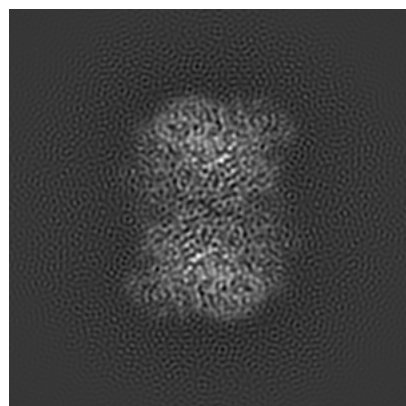
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4907. These allow visual inspection of the internal detail of the map and identification of artifacts.

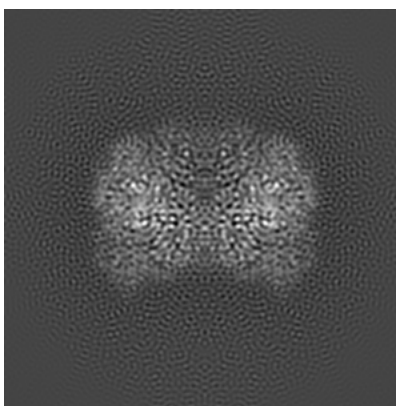
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

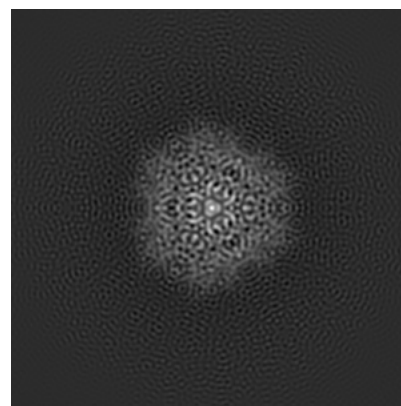
6.1.1 Primary map



X

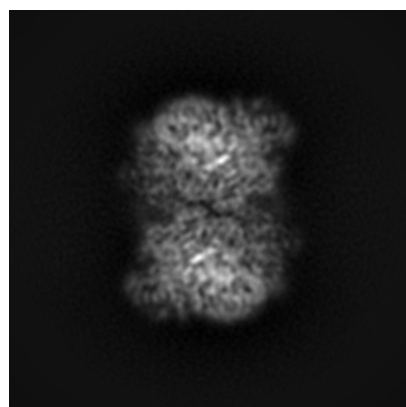


Y

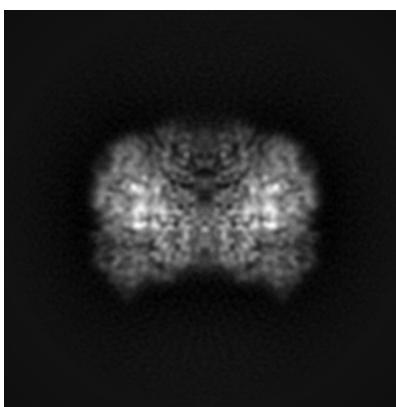


Z

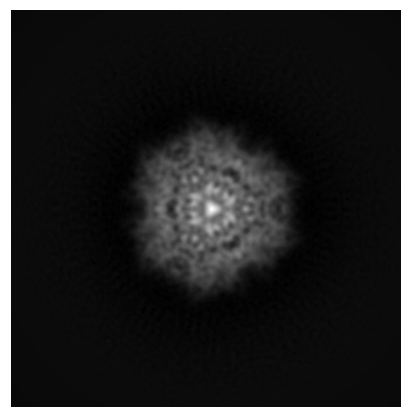
6.1.2 Raw map



X



Y

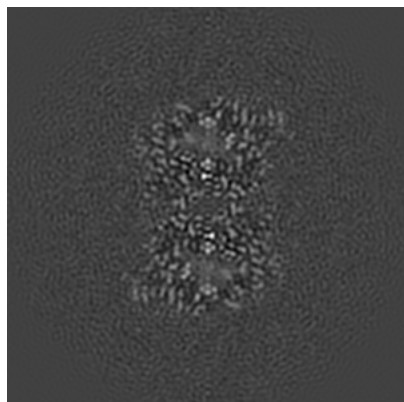


Z

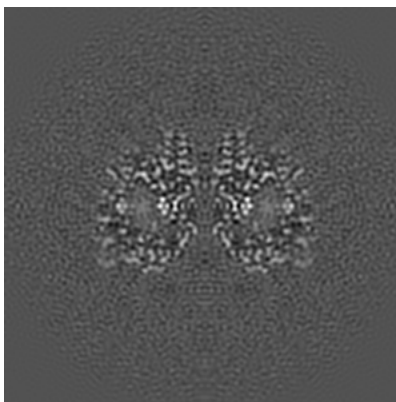
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

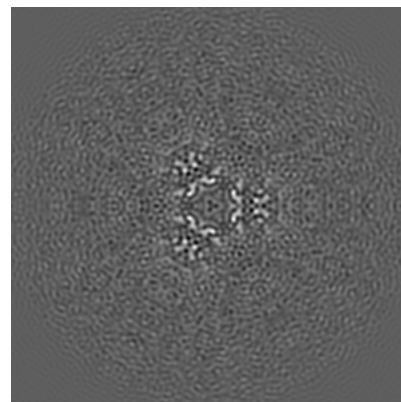
6.2.1 Primary map



X Index: 100

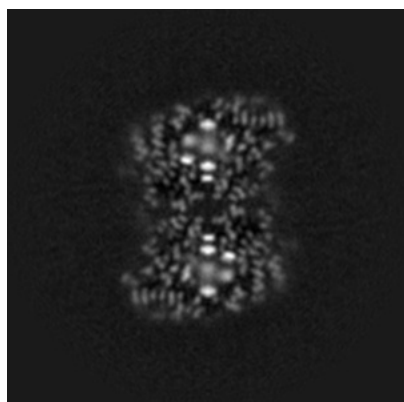


Y Index: 100

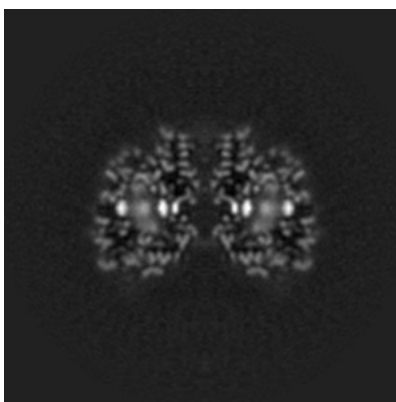


Z Index: 100

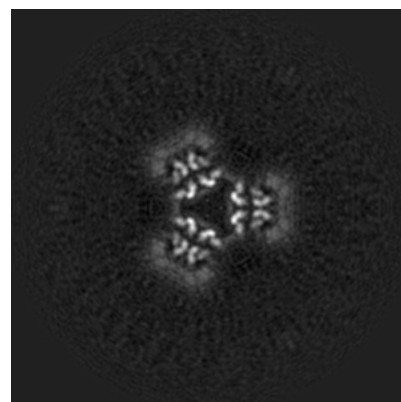
6.2.2 Raw map



X Index: 100



Y Index: 100

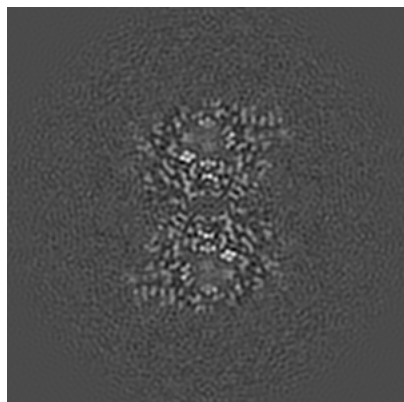


Z Index: 100

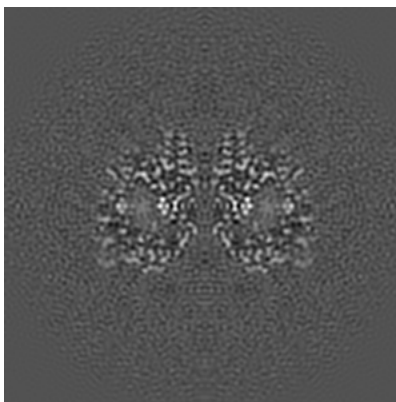
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

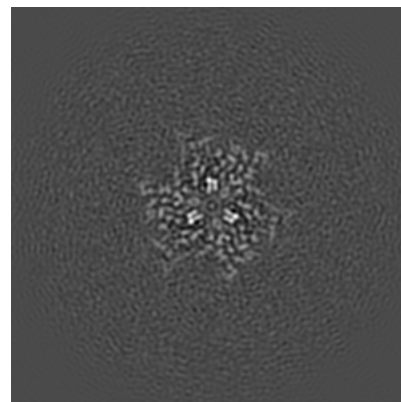
6.3.1 Primary map



X Index: 99

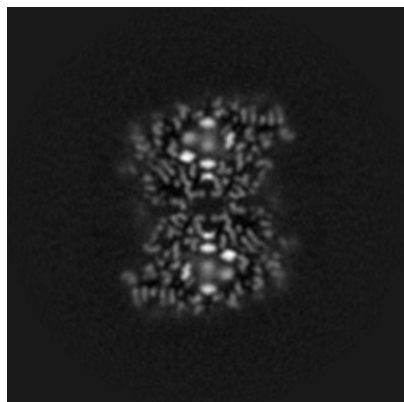


Y Index: 100

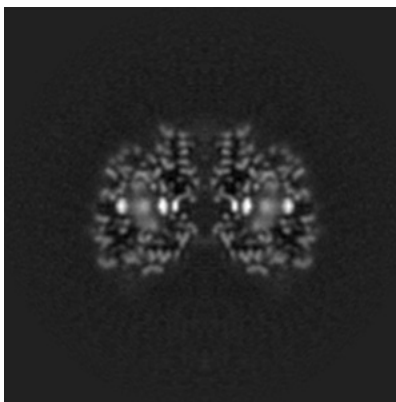


Z Index: 76

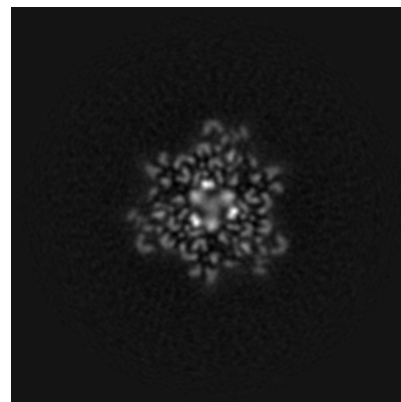
6.3.2 Raw map



X Index: 99



Y Index: 100

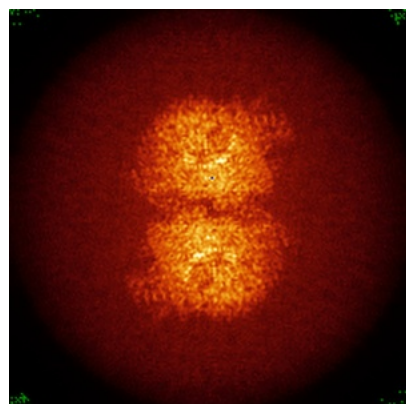


Z Index: 134

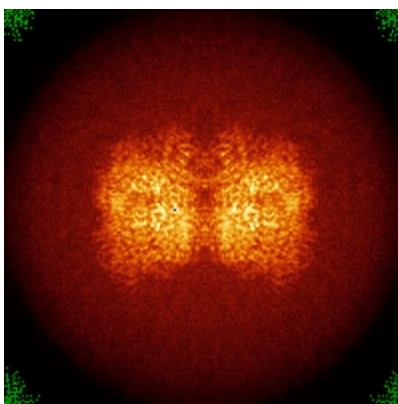
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

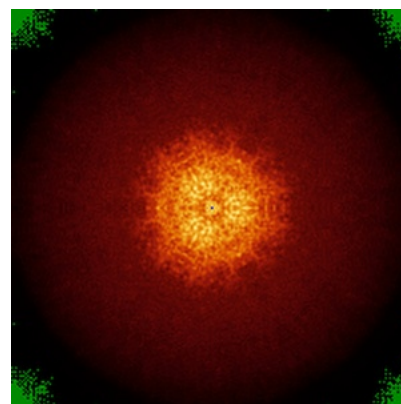
6.4.1 Primary map



X

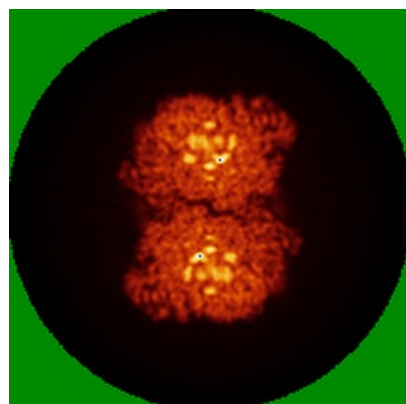


Y

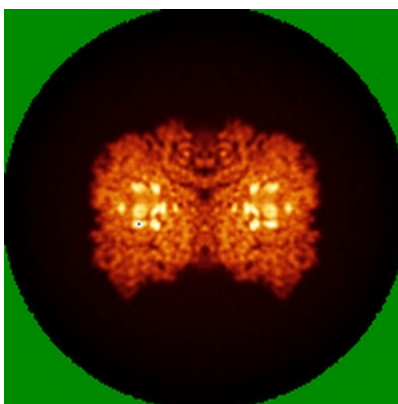


Z

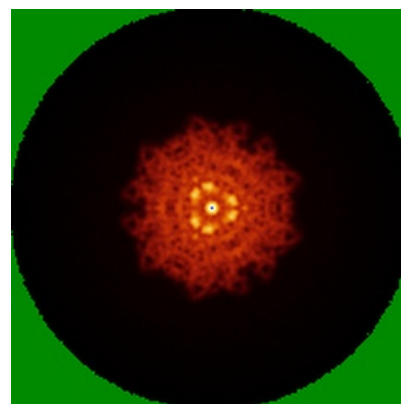
6.4.2 Raw map



X



Y



Z

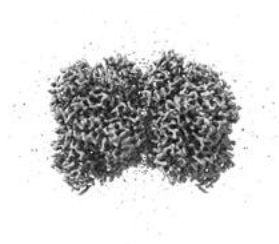
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

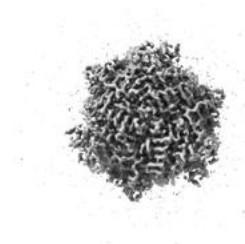
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

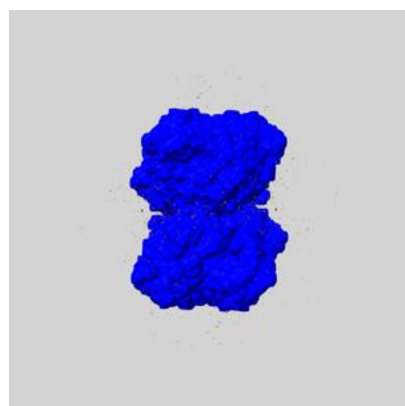
6.6 Mask visualisation [i](#)

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

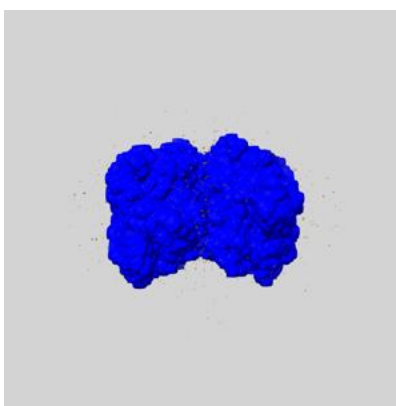
A mask typically either:

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

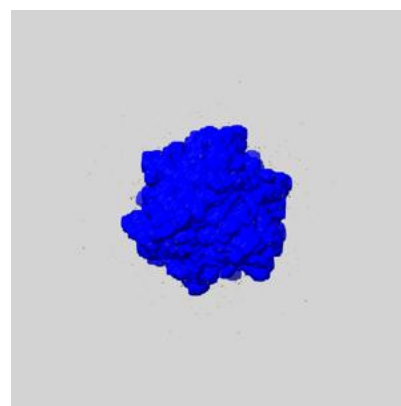
6.6.1 emd_4907_msk_1.map [i](#)



X



Y

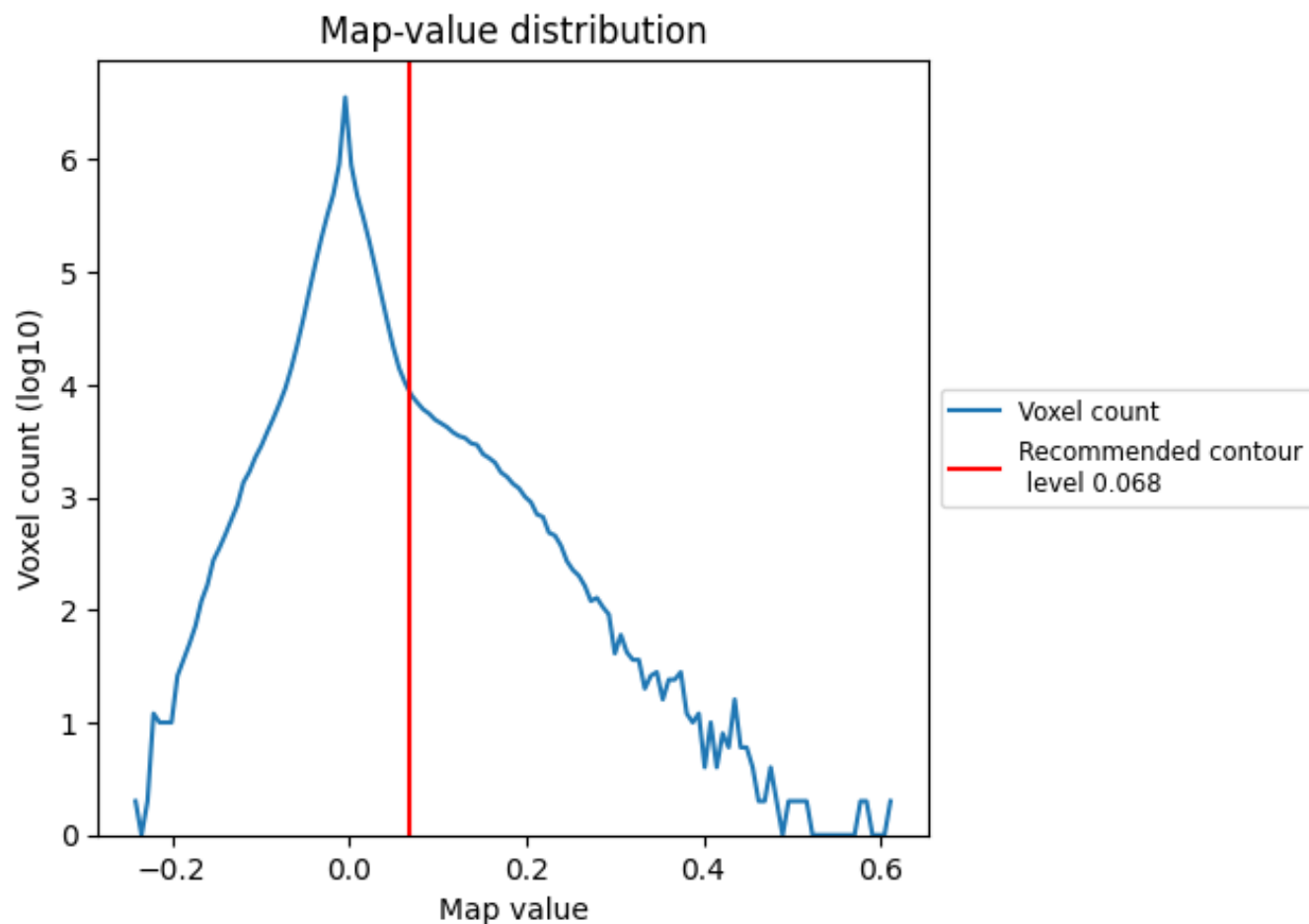


Z

7 Map analysis [i](#)

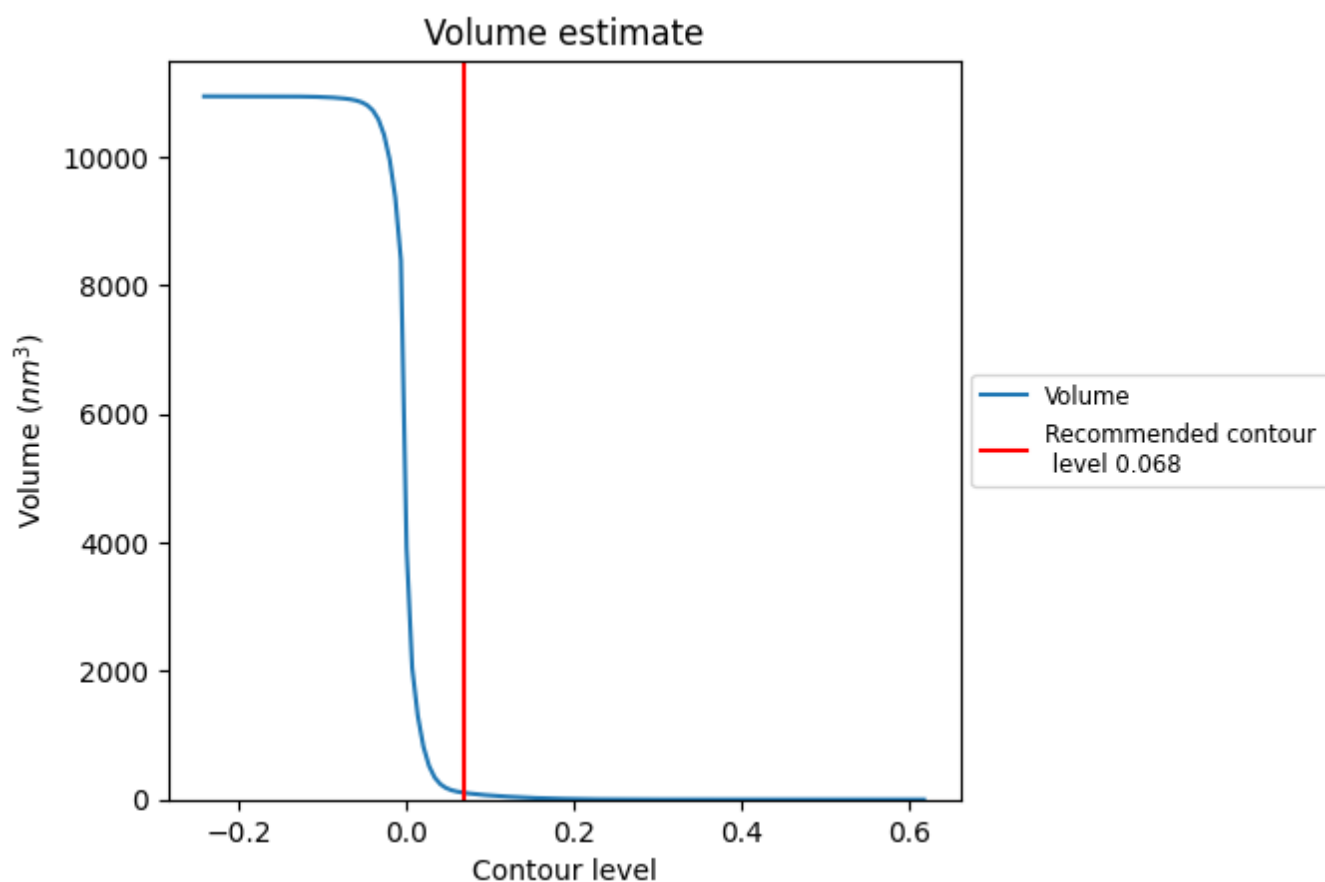
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

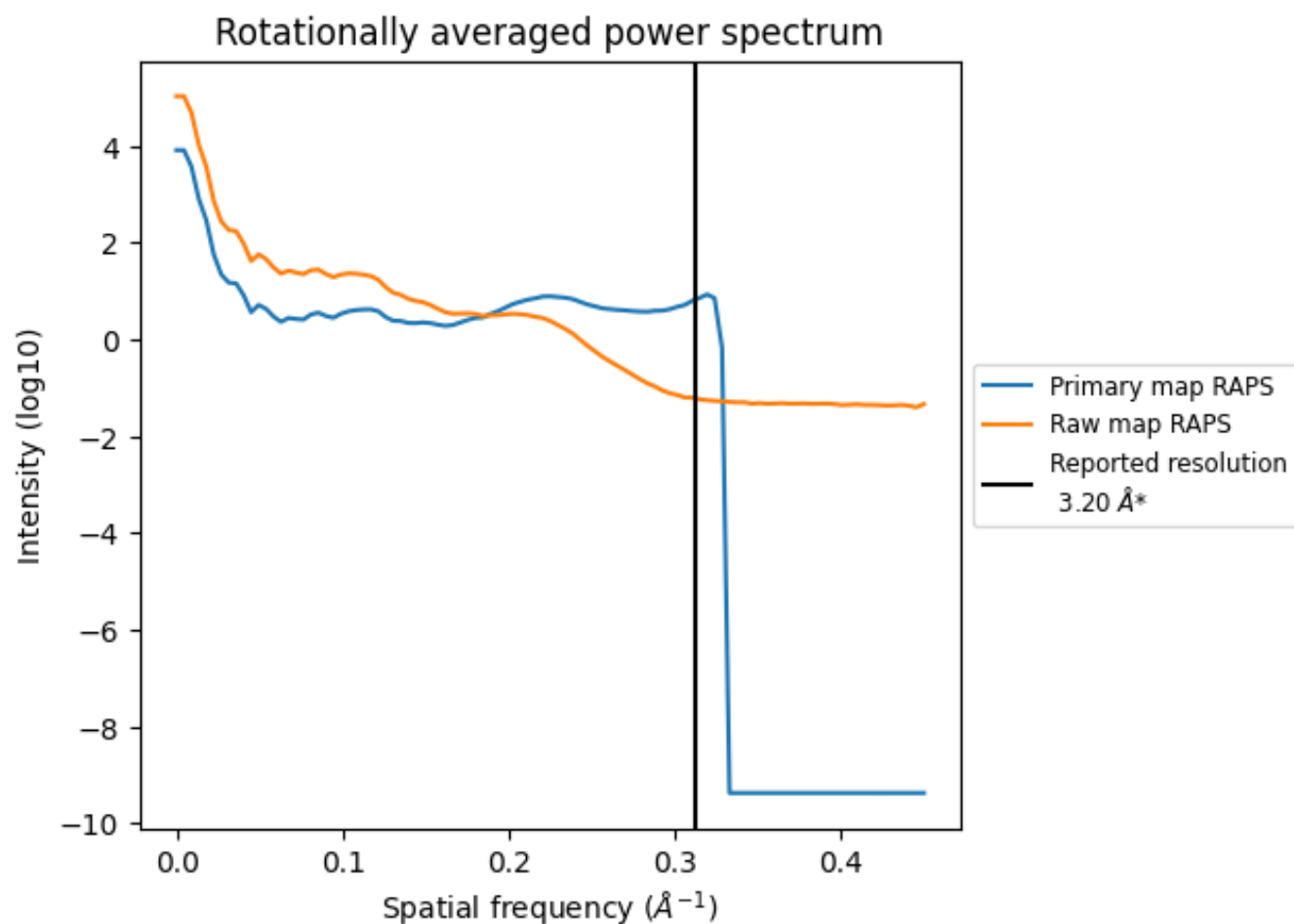
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 97 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 ⓘ

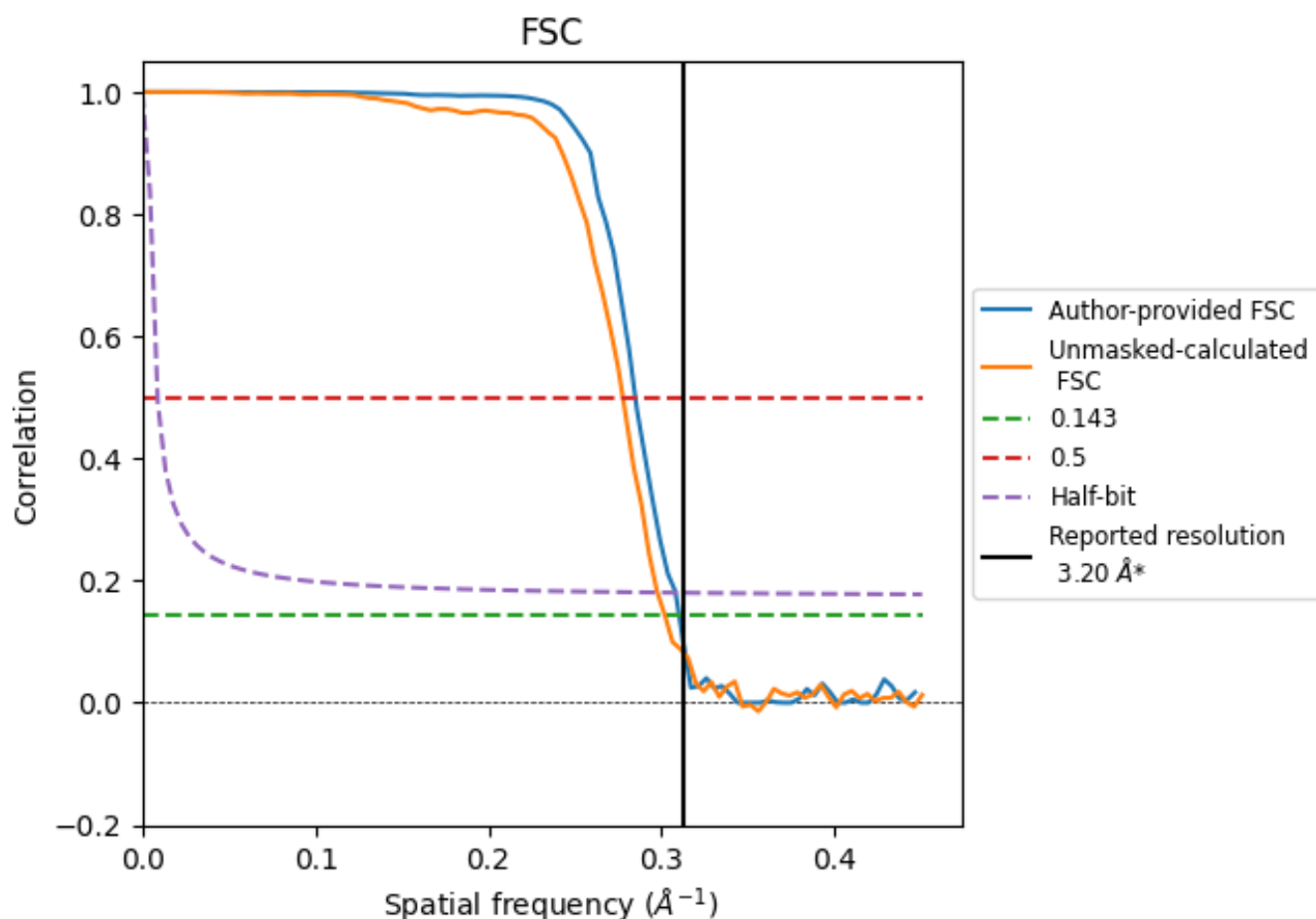


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

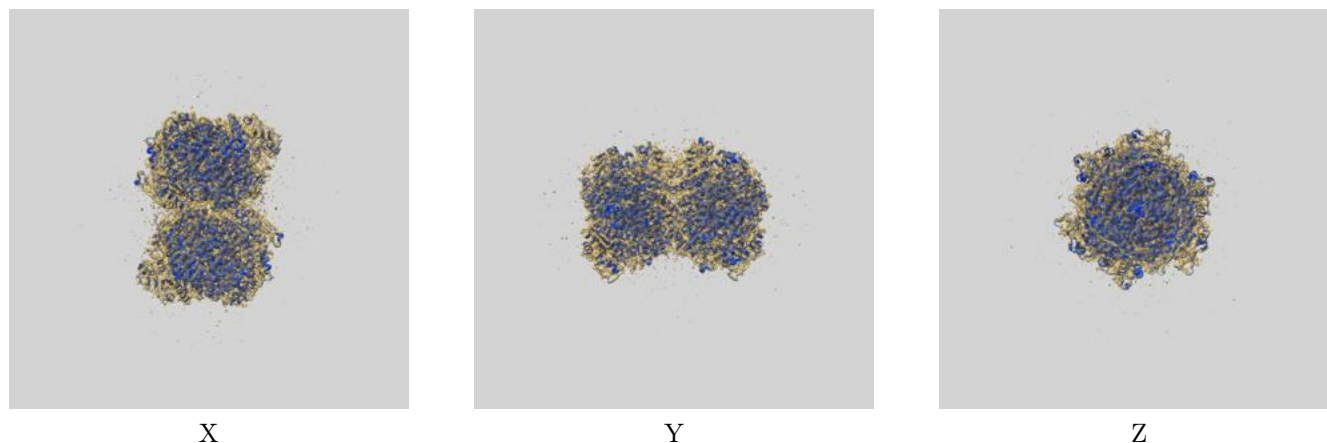
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.51	3.25
Unmasked-calculated*	3.31	3.60	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

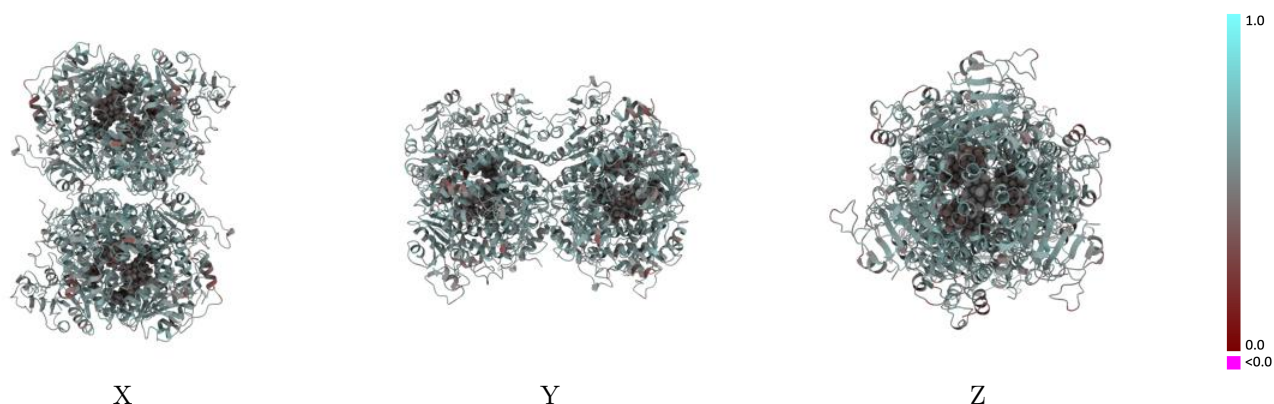
This section contains information regarding the fit between EMDB map EMD-4907 and PDB model 6RKD. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



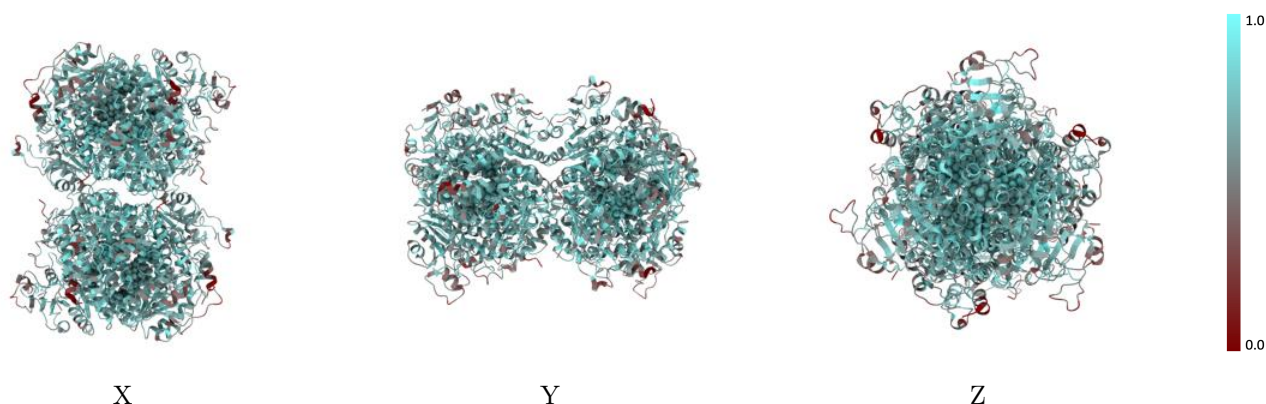
The images above show the 3D surface view of the map at the recommended contour level 0.068 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



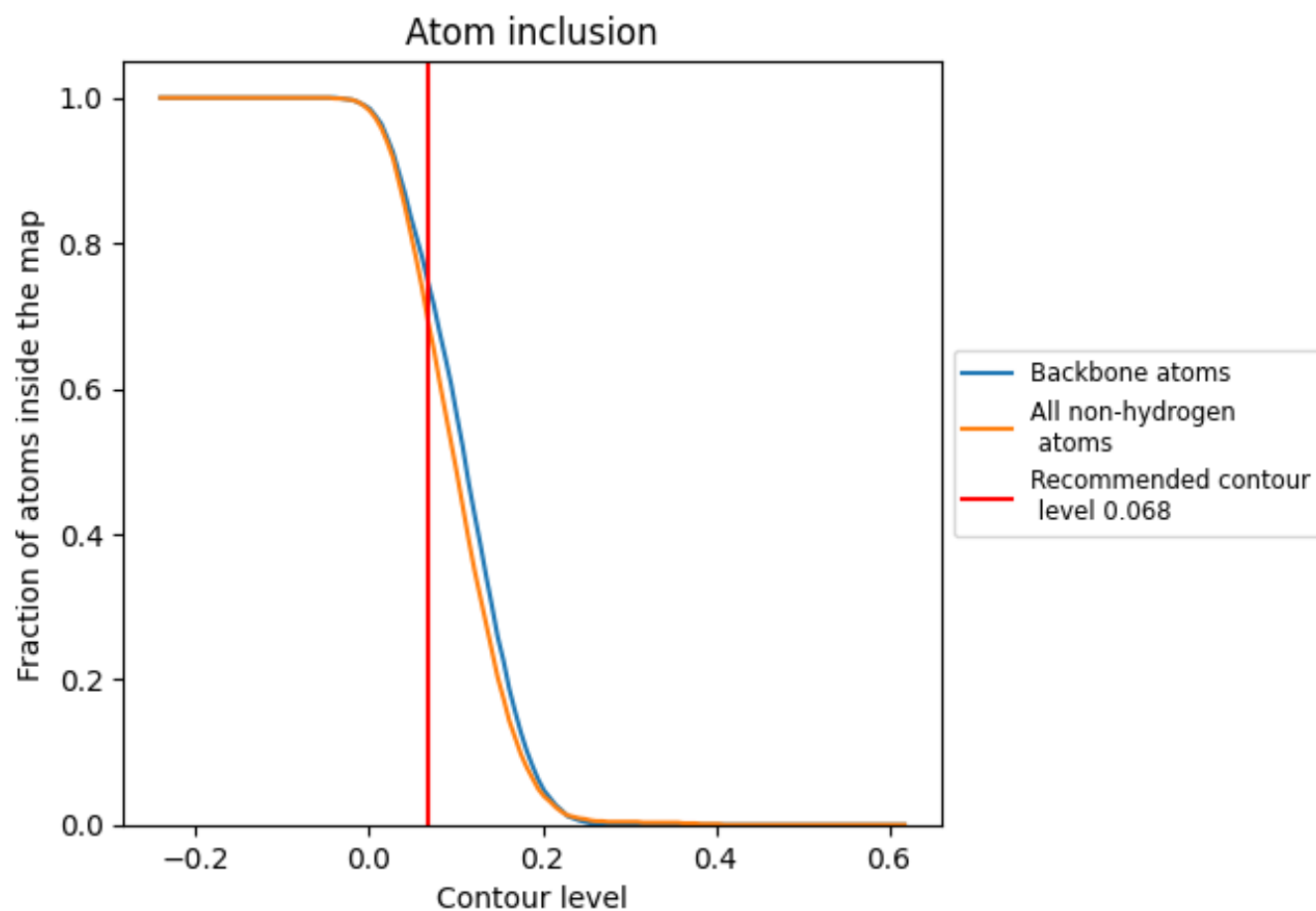
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.068).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.5460
A	0.7260	0.5540
B	0.6680	0.5410
C	0.7230	0.5520
D	0.6560	0.5370
E	0.7200	0.5520
F	0.6590	0.5380
G	0.7260	0.5560
H	0.6690	0.5400
I	0.7200	0.5510
J	0.6590	0.5380
K	0.7230	0.5520
L	0.6560	0.5380

1.0

0.0

<0.0