Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 09:27 am BST

PDB ID	:	6RKD
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:

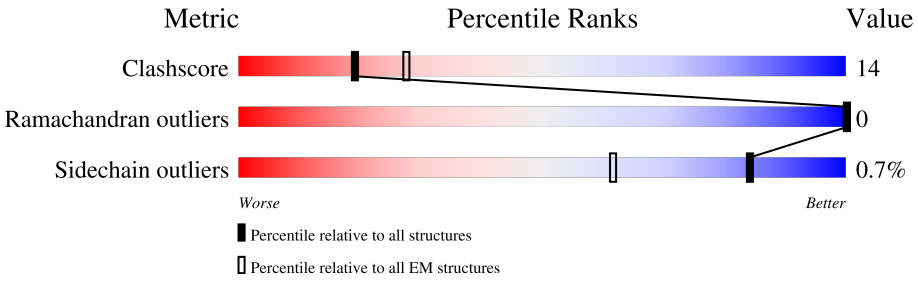
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	276	9% 83% 15% ·
1	C	276	9% 83% 15% ·
1	E	276	8% 83% 15% ·
1	G	276	9% 83% 15% ·
1	I	276	8% 83% 15% ·
1	K	276	9% 83% 15% ·
2	B	270	11% 81% 18% ·
2	D	270	12% 81% 19% ·

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Mol	Chain	Length	Quality of chain
2	F	270	13% 80% 19%
2	H	270	11% 80% 19%
2	J	270	13% 80% 19%
2	L	270	12% 81% 18%

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
3	ATP	B	805	-	-	X	-
3	ATP	D	906	-	-	X	-
3	ATP	F	905	-	-	X	-
3	ATP	H	805	-	-	X	-
3	ATP	J	804	-	-	X	-
3	ATP	L	905	-	-	X	-
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	-
7	MOO	F	902	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 (i)

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.

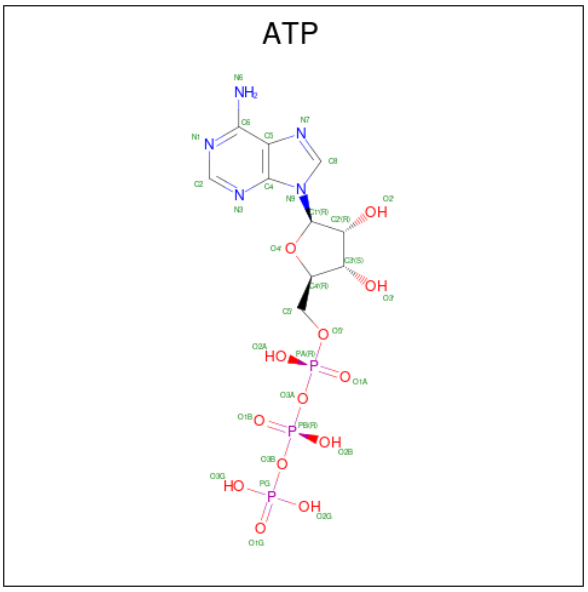
- Molecule 1 is a protein called Molybdenum storage protein subunit alpha.

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

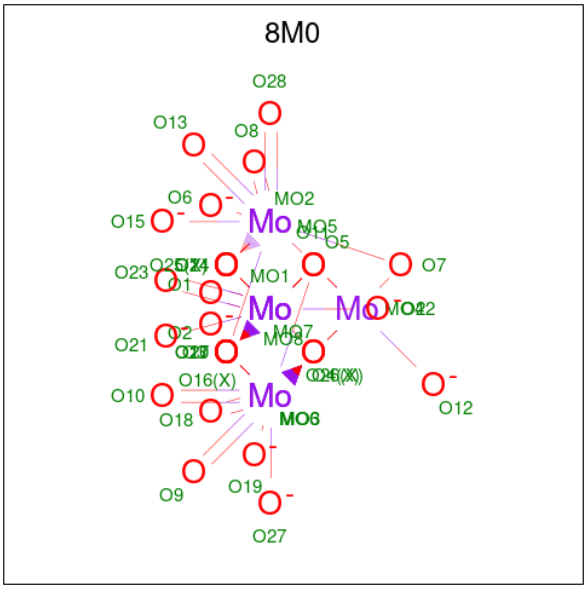


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is bis(mu4-oxo)-tetrakis(mu3-oxo)-hexakis(mu2-oxo)-hexadecaoxo-octamolybdenum (VI) (three-letter code: 8M0) (formula: Mo_8O_{28}).



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

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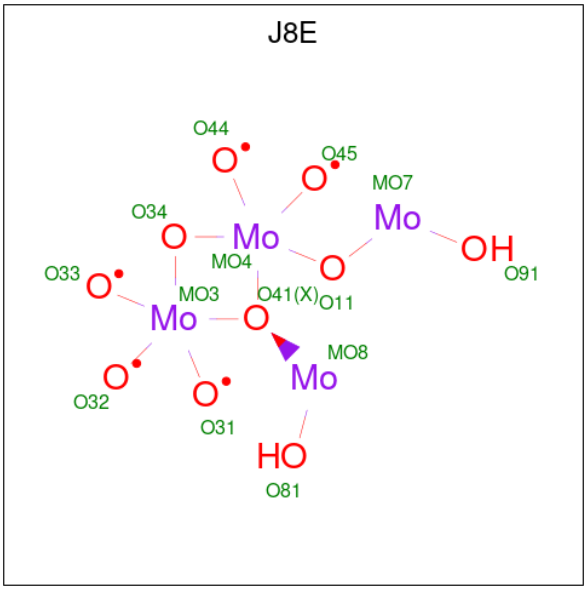
Mol	Chain	Residues	Atoms			AltConf
5	F	1	Total	Mo	O	0
			36	8	28	
5	G	1	Total	Mo	O	0
			34	8	26	
5	H	1	Total	Mo	O	0
			36	8	28	
5	I	1	Total	Mo	O	0
			34	8	26	
5	J	1	Total	Mo	O	0
			36	8	28	
5	K	1	Total	Mo	O	0
			34	8	26	
5	L	1	Total	Mo	O	0
			36	8	28	

- Molecule 6 is oxidanyl-[[2,2,4,4,4-pentakis($l^{1}-oxidanyl)-1-(oxidanylmolybdenio)-1$l^{3},3-dioxa-2$l^{5},4$l^{5}-dimolybdacyclobut-2-yl]oxy]molybdenum (three-letter code: J8E) (formula: $H_2Mo_4O_{10}$).



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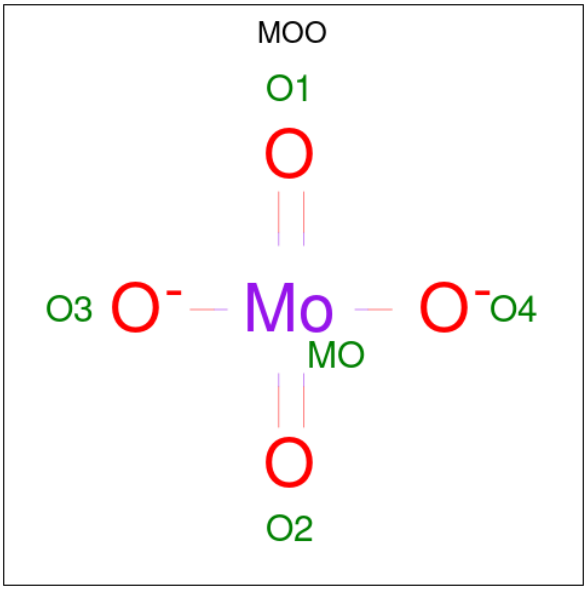
Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total Mo O 14 4 10	0
6	E	1	Total Mo O 14 4 10	0
6	F	1	Total Mo O 14 4 10	0
6	G	1	Total Mo O 14 4 10	0
6	H	1	Total Mo O 14 4 10	0
6	I	1	Total Mo O 14 4 10	0
6	J	1	Total Mo O 14 4 10	0
6	K	1	Total Mo O 14 4 10	0
6	L	1	Total Mo O 14 4 10	0

- Molecule 7 is MOLYBDATE ION (three-letter code: MOO) (formula: MoO_4).



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

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

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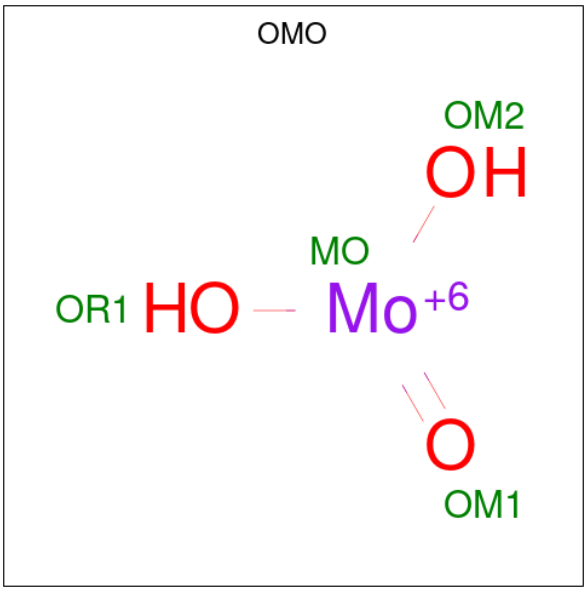
Mol	Chain	Residues	Atoms			AltConf
7	G	1	Total 5	Mo 1	O 4	0
7	H	1	Total 5	Mo 1	O 4	0
7	H	1	Total 5	Mo 1	O 4	0
7	H	1	Total 5	Mo 1	O 4	0
7	H	1	Total 5	Mo 1	O 4	0
7	H	1	Total 5	Mo 1	O 4	0
7	I	1	Total 5	Mo 1	O 4	0
7	I	1	Total 5	Mo 1	O 4	0
7	I	1	Total 5	Mo 1	O 4	0
7	J	1	Total 5	Mo 1	O 4	0
7	J	1	Total 5	Mo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

- Molecule 8 is MO(VI)(=O)(OH)2 CLUSTER (three-letter code: OMO) (formula: H_2MoO_3).



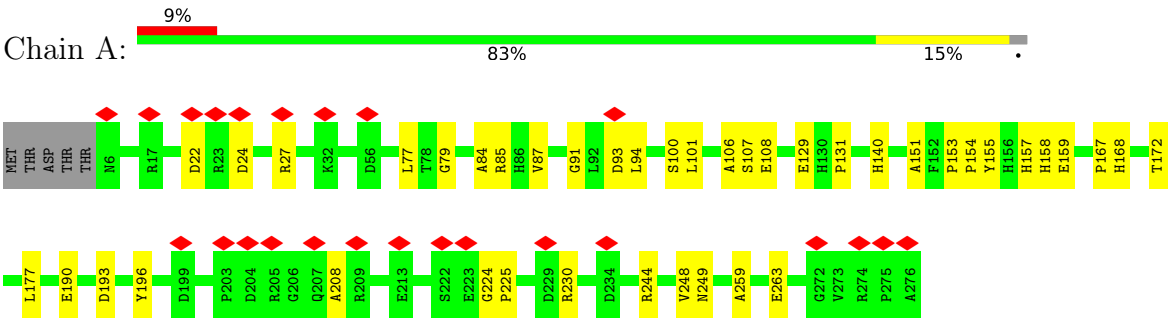
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total 4	Mo 1	O 3	0
8	C	1	Total 4	Mo 1	O 3	0
8	E	1	Total 4	Mo 1	O 3	0
8	G	1	Total 4	Mo 1	O 3	0
8	I	1	Total 4	Mo 1	O 3	0
8	K	1	Total 4	Mo 1	O 3	0

3 Residue-property plots (i)

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

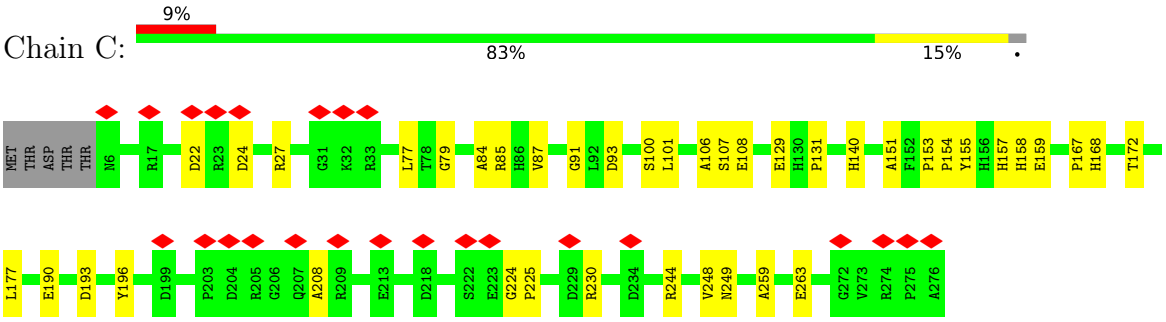
• Molecule 1: Molybdenum storage protein subunit alpha

Chain A:



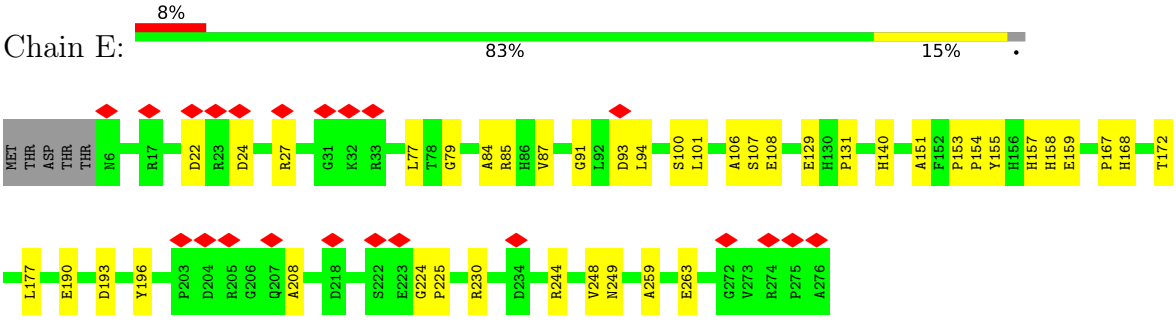
• Molecule 1: Molybdenum storage protein subunit alpha

Chain C:



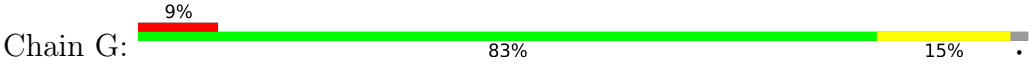
• Molecule 1: Molybdenum storage protein subunit alpha

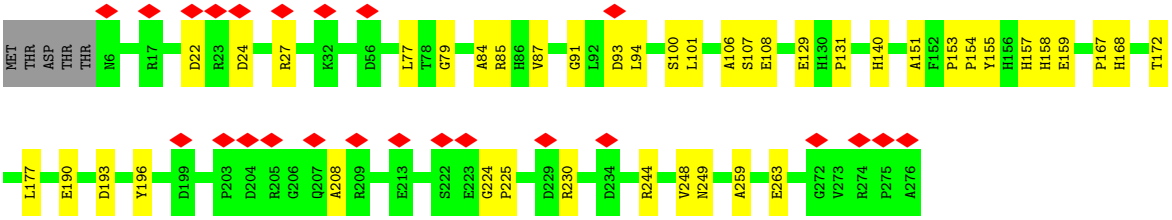
Chain E:



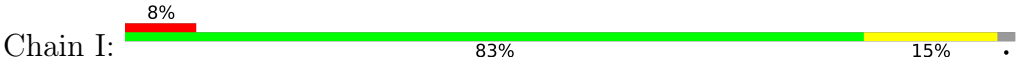
• Molecule 1: Molybdenum storage protein subunit alpha

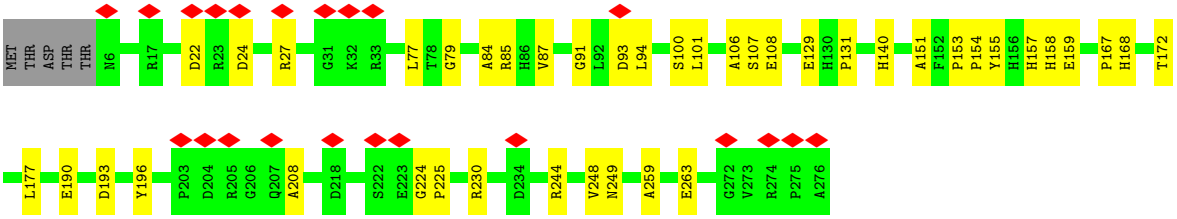
Chain G:



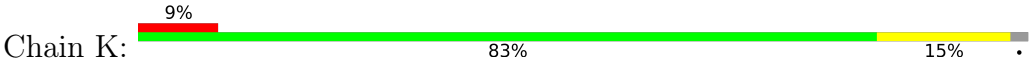


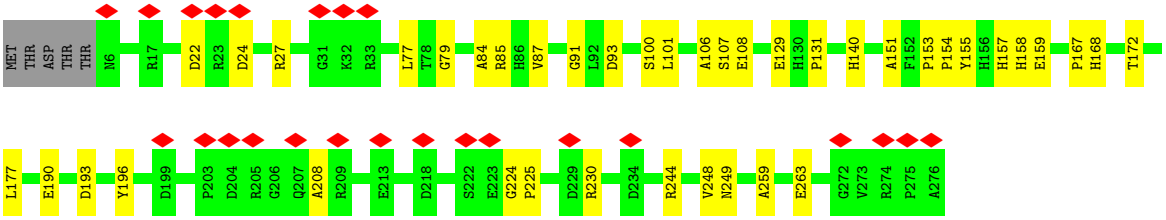
• Molecule 1: Molybdenum storage protein subunit alpha



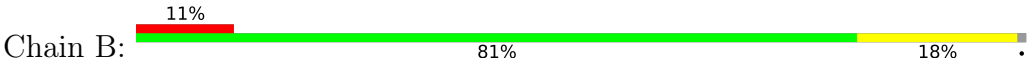


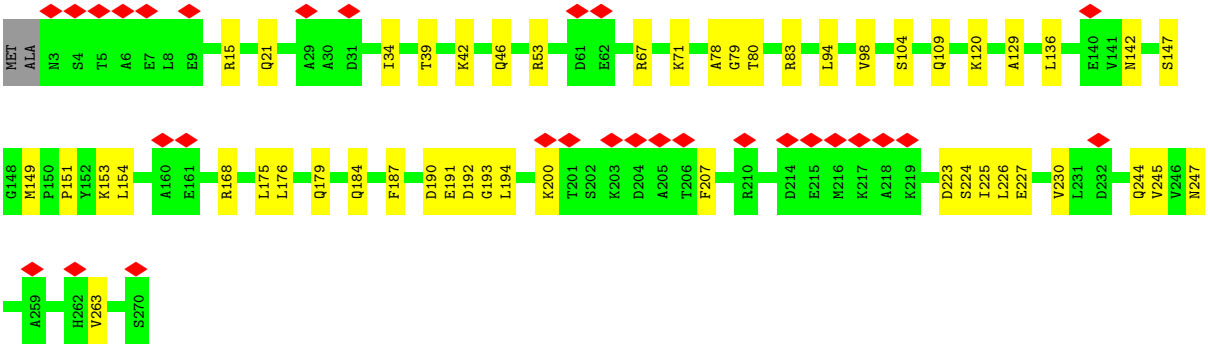
• Molecule 1: Molybdenum storage protein subunit alpha



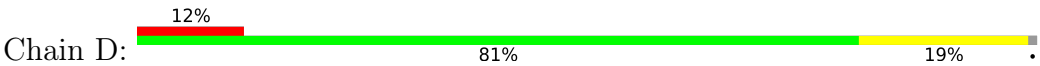


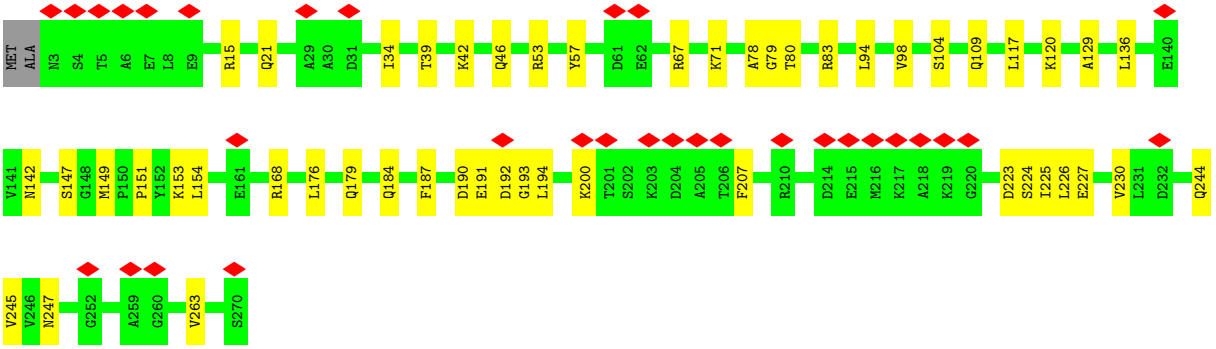
• Molecule 2: Molybdenum storage protein subunit beta



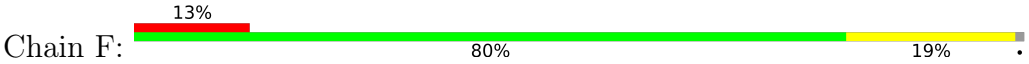


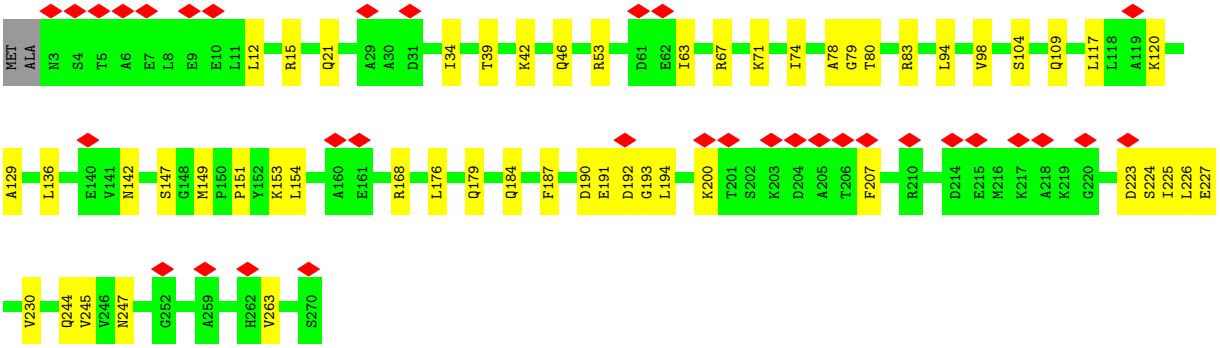
• Molecule 2: Molybdenum storage protein subunit beta



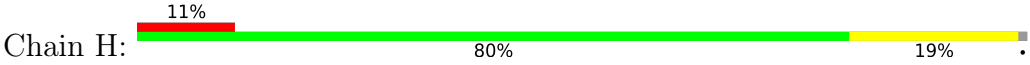


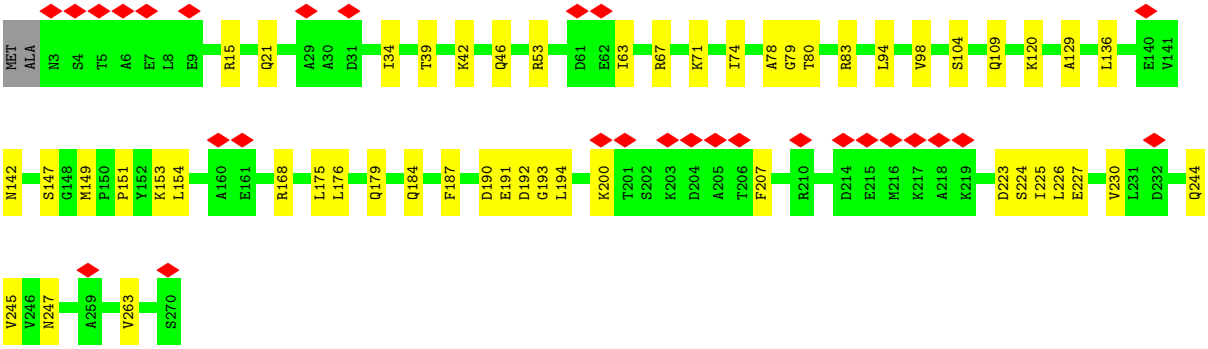
• Molecule 2: Molybdenum storage protein subunit beta



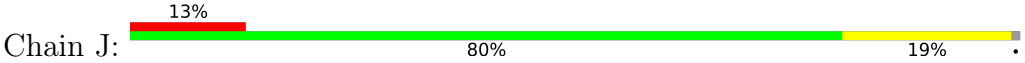


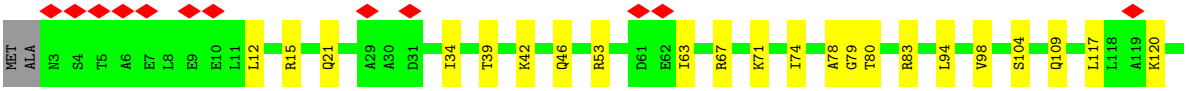
• Molecule 2: Molybdenum storage protein subunit beta

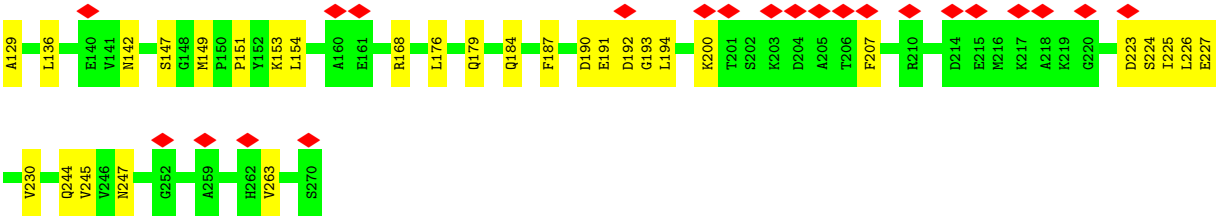




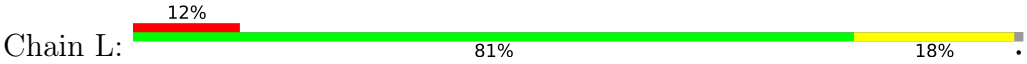
• Molecule 2: Molybdenum storage protein subunit beta

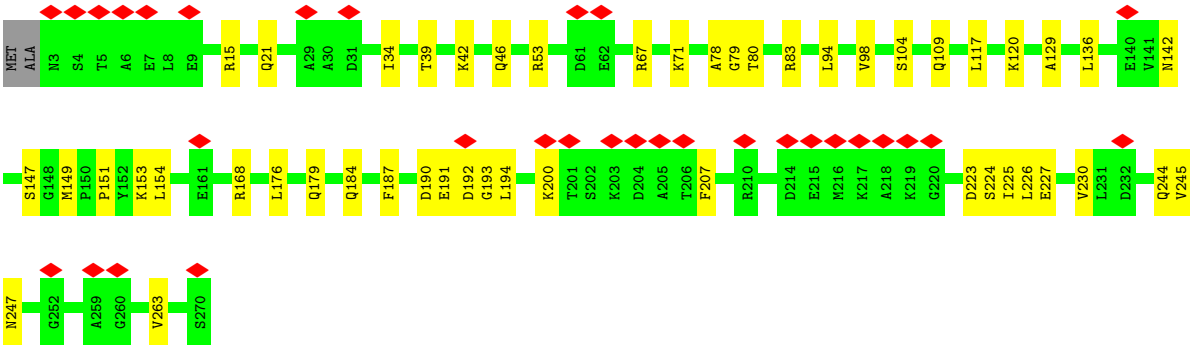






• Molecule 2: Molybdenum storage protein subunit beta





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	222.0, 222.0, 222.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MOO, OMO, 8M0, J8E, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	1/2081 (0.0%)	0.63	0/2836
1	C	0.48	1/2081 (0.0%)	0.63	0/2836
1	E	0.48	1/2081 (0.0%)	0.63	0/2836
1	G	0.48	1/2081 (0.0%)	0.63	0/2836
1	I	0.48	1/2081 (0.0%)	0.63	0/2836
1	K	0.48	1/2081 (0.0%)	0.63	0/2836
2	B	0.40	0/2041	0.59	0/2773
2	D	0.40	0/2041	0.58	0/2773
2	F	0.40	0/2041	0.59	0/2773
2	H	0.40	0/2041	0.59	0/2773
2	J	0.40	0/2041	0.59	0/2773
2	L	0.40	0/2041	0.58	0/2773
All	All	0.44	6/24732 (0.0%)	0.61	0/33654

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	PRO	C-N	7.46	1.51	1.34
1	G	154	PRO	C-N	7.46	1.51	1.34
1	E	154	PRO	C-N	7.45	1.51	1.34
1	I	154	PRO	C-N	7.45	1.51	1.34
1	C	154	PRO	C-N	7.43	1.51	1.34
1	K	154	PRO	C-N	7.43	1.51	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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	10	0
3	C	31	0	12	5	0
3	D	31	0	12	10	0
3	E	31	0	12	5	0
3	F	31	0	12	10	0
3	G	31	0	12	5	0
3	H	31	0	12	10	0
3	I	31	0	12	5	0
3	J	31	0	12	10	0
3	K	31	0	12	5	0
3	L	31	0	12	10	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	2	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	713	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 (713) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:805:ATP:N3	3:H:805:ATP:H2'	1.96	0.80
3:B:805:ATP:N3	3:B:805:ATP:H2'	1.96	0.80
3:D:906:ATP:N3	3:D:906:ATP:H2'	1.96	0.80
7:B:801:MOO:O4	5:B:806:8M0:O19	2.00	0.79
3:F:905:ATP:N3	3:F:905:ATP:H2'	1.96	0.79
3:J:804:ATP:H2'	3:J:804:ATP:N3	1.96	0.79
7:H:801:MOO:O4	5:H:806:8M0:O19	2.00	0.79
3:L:905:ATP:H2'	3:L:905:ATP:N3	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
7:I:306:MOO:MO	7:I:306:MOO:O1	1.69	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:200:LYS:NZ	3:B:805:ATP:O2'	2.28	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
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
7:L:902:MOO:MO	7:L:902:MOO:O1	1.69	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ALA:C	5:E:304:8M0:O6	2.42	0.57
1:I:106:ALA:C	5:I:304:8M0:O6	2.42	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:106:ALA:C	5:A:303:8M0:O6	2.42	0.57
1:G:106:ALA:C	5:G:303:8M0:O6	2.42	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:C:106:ALA:C	5:C:303:8M0:O6	2.42	0.57
1:G:158:HIS:ND1	5:H:806:8M0:O8	2.37	0.57
1:K:106:ALA:C	5:K:304:8M0:O6	2.42	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:200:LYS:NZ	3:D:906:ATP:O2'	2.28	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
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
3:D:906:ATP:N3	3:D:906:ATP:C2'	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:HIS:ND1	5:L:906:8M0:O8	2.37	0.50
3:L:905:ATP:N3	3:L:905:ATP:C2'	2.73	0.50
3:F:905:ATP:N3	3:F:905:ATP:C2'	2.73	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
3:J:804:ATP:N3	3:J:804:ATP:C2'	2.73	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
3:B:805:ATP:N3	3:B:805:ATP:C2'	2.73	0.49
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
3:H:805:ATP:N3	3:H:805:ATP:C2'	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	270/276 (98%)	262 (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	3234/3276 (99%)	3136 (97%)	98 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	205 (99%)	3 (1%)	67	86
2	D	208/206 (101%)	205 (99%)	3 (1%)	67	86
2	F	208/206 (101%)	205 (99%)	3 (1%)	67	86
2	H	208/206 (101%)	205 (99%)	3 (1%)	67	86
2	J	208/206 (101%)	205 (99%)	3 (1%)	67	86
2	L	208/206 (101%)	205 (99%)	3 (1%)	67	86
All	All	2520/2532 (100%)	2502 (99%)	18 (1%)	84	94

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	ARG
2	B	142	ASN
2	B	153	LYS
2	D	67	ARG
2	D	142	ASN
2	D	153	LYS
2	F	67	ARG
2	F	142	ASN
2	F	153	LYS
2	H	67	ARG
2	H	142	ASN
2	H	153	LYS
2	J	67	ARG
2	J	142	ASN

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Mol	Chain	Res	Type
2	J	153	LYS
2	L	67	ARG
2	L	142	ASN
2	L	153	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	21	GLN
1	A	86	HIS
1	A	111	GLN
1	A	246	GLN
2	B	142	ASN
2	B	179	GLN
1	C	10	HIS
1	C	21	GLN
1	C	86	HIS
1	C	111	GLN
1	C	246	GLN
2	D	142	ASN
2	D	179	GLN
1	E	10	HIS
1	E	21	GLN
1	E	86	HIS
1	E	111	GLN
1	E	246	GLN
2	F	142	ASN
2	F	179	GLN
1	G	10	HIS
1	G	21	GLN
1	G	86	HIS
1	G	111	GLN
1	G	246	GLN
2	H	142	ASN
2	H	179	GLN
1	I	10	HIS
1	I	21	GLN
1	I	86	HIS
1	I	111	GLN
1	I	246	GLN
2	J	142	ASN

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Mol	Chain	Res	Type
2	J	179	GLN
1	K	10	HIS
1	K	21	GLN
1	K	86	HIS
1	K	111	GLN
1	K	246	GLN
2	L	142	ASN
2	L	179	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 monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	8M0	H	806	-	22,48,48	8.03	12 (54%)	-		
7	MOO	G	306	-	2,4,4	1.35	0	-		
7	MOO	I	308	-	2,4,4	1.33	0	-		
8	OMO	A	307	-	0,3,3	-	-	-		
7	MOO	A	308	-	2,4,4	1.32	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	8M0	A	303	-	17,46,48	8.30	8 (47%)	-		
3	ATP	F	905	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
3	ATP	E	302	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)
7	MOO	H	803	-	2,4,4	1.35	0	-		
7	MOO	I	306	-	2,4,4	1.33	0	-		
3	ATP	L	905	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
5	8M0	L	906	-	22,48,48	8.04	12 (54%)	-		
6	J8E	L	901	-	0,14,14	-	-	-		
5	8M0	K	304	-	17,46,48	8.29	8 (47%)	-		
6	J8E	A	304	-	0,14,14	-	-	-		
3	ATP	K	302	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)
5	8M0	E	304	-	17,46,48	8.31	8 (47%)	-		
6	J8E	C	304	-	0,14,14	-	-	-		
7	MOO	H	801	-	2,4,4	1.34	0	-		
7	MOO	H	802	-	2,4,4	1.34	0	-		
7	MOO	B	801	-	2,4,4	1.34	0	-		
7	MOO	B	802	-	2,4,4	1.34	0	-		
3	ATP	I	302	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)
7	MOO	C	306	-	2,4,4	1.34	0	-		
7	MOO	D	905	-	2,4,4	1.33	0	-		
7	MOO	L	907	3	2,4,4	1.34	0	-		
6	J8E	K	305	-	0,14,14	-	-	-		
6	J8E	H	808	-	0,14,14	-	-	-		
5	8M0	B	806	-	22,48,48	8.03	12 (54%)	-		
6	J8E	E	305	-	0,14,14	-	-	-		
7	MOO	D	902	-	2,4,4	1.34	0	-		
5	8M0	G	303	-	17,46,48	8.30	8 (47%)	-		
8	OMO	E	301	-	0,3,3	-	-	-		
7	MOO	J	803	-	2,4,4	1.34	0	-		
5	8M0	J	805	-	22,48,48	8.03	12 (54%)	-		
7	MOO	I	307	-	2,4,4	1.34	0	-		
5	8M0	C	303	-	17,46,48	8.29	8 (47%)	-		
7	MOO	E	307	-	2,4,4	1.34	0	-		
6	J8E	B	808	-	0,14,14	-	-	-		
7	MOO	D	908	3	2,4,4	1.34	0	-		
8	OMO	I	301	-	0,3,3	-	-	-		
6	J8E	F	901	-	0,14,14	-	-	-		
7	MOO	L	904	-	2,4,4	1.33	0	-		
7	MOO	D	904	-	2,4,4	1.33	0	-		
7	MOO	A	306	-	2,4,4	1.35	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	8M0	I	304	-	17,46,48	8.31	8 (47%)	-		
7	MOO	E	306	-	2,4,4	1.33	0	-		
7	MOO	F	902	-	2,4,4	1.35	0	-		
7	MOO	G	305	-	2,4,4	1.33	0	-		
3	ATP	A	301	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)
3	ATP	H	805	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
7	MOO	B	804	-	2,4,4	1.33	0	-		
7	MOO	G	307	-	2,4,4	1.32	0	-		
7	MOO	K	307	-	2,4,4	1.34	0	-		
8	OMO	G	308	-	0,3,3	-	-	-		
7	MOO	K	306	-	2,4,4	1.33	0	-		
6	J8E	G	304	-	0,14,14	-	-	-		
3	ATP	J	804	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
7	MOO	H	804	-	2,4,4	1.33	0	-		
7	MOO	B	803	-	2,4,4	1.35	0	-		
7	MOO	F	903	-	2,4,4	1.33	0	-		
6	J8E	I	305	-	0,14,14	-	-	-		
5	8M0	F	906	-	22,48,48	8.03	12 (54%)	-		
7	MOO	A	305	-	2,4,4	1.33	0	-		
7	MOO	B	807	3	2,4,4	1.34	0	-		
6	J8E	D	901	-	0,14,14	-	-	-		
3	ATP	C	301	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)
7	MOO	C	305	-	2,4,4	1.33	0	-		
6	J8E	J	807	-	0,14,14	-	-	-		
7	MOO	F	904	-	2,4,4	1.34	0	-		
8	OMO	C	307	-	0,3,3	-	-	-		
3	ATP	D	906	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
7	MOO	F	907	3	2,4,4	1.34	0	-		
7	MOO	L	902	-	2,4,4	1.34	0	-		
7	MOO	H	807	3	2,4,4	1.34	0	-		
7	MOO	J	806	3	2,4,4	1.34	0	-		
7	MOO	L	903	-	2,4,4	1.33	0	-		
3	ATP	B	805	7	26,33,33	0.68	0	31,52,52	0.93	2 (6%)
8	OMO	K	301	-	0,3,3	-	-	-		
7	MOO	D	903	-	2,4,4	1.33	0	-		
7	MOO	J	801	-	2,4,4	1.35	0	-		
5	8M0	D	907	-	22,48,48	8.04	12 (54%)	-		
7	MOO	J	802	-	2,4,4	1.33	0	-		
3	ATP	G	301	4	26,33,33	1.24	3 (11%)	31,52,52	1.49	3 (9%)

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	I	302	4	-	1/18/38/38	0/3/3/3
6	J8E	I	305	-	-	-	0/1/1/1
6	J8E	K	305	-	-	-	0/1/1/1
6	J8E	H	808	-	-	-	0/1/1/1
6	J8E	D	901	-	-	-	0/1/1/1
3	ATP	C	301	4	-	1/18/38/38	0/3/3/3
6	J8E	E	305	-	-	-	0/1/1/1
3	ATP	F	905	7	-	1/18/38/38	0/3/3/3
3	ATP	A	301	4	-	1/18/38/38	0/3/3/3
3	ATP	H	805	7	-	1/18/38/38	0/3/3/3
3	ATP	E	302	4	-	1/18/38/38	0/3/3/3
6	J8E	J	807	-	-	-	0/1/1/1
3	ATP	L	905	7	-	1/18/38/38	0/3/3/3
6	J8E	L	901	-	-	-	0/1/1/1
6	J8E	A	304	-	-	-	0/1/1/1
3	ATP	D	906	7	-	1/18/38/38	0/3/3/3
3	ATP	K	302	4	-	1/18/38/38	0/3/3/3
6	J8E	C	304	-	-	-	0/1/1/1
3	ATP	B	805	7	-	1/18/38/38	0/3/3/3
6	J8E	B	808	-	-	-	0/1/1/1
6	J8E	G	304	-	-	-	0/1/1/1
3	ATP	J	804	7	-	1/18/38/38	0/3/3/3
6	J8E	F	901	-	-	-	0/1/1/1
3	ATP	G	301	4	-	1/18/38/38	0/3/3/3

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	304	8M0	O20-MO8	22.85	1.96	1.74
5	I	304	8M0	O20-MO8	22.85	1.96	1.74
5	A	303	8M0	O20-MO8	22.81	1.96	1.74
5	G	303	8M0	O20-MO8	22.81	1.96	1.74
5	C	303	8M0	O20-MO8	22.78	1.96	1.74
5	K	304	8M0	O20-MO8	22.78	1.96	1.74
5	E	304	8M0	O7-MO4	21.29	1.95	1.74
5	I	304	8M0	O7-MO4	21.29	1.95	1.74
5	A	303	8M0	O7-MO4	21.27	1.95	1.74
5	G	303	8M0	O7-MO4	21.27	1.95	1.74
5	C	303	8M0	O7-MO4	21.26	1.95	1.74
5	K	304	8M0	O7-MO4	21.26	1.95	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	806	8M0	O7-MO4	17.77	1.91	1.74
5	H	806	8M0	O7-MO4	17.77	1.91	1.74
5	D	907	8M0	O7-MO4	17.75	1.91	1.74
5	L	906	8M0	O7-MO4	17.75	1.91	1.74
5	F	906	8M0	O7-MO4	17.70	1.91	1.74
5	J	805	8M0	O7-MO4	17.70	1.91	1.74
5	D	907	8M0	O20-MO8	15.94	1.89	1.74
5	L	906	8M0	O20-MO8	15.94	1.89	1.74
5	B	806	8M0	O20-MO8	15.93	1.89	1.74
5	H	806	8M0	O20-MO8	15.93	1.89	1.74
5	F	906	8M0	O20-MO8	15.92	1.89	1.74
5	J	805	8M0	O20-MO8	15.92	1.89	1.74
5	D	907	8M0	O9-MO3	15.57	1.90	1.71
5	L	906	8M0	O9-MO3	15.57	1.90	1.71
5	F	906	8M0	O9-MO3	15.53	1.90	1.71
5	J	805	8M0	O9-MO3	15.53	1.90	1.71
5	B	806	8M0	O9-MO3	15.53	1.90	1.71
5	H	806	8M0	O9-MO3	15.53	1.90	1.71
5	D	907	8M0	O10-MO3	12.67	1.87	1.71
5	F	906	8M0	O10-MO3	12.67	1.87	1.71
5	J	805	8M0	O10-MO3	12.67	1.87	1.71
5	L	906	8M0	O10-MO3	12.67	1.87	1.71
5	B	806	8M0	O10-MO3	12.67	1.87	1.71
5	H	806	8M0	O10-MO3	12.67	1.87	1.71
5	F	906	8M0	O23-MO7	11.25	1.88	1.68
5	J	805	8M0	O23-MO7	11.25	1.88	1.68
5	D	907	8M0	O23-MO7	11.25	1.88	1.68
5	L	906	8M0	O23-MO7	11.25	1.88	1.68
5	B	806	8M0	O23-MO7	11.25	1.88	1.68
5	H	806	8M0	O23-MO7	11.25	1.88	1.68
5	F	906	8M0	O1-MO1	10.29	1.86	1.68
5	J	805	8M0	O1-MO1	10.29	1.86	1.68
5	D	907	8M0	O1-MO1	10.29	1.86	1.68
5	L	906	8M0	O1-MO1	10.29	1.86	1.68
5	B	806	8M0	O1-MO1	10.29	1.86	1.68
5	H	806	8M0	O1-MO1	10.29	1.86	1.68
5	B	806	8M0	O28-MO5	8.34	1.81	1.71
5	H	806	8M0	O28-MO5	8.34	1.81	1.71
5	D	907	8M0	O28-MO5	8.34	1.81	1.71
5	L	906	8M0	O28-MO5	8.34	1.81	1.71
5	F	906	8M0	O28-MO5	8.33	1.81	1.71
5	J	805	8M0	O28-MO5	8.33	1.81	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	304	8M0	O18-MO6	7.64	1.81	1.68
5	I	304	8M0	O18-MO6	7.64	1.81	1.68
5	C	303	8M0	O18-MO6	7.64	1.81	1.68
5	K	304	8M0	O18-MO6	7.64	1.81	1.68
5	A	303	8M0	O18-MO6	7.62	1.81	1.68
5	G	303	8M0	O18-MO6	7.62	1.81	1.68
5	A	303	8M0	O23-MO7	7.47	1.81	1.68
5	G	303	8M0	O23-MO7	7.47	1.81	1.68
5	E	304	8M0	O23-MO7	7.46	1.81	1.68
5	I	304	8M0	O23-MO7	7.46	1.81	1.68
5	C	303	8M0	O23-MO7	7.46	1.81	1.68
5	K	304	8M0	O23-MO7	7.46	1.81	1.68
5	B	806	8M0	O18-MO6	7.01	1.80	1.68
5	H	806	8M0	O18-MO6	7.01	1.80	1.68
5	D	907	8M0	O18-MO6	7.00	1.80	1.68
5	L	906	8M0	O18-MO6	7.00	1.80	1.68
5	F	906	8M0	O18-MO6	6.96	1.80	1.68
5	J	805	8M0	O18-MO6	6.96	1.80	1.68
5	A	303	8M0	O13-MO5	6.49	1.81	1.67
5	G	303	8M0	O13-MO5	6.49	1.81	1.67
5	C	303	8M0	O13-MO5	6.48	1.81	1.67
5	K	304	8M0	O13-MO5	6.48	1.81	1.67
5	E	304	8M0	O13-MO5	6.46	1.81	1.67
5	I	304	8M0	O13-MO5	6.46	1.81	1.67
5	F	906	8M0	O26-MO4	5.89	2.18	1.88
5	J	805	8M0	O26-MO4	5.89	2.18	1.88
5	B	806	8M0	O26-MO4	5.89	2.18	1.88
5	H	806	8M0	O26-MO4	5.89	2.18	1.88
5	D	907	8M0	O26-MO4	5.88	2.18	1.88
5	L	906	8M0	O26-MO4	5.88	2.18	1.88
5	F	906	8M0	O25-MO8	5.01	2.14	1.88
5	J	805	8M0	O25-MO8	5.01	2.14	1.88
5	B	806	8M0	O25-MO8	5.01	2.14	1.88
5	H	806	8M0	O25-MO8	5.01	2.14	1.88
5	D	907	8M0	O25-MO8	5.01	2.14	1.88
5	L	906	8M0	O25-MO8	5.01	2.14	1.88
5	F	906	8M0	O13-MO5	4.93	1.77	1.71
5	J	805	8M0	O13-MO5	4.93	1.77	1.71
5	D	907	8M0	O13-MO5	4.88	1.77	1.71
5	L	906	8M0	O13-MO5	4.88	1.77	1.71
5	B	806	8M0	O13-MO5	4.86	1.77	1.71
5	H	806	8M0	O13-MO5	4.86	1.77	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	8M0	O8-MO2	4.02	1.75	1.68
5	G	303	8M0	O8-MO2	4.02	1.75	1.68
5	E	304	8M0	O8-MO2	4.01	1.75	1.68
5	I	304	8M0	O8-MO2	4.01	1.75	1.68
5	C	303	8M0	O8-MO2	4.00	1.75	1.68
5	K	304	8M0	O8-MO2	4.00	1.75	1.68
3	A	301	ATP	C2-N3	3.52	1.37	1.32
3	G	301	ATP	C2-N3	3.52	1.37	1.32
3	C	301	ATP	C2-N3	3.48	1.37	1.32
3	K	302	ATP	C2-N3	3.48	1.37	1.32
3	E	302	ATP	C2-N3	3.48	1.37	1.32
3	I	302	ATP	C2-N3	3.48	1.37	1.32
5	B	806	8M0	O8-MO2	3.38	1.74	1.68
5	H	806	8M0	O8-MO2	3.38	1.74	1.68
5	D	907	8M0	O8-MO2	3.38	1.74	1.68
5	L	906	8M0	O8-MO2	3.38	1.74	1.68
5	F	906	8M0	O8-MO2	3.37	1.74	1.68
5	J	805	8M0	O8-MO2	3.37	1.74	1.68
5	A	303	8M0	O1-MO1	3.19	1.73	1.68
5	G	303	8M0	O1-MO1	3.19	1.73	1.68
5	E	304	8M0	O1-MO1	3.19	1.73	1.68
5	I	304	8M0	O1-MO1	3.19	1.73	1.68
5	C	303	8M0	O1-MO1	3.18	1.73	1.68
5	K	304	8M0	O1-MO1	3.18	1.73	1.68
5	E	304	8M0	O14-MO5	3.09	2.01	1.89
5	I	304	8M0	O14-MO5	3.09	2.01	1.89
5	A	303	8M0	O14-MO5	3.08	2.01	1.89
5	G	303	8M0	O14-MO5	3.08	2.01	1.89
5	C	303	8M0	O14-MO5	3.07	2.01	1.89
5	K	304	8M0	O14-MO5	3.07	2.01	1.89
3	E	302	ATP	C5-C4	2.14	1.46	1.40
3	I	302	ATP	C5-C4	2.14	1.46	1.40
3	A	301	ATP	C5-C4	2.14	1.46	1.40
3	G	301	ATP	C5-C4	2.14	1.46	1.40
3	C	301	ATP	C5-C4	2.13	1.46	1.40
3	K	302	ATP	C5-C4	2.13	1.46	1.40
3	A	301	ATP	PG-O3G	-2.11	1.46	1.54
3	G	301	ATP	PG-O3G	-2.11	1.46	1.54
3	C	301	ATP	PG-O3G	-2.11	1.46	1.54
3	K	302	ATP	PG-O3G	-2.11	1.46	1.54
3	E	302	ATP	PG-O3G	-2.10	1.46	1.54
3	I	302	ATP	PG-O3G	-2.10	1.46	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	ATP	N3-C2-N1	-4.96	120.92	128.68
3	K	302	ATP	N3-C2-N1	-4.96	120.92	128.68
3	E	302	ATP	N3-C2-N1	-4.96	120.93	128.68
3	I	302	ATP	N3-C2-N1	-4.96	120.93	128.68
3	A	301	ATP	N3-C2-N1	-4.95	120.94	128.68
3	G	301	ATP	N3-C2-N1	-4.95	120.94	128.68
3	A	301	ATP	C2-N1-C6	3.08	124.02	118.75
3	G	301	ATP	C2-N1-C6	3.08	124.02	118.75
3	C	301	ATP	C2-N1-C6	3.06	123.99	118.75
3	K	302	ATP	C2-N1-C6	3.06	123.99	118.75
3	E	302	ATP	C2-N1-C6	3.06	123.98	118.75
3	I	302	ATP	C2-N1-C6	3.06	123.98	118.75
3	D	906	ATP	C5-C6-N6	2.43	124.05	120.35
3	L	905	ATP	C5-C6-N6	2.43	124.05	120.35
3	F	905	ATP	C5-C6-N6	2.43	124.04	120.35
3	J	804	ATP	C5-C6-N6	2.43	124.04	120.35
3	B	805	ATP	C5-C6-N6	2.43	124.04	120.35
3	H	805	ATP	C5-C6-N6	2.43	124.04	120.35
3	C	301	ATP	O5'-C5'-C4'	-2.28	101.13	108.99
3	K	302	ATP	O5'-C5'-C4'	-2.28	101.13	108.99
3	E	302	ATP	O5'-C5'-C4'	-2.28	101.15	108.99
3	I	302	ATP	O5'-C5'-C4'	-2.28	101.15	108.99
3	A	301	ATP	O5'-C5'-C4'	-2.28	101.16	108.99
3	G	301	ATP	O5'-C5'-C4'	-2.28	101.16	108.99
3	B	805	ATP	C3'-C2'-C1'	2.08	104.10	100.98
3	F	905	ATP	C3'-C2'-C1'	2.08	104.10	100.98
3	H	805	ATP	C3'-C2'-C1'	2.08	104.10	100.98
3	J	804	ATP	C3'-C2'-C1'	2.08	104.10	100.98
3	D	906	ATP	C3'-C2'-C1'	2.07	104.10	100.98
3	L	905	ATP	C3'-C2'-C1'	2.07	104.10	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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Mol	Chain	Res	Type	Atoms
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

There are no ring outliers.

78 monomers are involved in 463 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	806	8M0	8	0
7	G	306	MOO	8	0
7	I	308	MOO	9	0
8	A	307	OMO	5	0
7	A	308	MOO	9	0
5	A	303	8M0	2	0
3	F	905	ATP	10	0
3	E	302	ATP	5	0
7	H	803	MOO	9	0
7	I	306	MOO	11	0
3	L	905	ATP	10	0
5	L	906	8M0	8	0
5	K	304	8M0	1	0
6	A	304	J8E	3	0
3	K	302	ATP	5	0
5	E	304	8M0	2	0
6	C	304	J8E	3	0
7	H	801	MOO	7	0
7	H	802	MOO	3	0
7	B	801	MOO	7	0
7	B	802	MOO	3	0
3	I	302	ATP	5	0
7	C	306	MOO	8	0
7	D	905	MOO	7	0
7	L	907	MOO	9	0
6	K	305	J8E	3	0
5	B	806	8M0	8	0
6	E	305	J8E	3	0
7	D	902	MOO	8	0
5	G	303	8M0	2	0
8	E	301	OMO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	803	MOO	7	0
5	J	805	8M0	8	0
7	I	307	MOO	8	0
5	C	303	8M0	1	0
7	E	307	MOO	8	0
7	D	908	MOO	9	0
8	I	301	OMO	5	0
7	L	904	MOO	7	0
7	D	904	MOO	9	0
7	A	306	MOO	8	0
5	I	304	8M0	2	0
7	E	306	MOO	11	0
7	F	902	MOO	8	0
7	G	305	MOO	11	0
3	A	301	ATP	5	0
3	H	805	ATP	10	0
7	B	804	MOO	7	0
7	G	307	MOO	9	0
7	K	307	MOO	8	0
8	G	308	OMO	5	0
7	K	306	MOO	11	0
6	G	304	J8E	3	0
3	J	804	ATP	10	0
7	H	804	MOO	7	0
7	B	803	MOO	9	0
7	F	903	MOO	3	0
6	I	305	J8E	3	0
5	F	906	8M0	8	0
7	A	305	MOO	11	0
7	B	807	MOO	9	0
3	C	301	ATP	5	0
7	C	305	MOO	11	0
7	F	904	MOO	7	0
8	C	307	OMO	5	0
3	D	906	ATP	10	0
7	F	907	MOO	9	0
7	L	902	MOO	7	0
7	H	807	MOO	9	0
7	J	806	MOO	9	0
7	L	903	MOO	3	0
3	B	805	ATP	10	0
8	K	301	OMO	5	0

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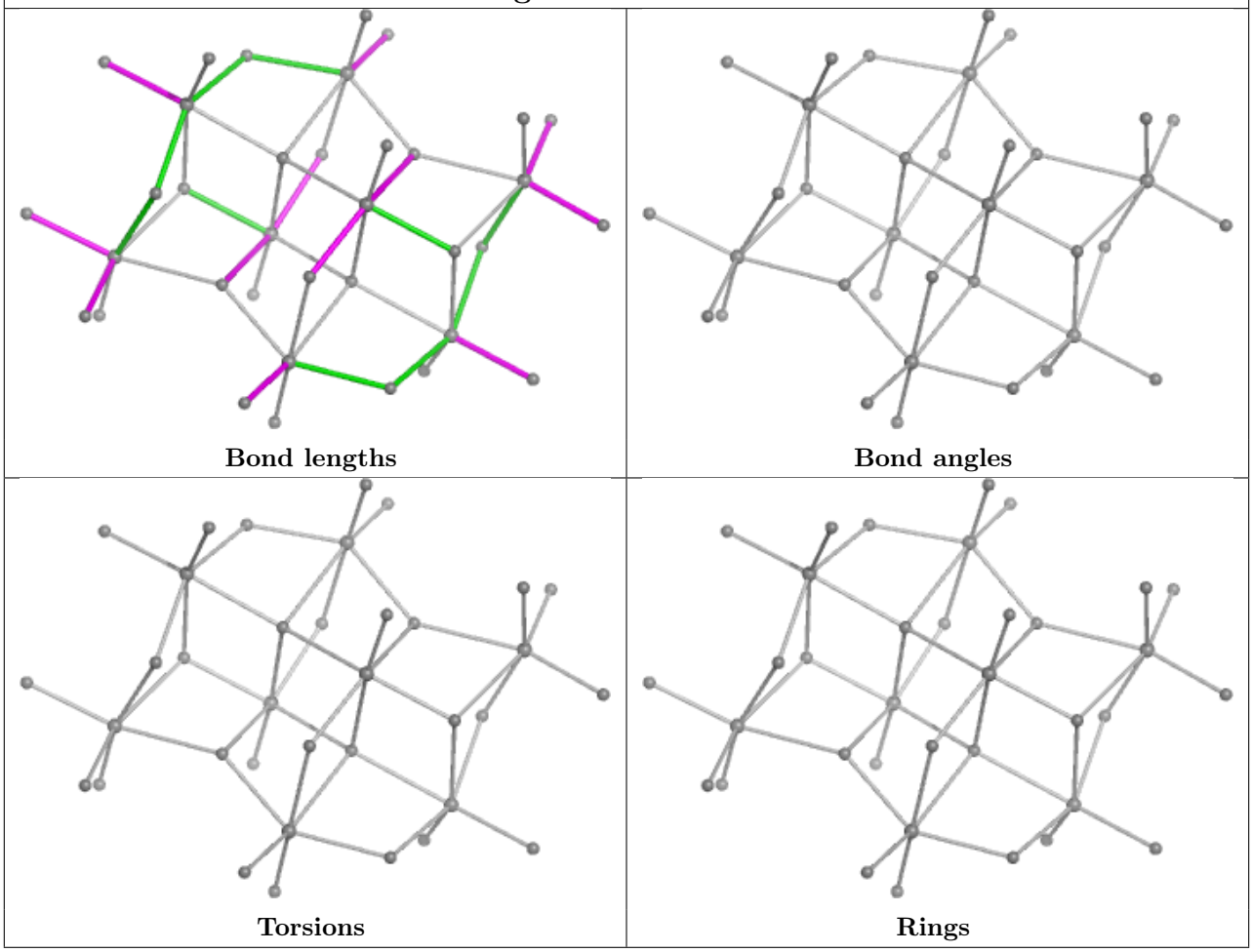
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	903	MOO	3	0
7	J	801	MOO	8	0
5	D	907	8M0	8	0
7	J	802	MOO	3	0
3	G	301	ATP	5	0

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.

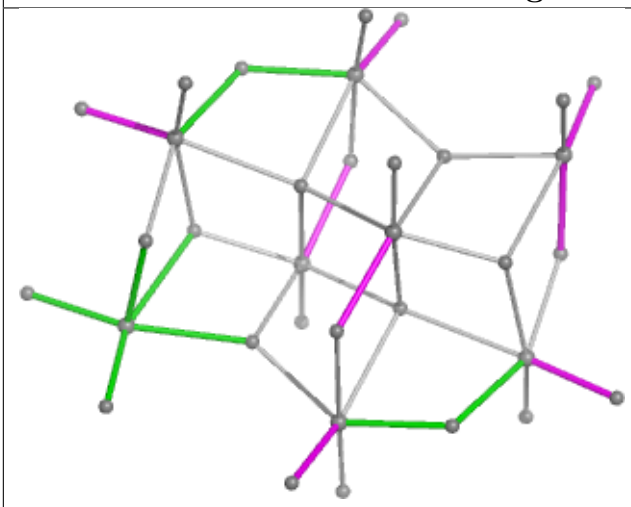
Ligand 8M0 H 806



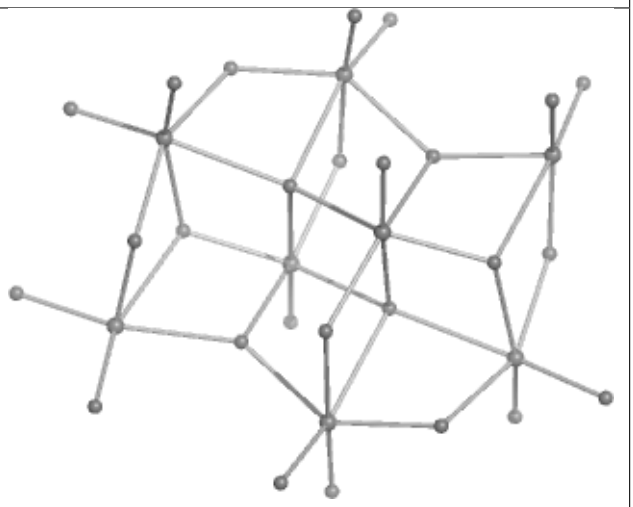
Bond lengths **Bond angles**

Torsions **Rings**

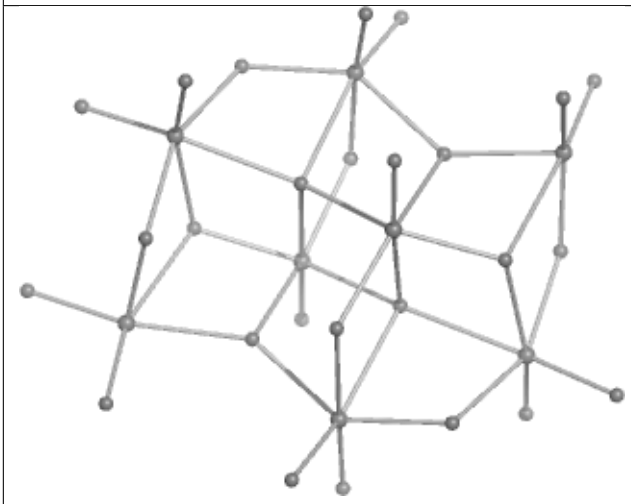
Ligand 8M0 A 303



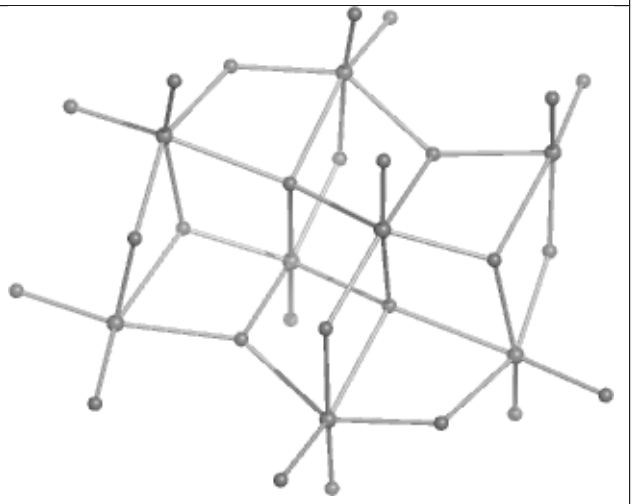
Bond lengths



Bond angles

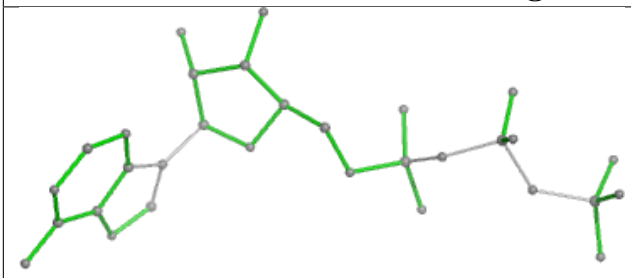


Torsions

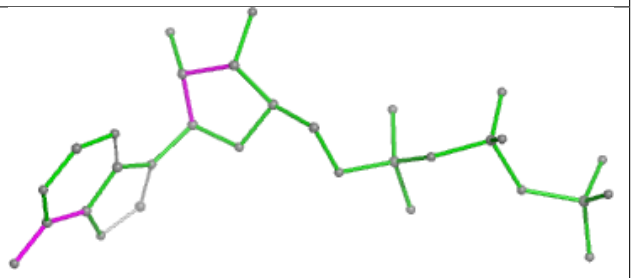


Rings

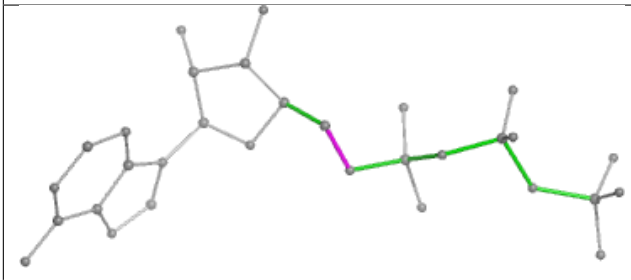
Ligand ATP F 905



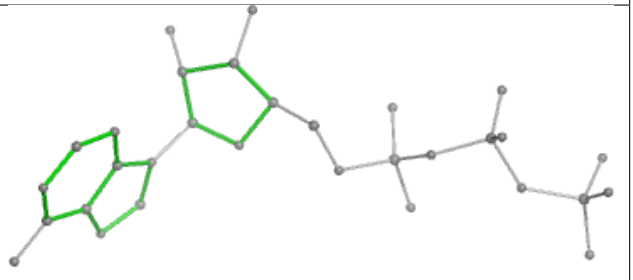
Bond lengths



Bond angles

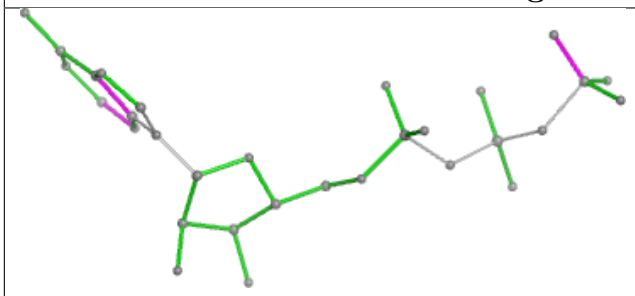


Torsions

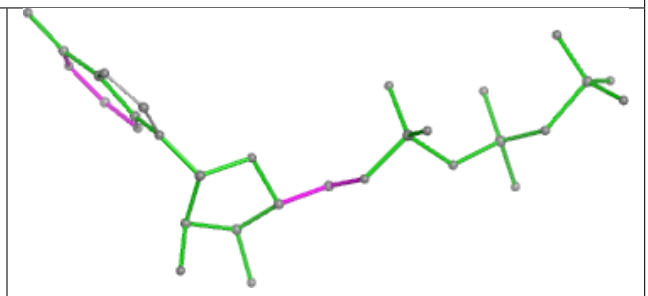


Rings

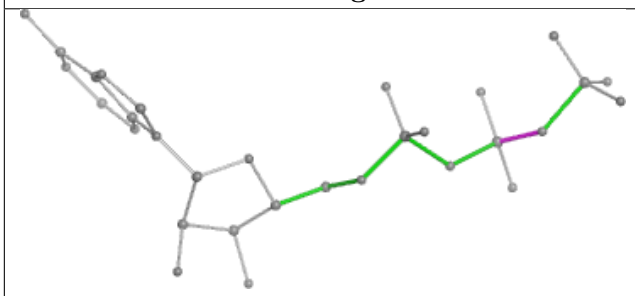
Ligand ATP E 302



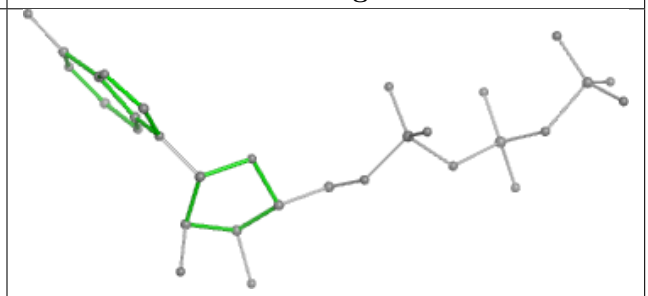
Bond lengths



Bond angles

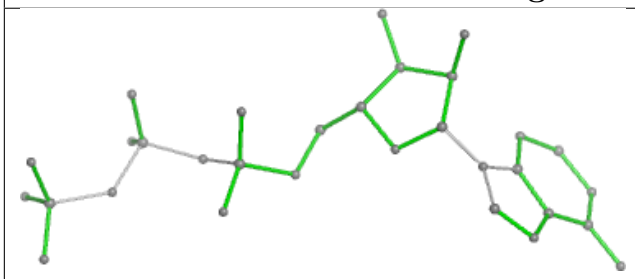


Torsions

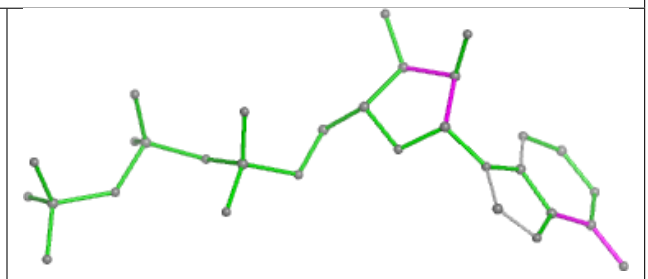


Rings

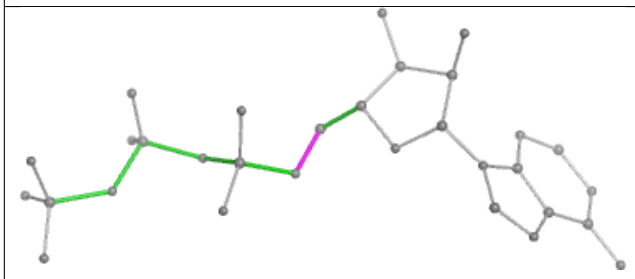
Ligand ATP L 905



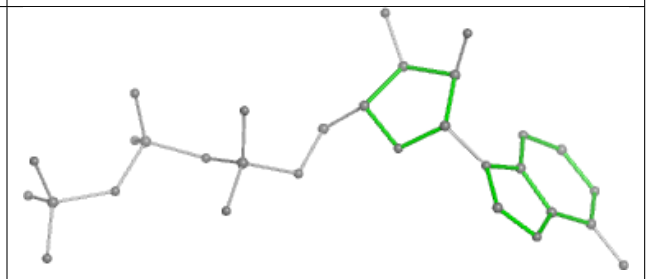
Bond lengths



Bond angles

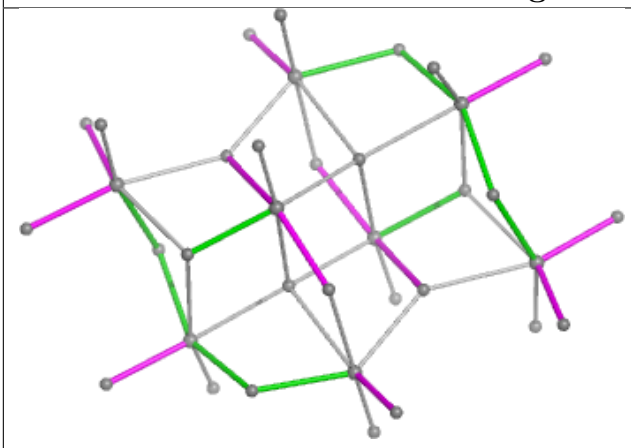


Torsions

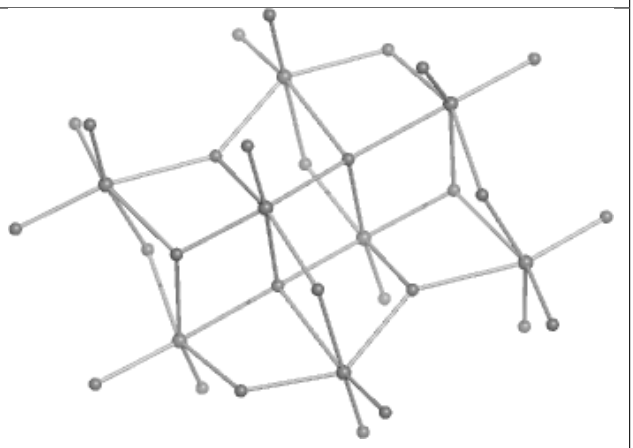


Rings

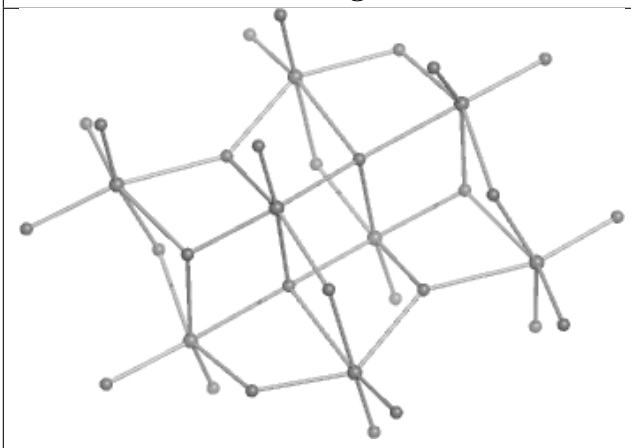
Ligand 8M0 L 906



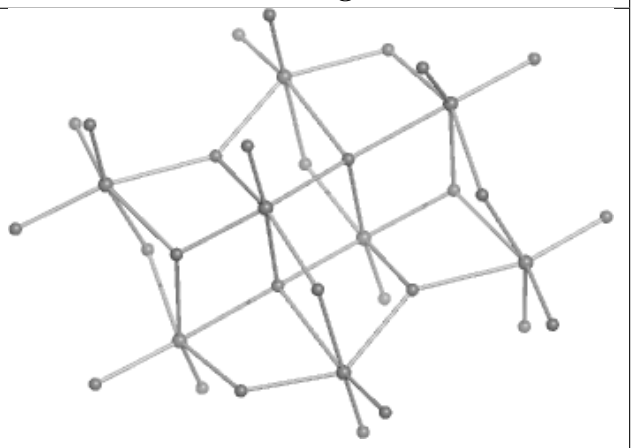
Bond lengths



Bond angles

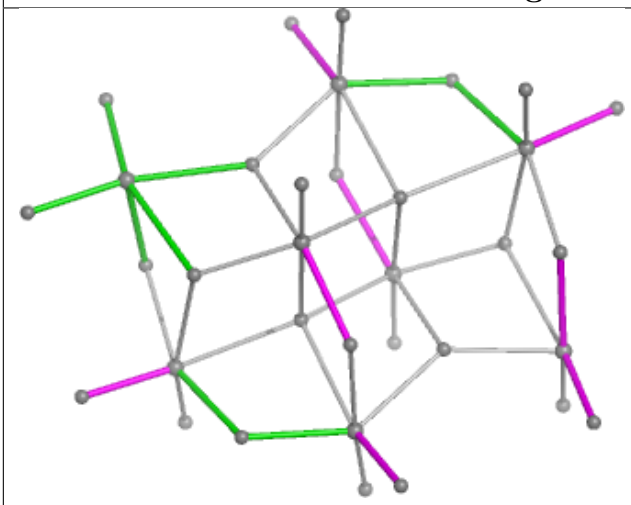


Torsions



Rings

Ligand 8M0 K 304



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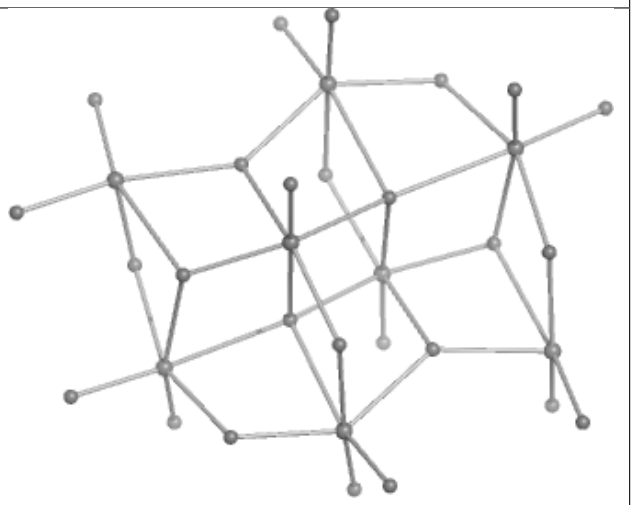
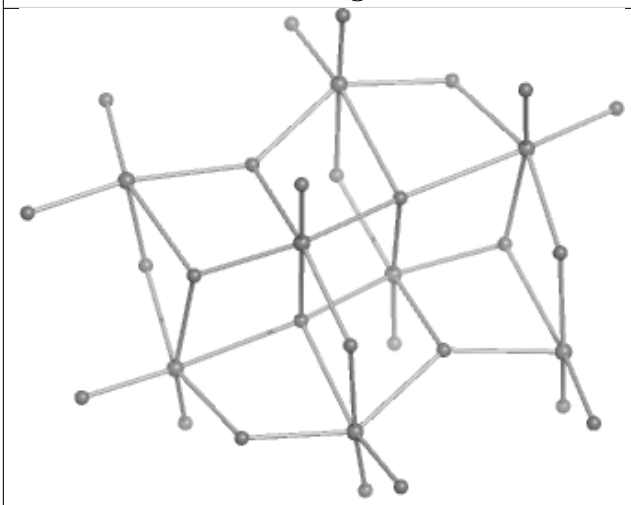
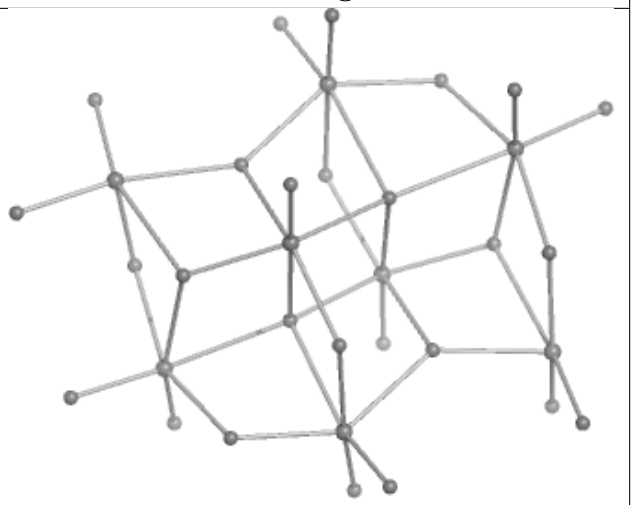


Bond angles

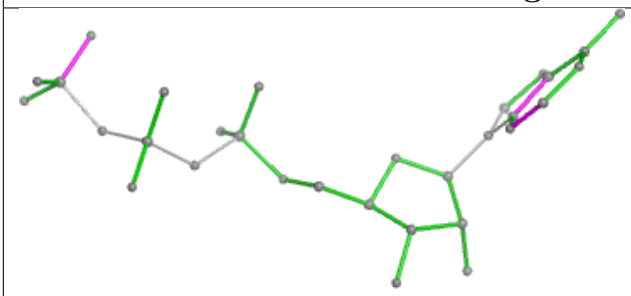


Torsions



Rings

Ligand ATP K 302



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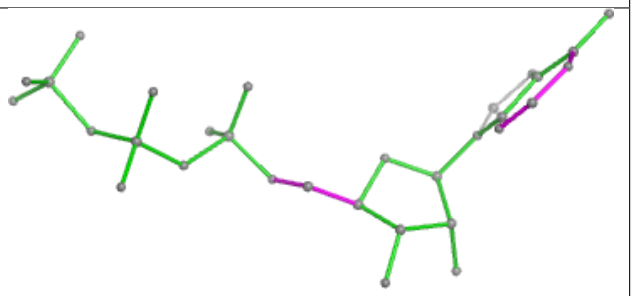
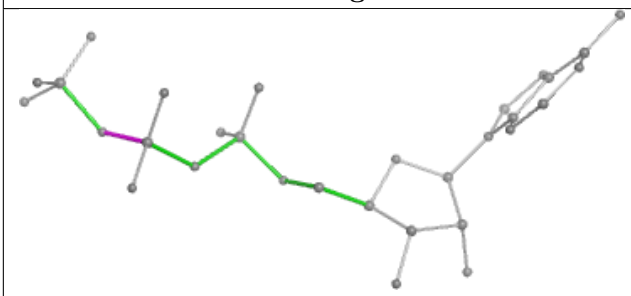
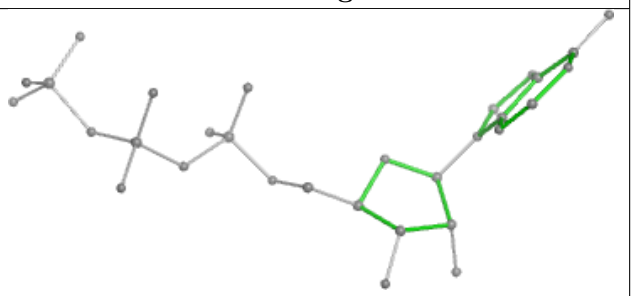


Bond angles

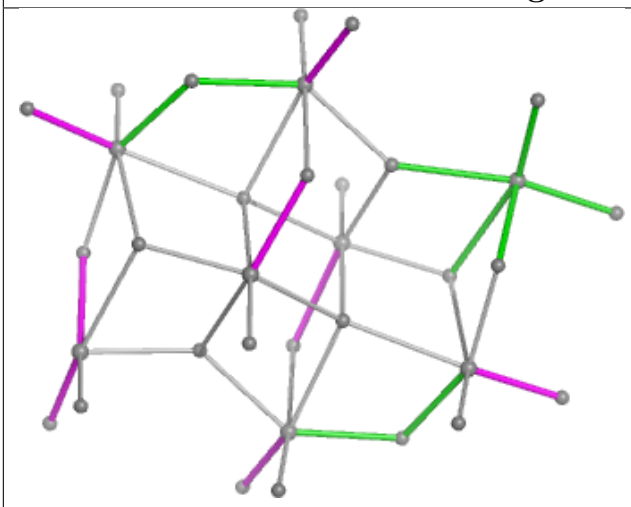


Torsions



Rings

Ligand 8M0 E 304



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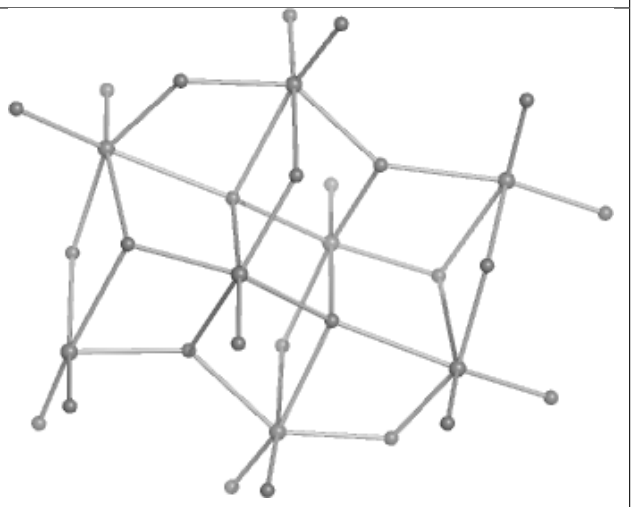
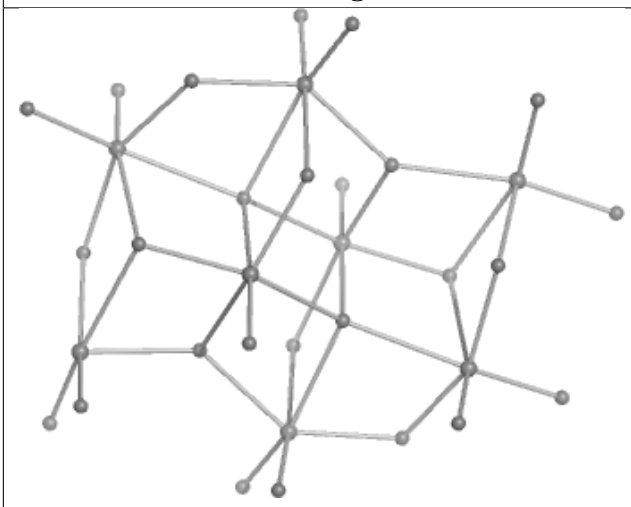
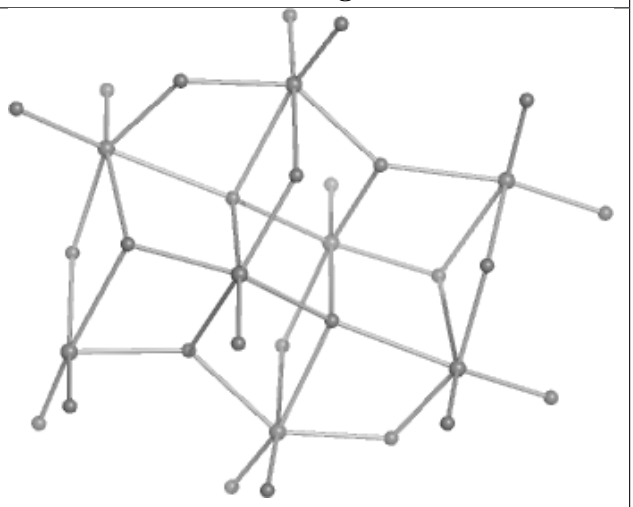


Bond angles

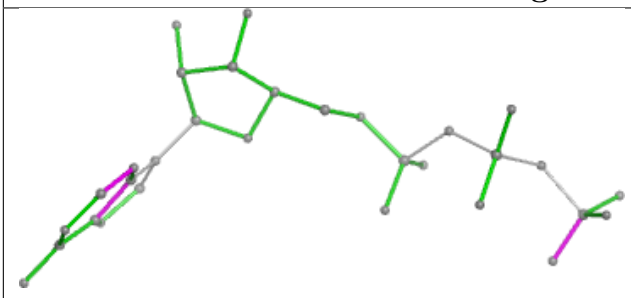


Torsions



Rings

Ligand ATP I 302



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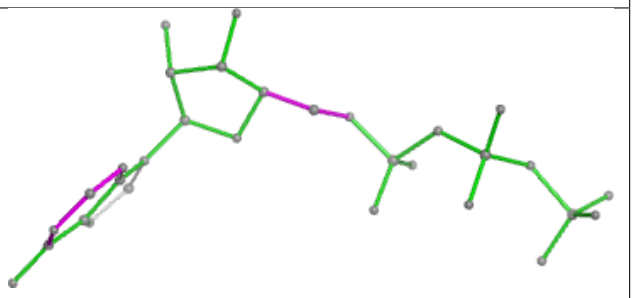
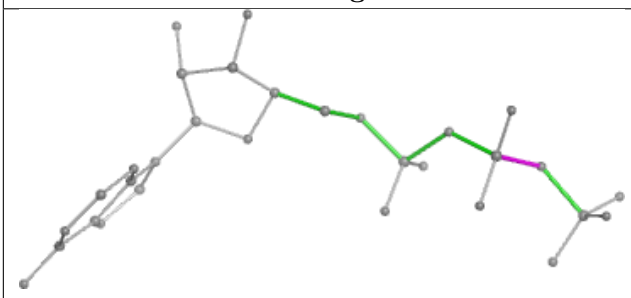


Bond angles



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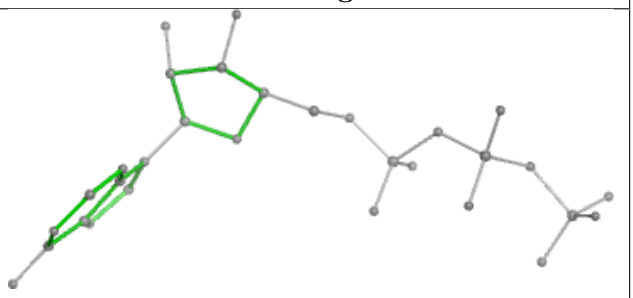
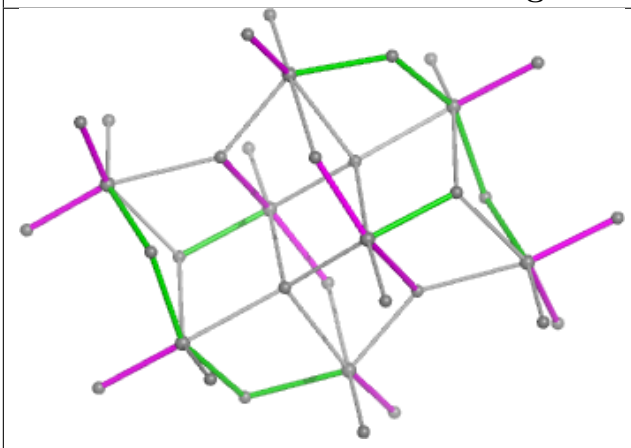
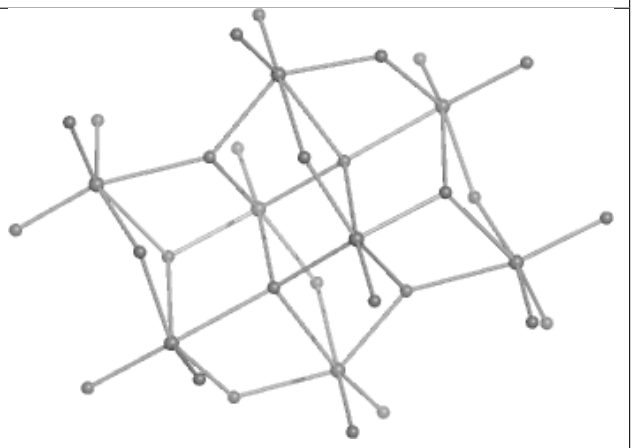


Rings

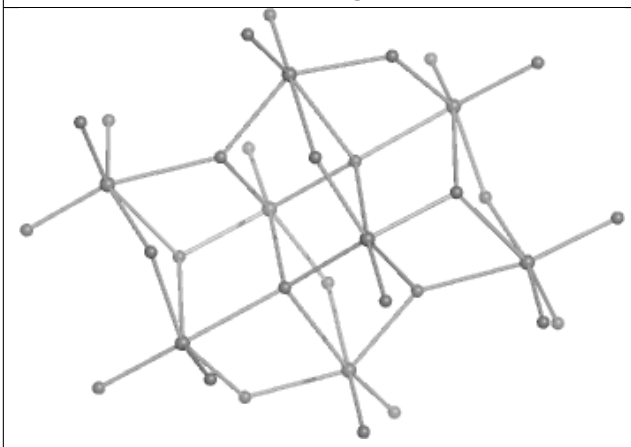
Ligand 8M0 B 806



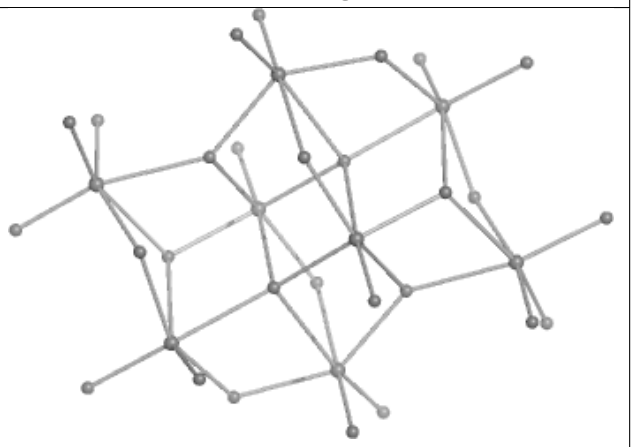
Bond lengths



Bond angles

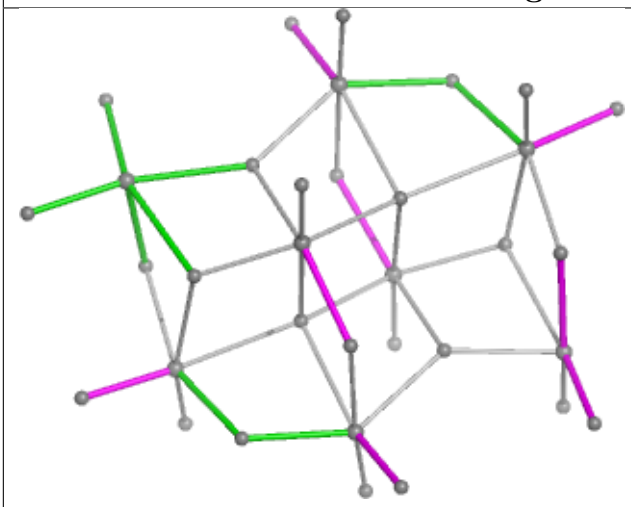


Torsions



Rings

Ligand 8M0 G 303



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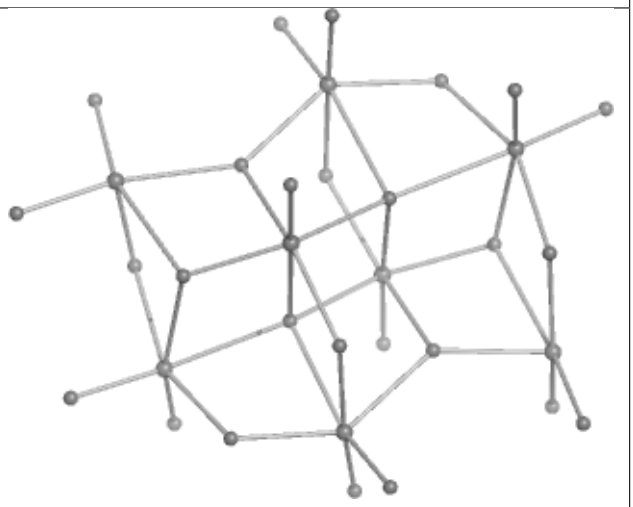
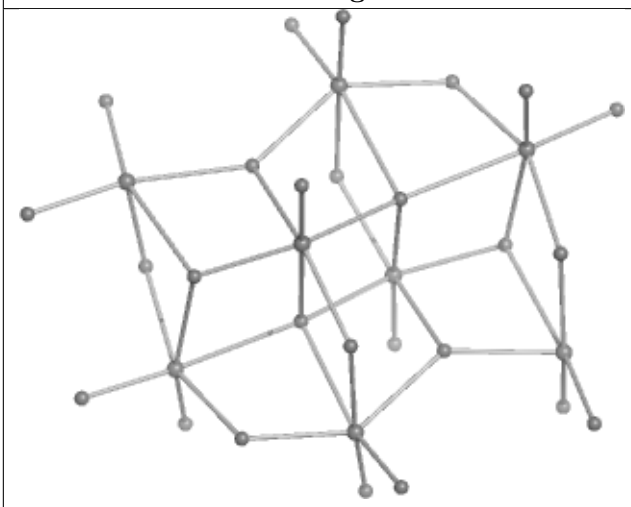
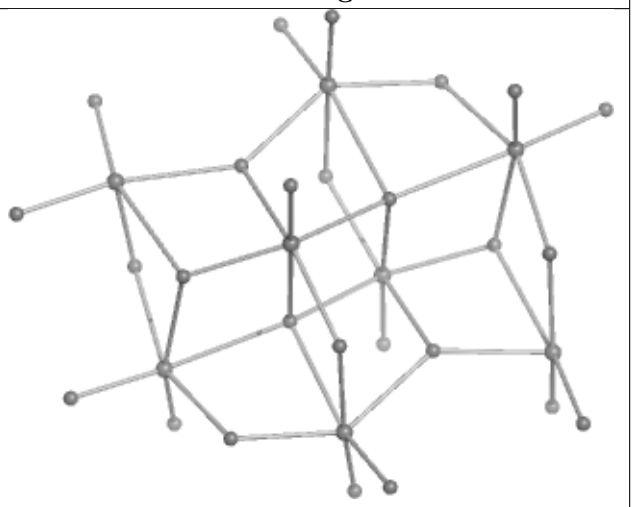


Bond angles

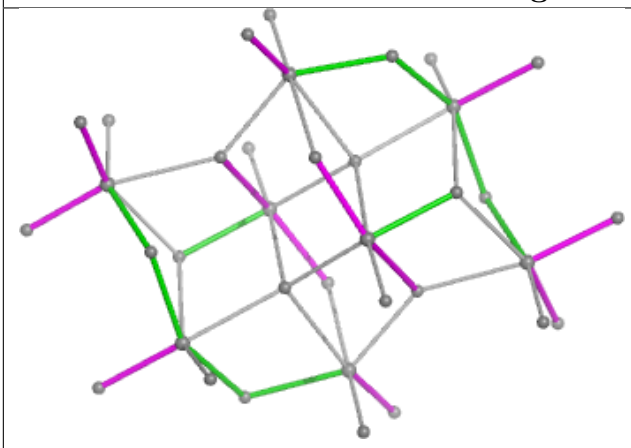


Torsions

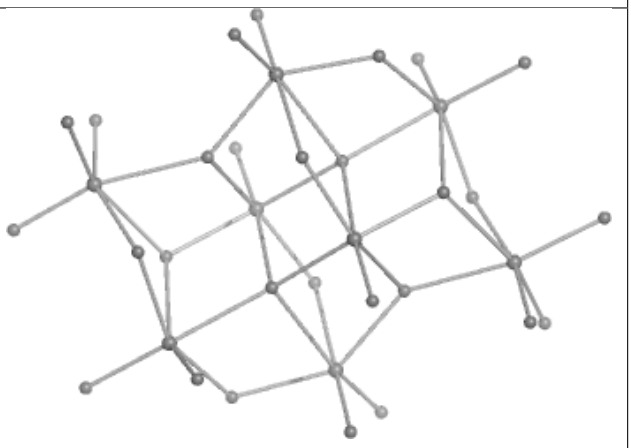


Rings

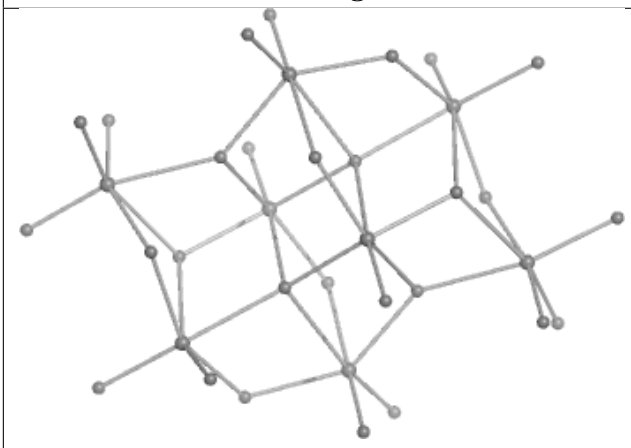
Ligand 8M0 J 805



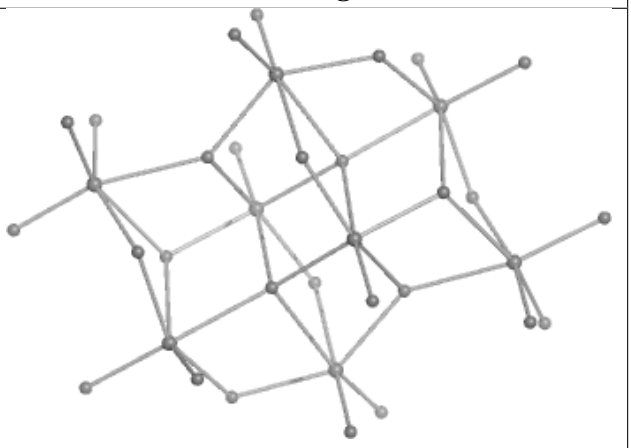
Bond lengths



Bond angles

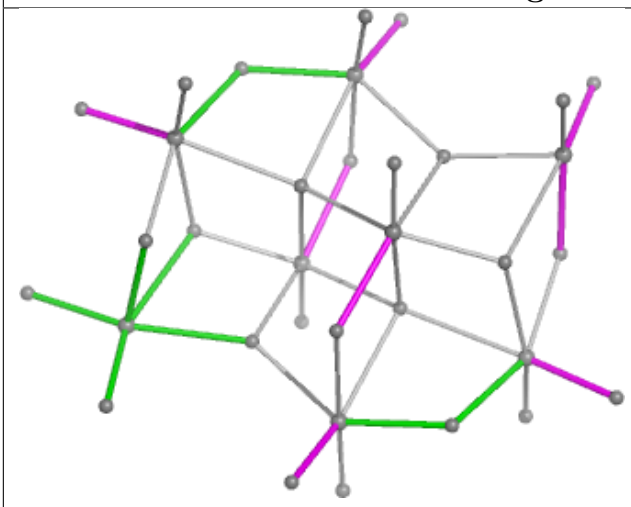


Torsions



Rings

Ligand 8M0 C 303



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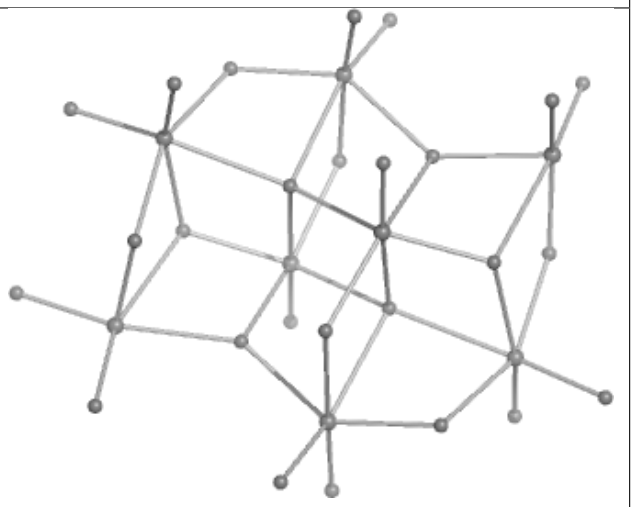
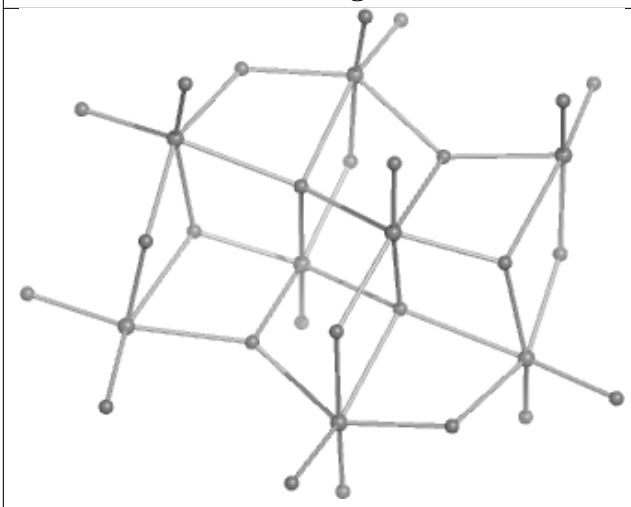


Bond angles



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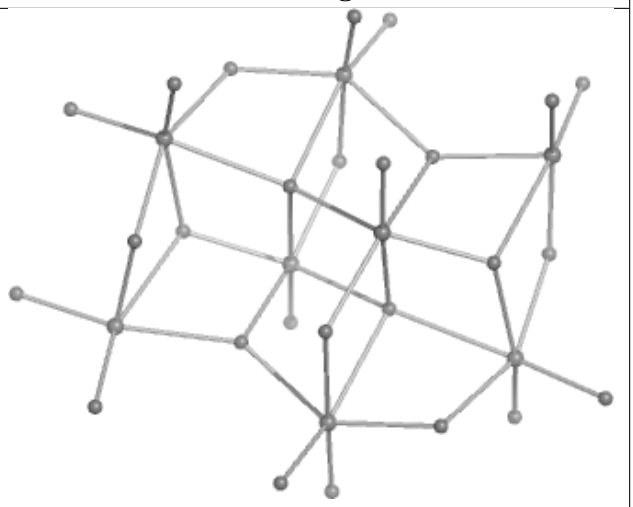
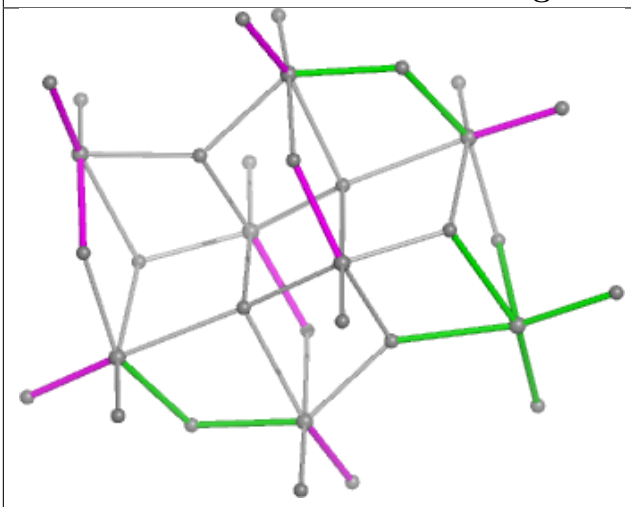


Rings

Ligand 8M0 I 304



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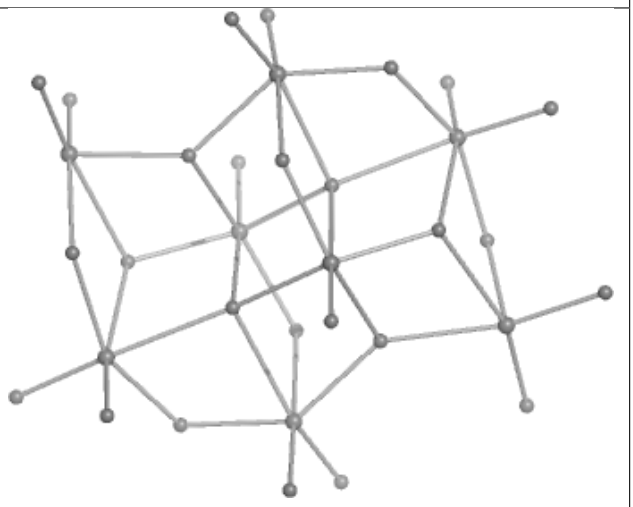
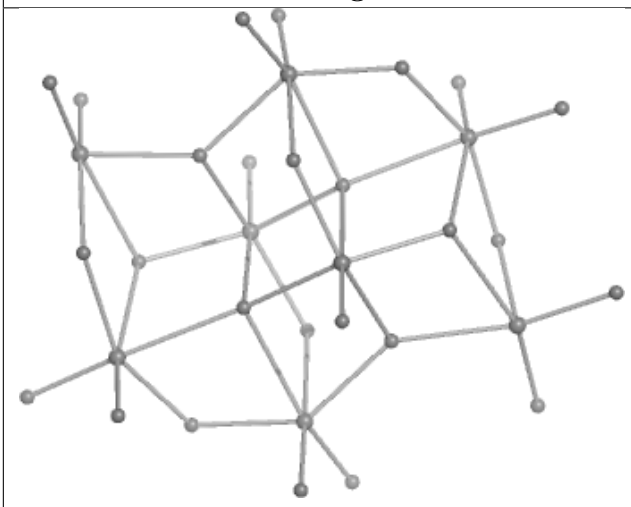
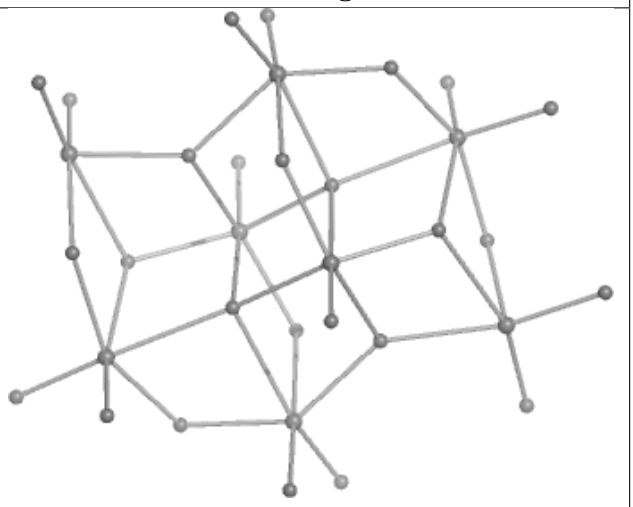


Bond angles

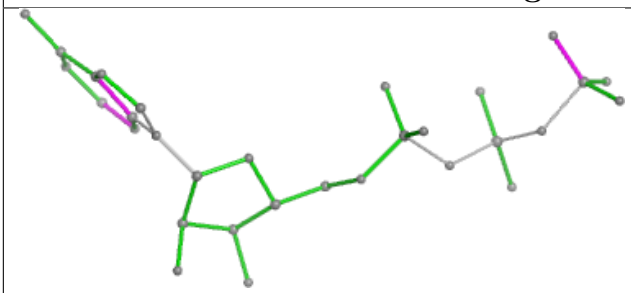


Torsions



Rings

Ligand ATP A 301



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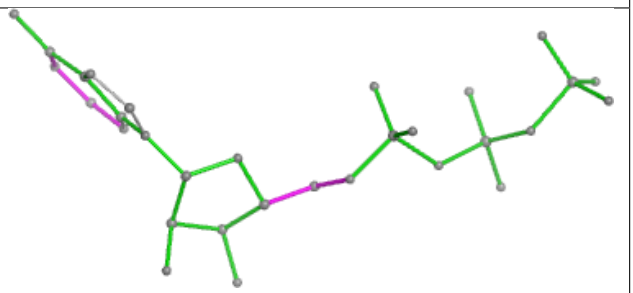
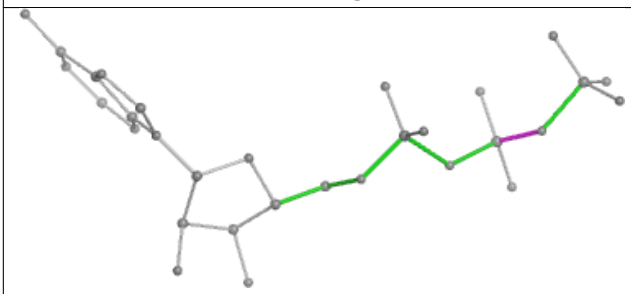
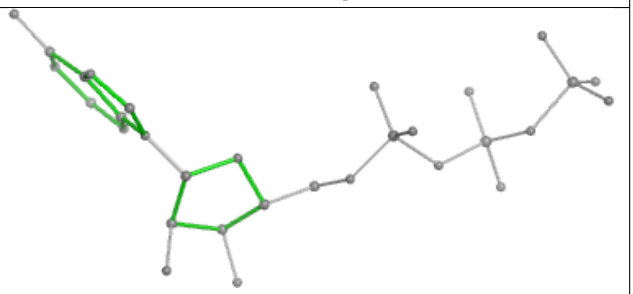


Bond angles

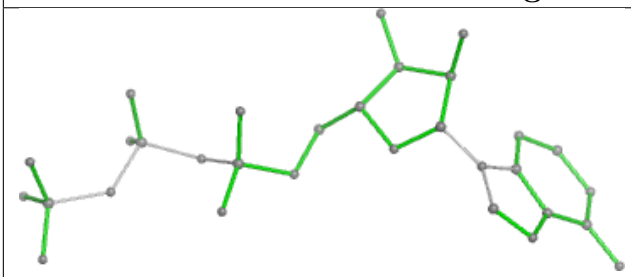


Torsions

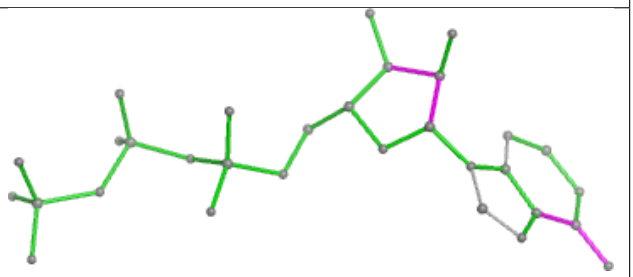


Rings

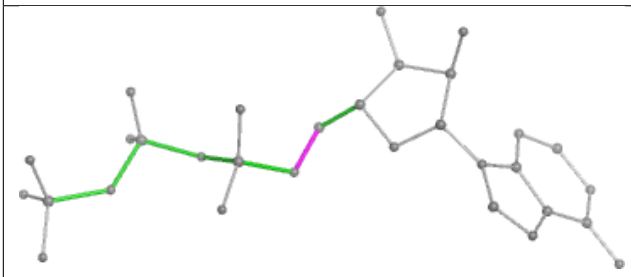
Ligand ATP H 805



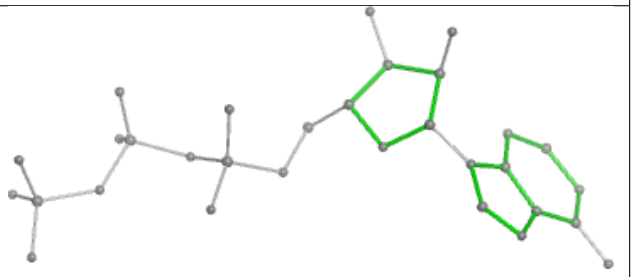
Bond lengths



Bond angles

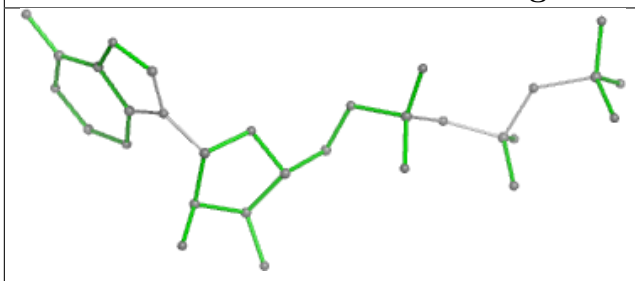


Torsions

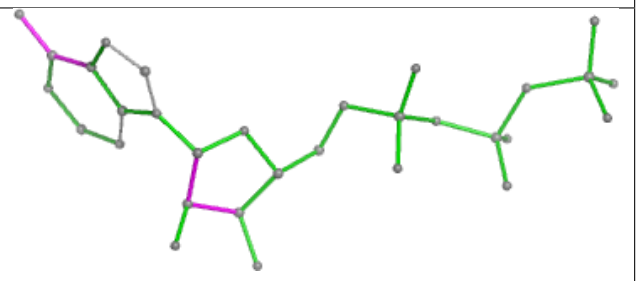


Rings

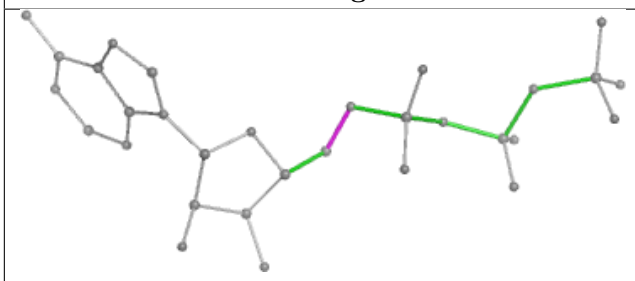
Ligand ATP J 804



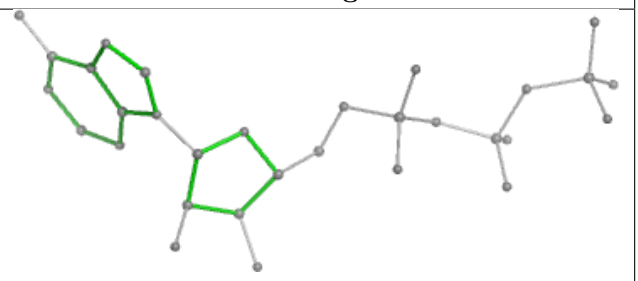
Bond lengths



Bond angles

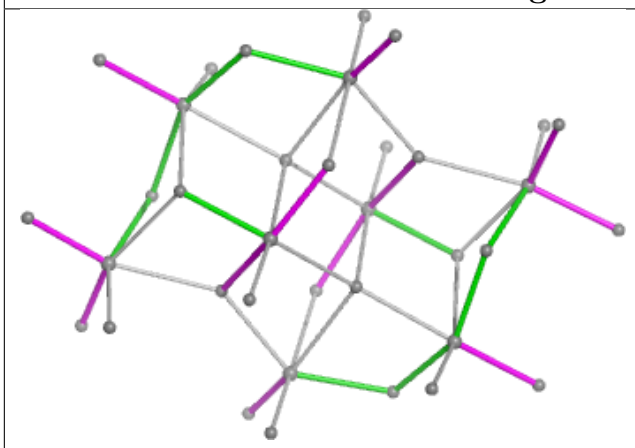


Torsions

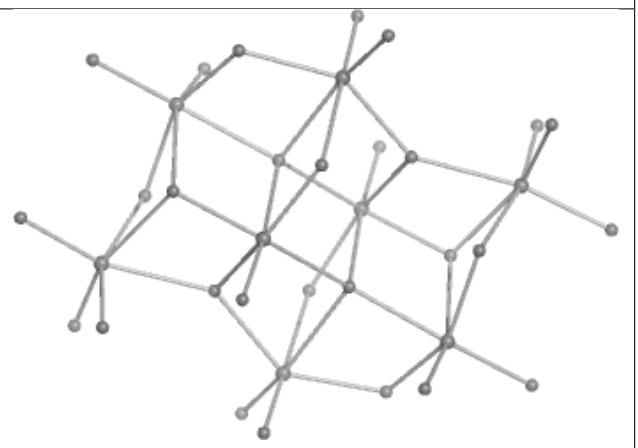


Rings

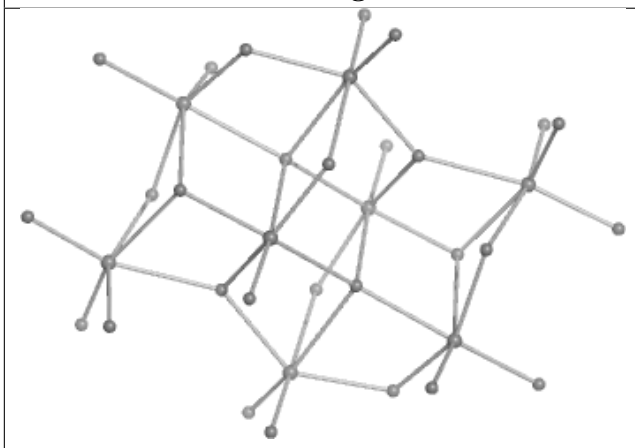
Ligand 8M0 F 906



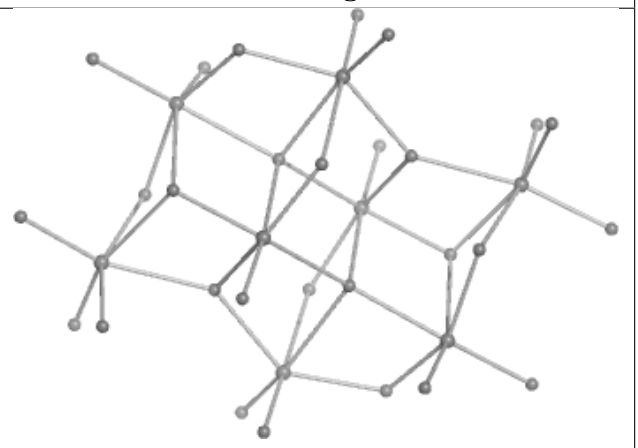
Bond lengths



Bond angles

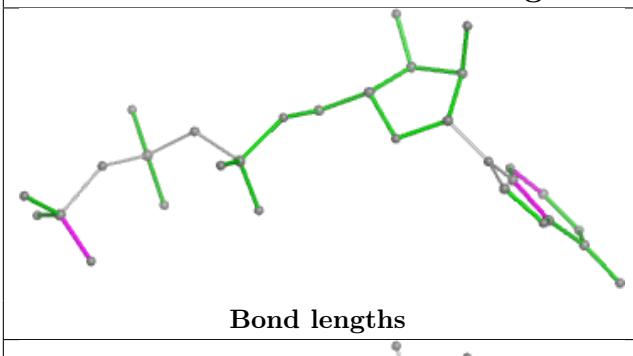


Torsions

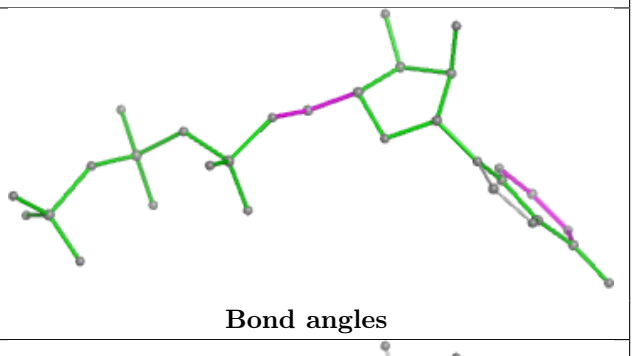


Rings

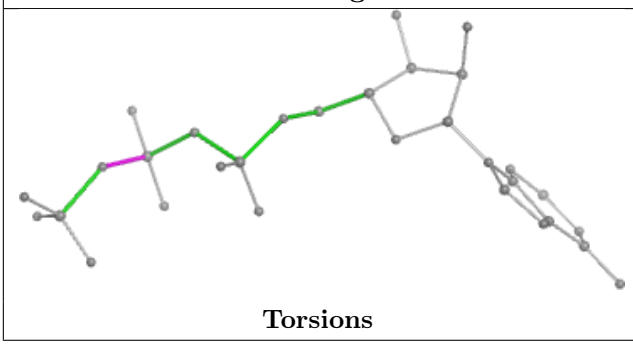
Ligand ATP C 301



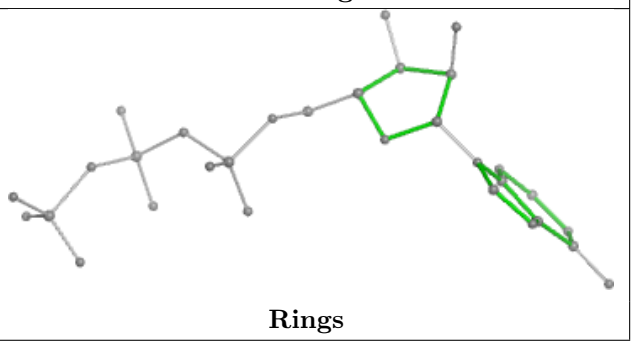
Bond lengths



Bond angles

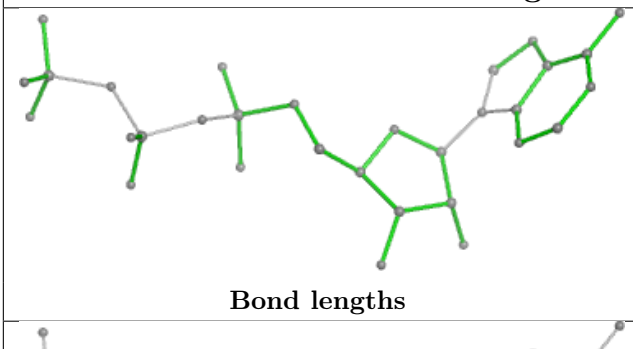


Torsions

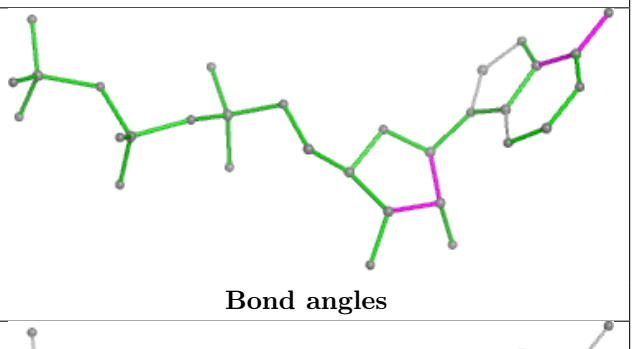


Rings

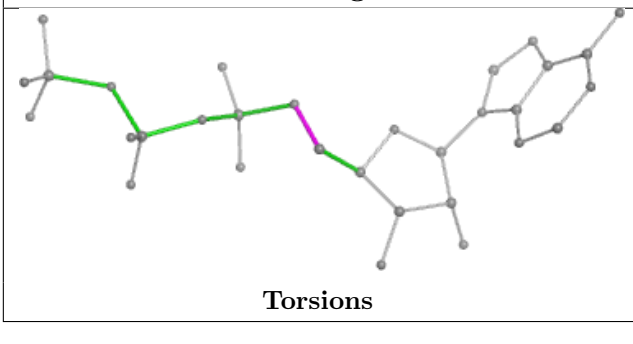
Ligand ATP D 906



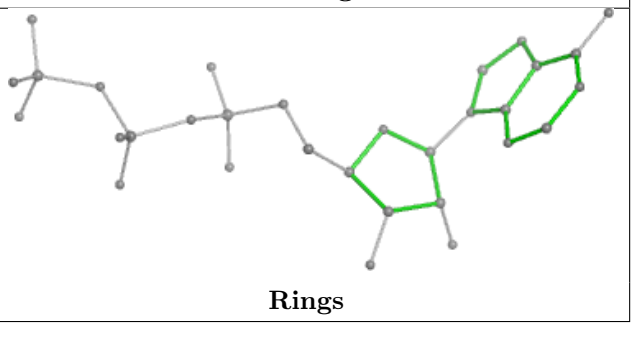
Bond lengths



Bond angles

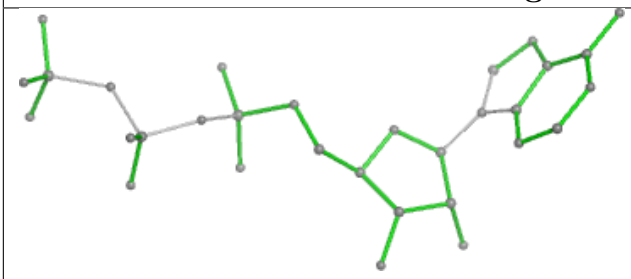


Torsions

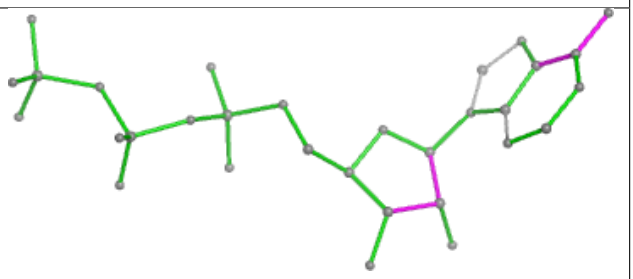


Rings

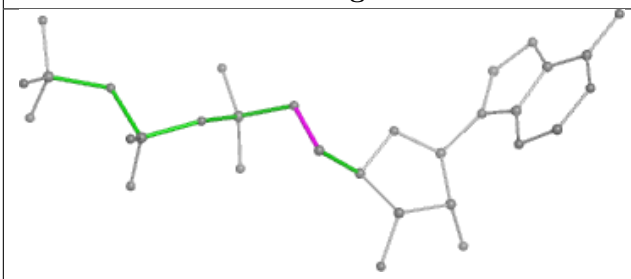
Ligand ATP B 805



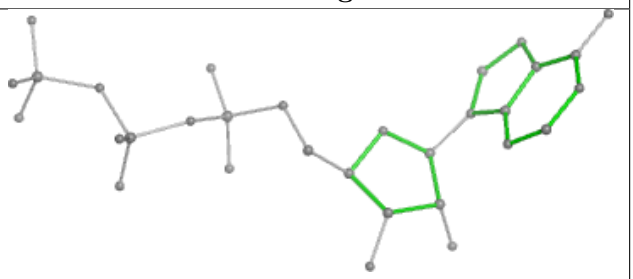
Bond lengths



Bond angles

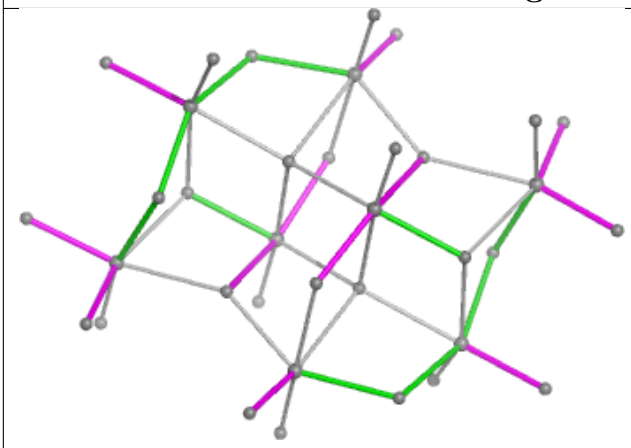


Torsions

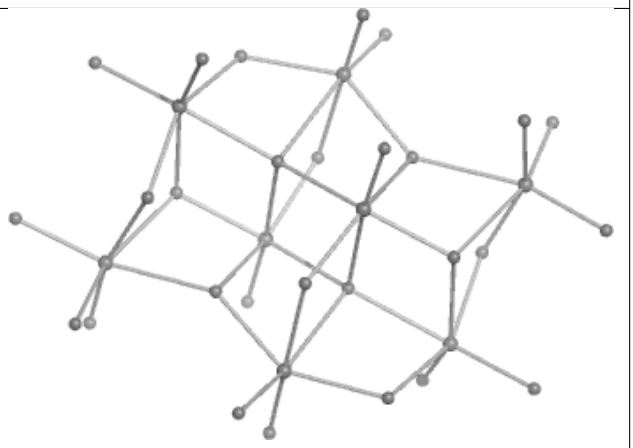


Rings

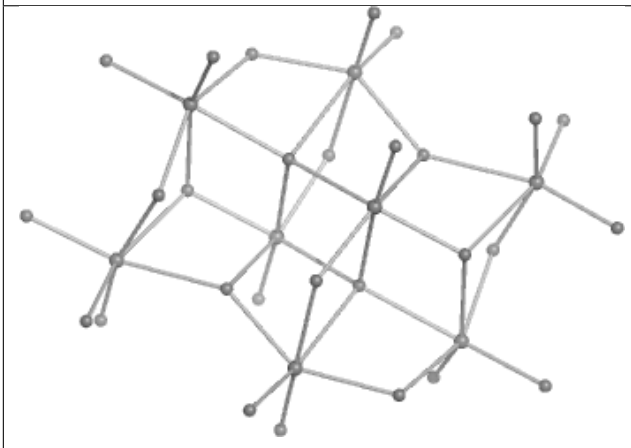
Ligand 8M0 D 907



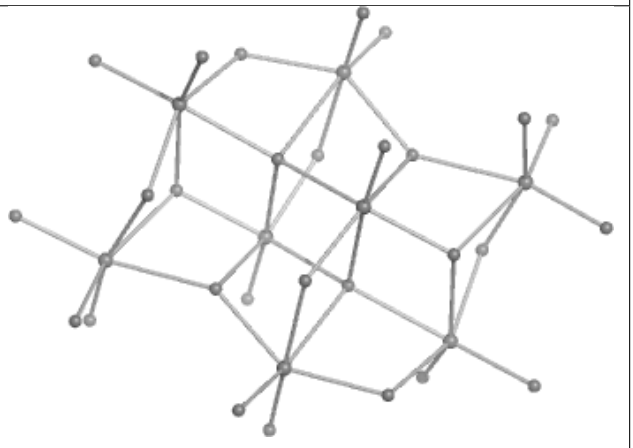
Bond lengths



Bond angles

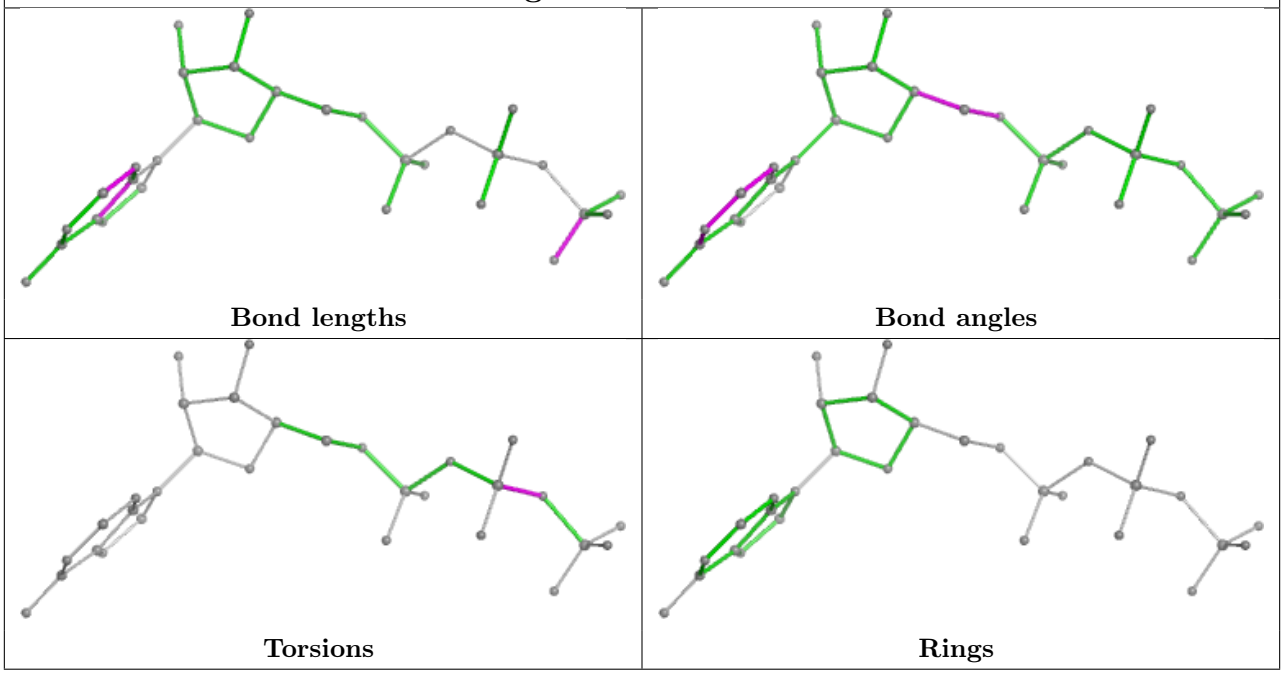


Torsions



Rings

Ligand ATP G 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

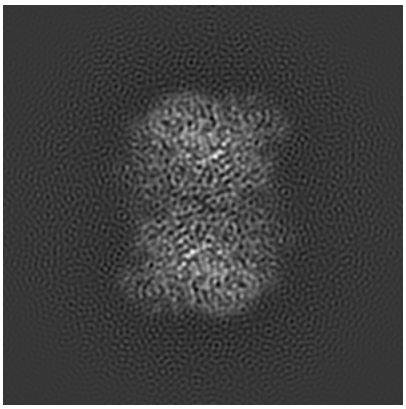
6 Map visualisation

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

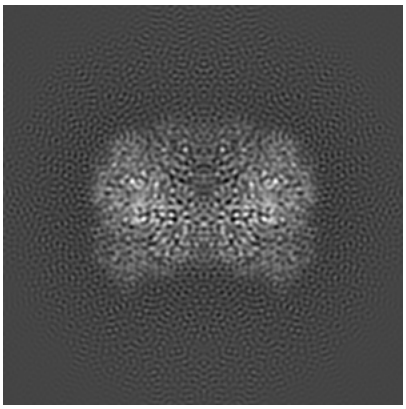
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

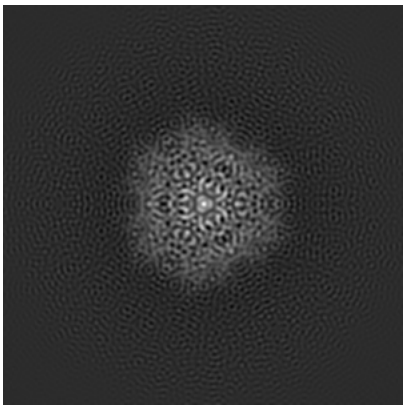
6.1.1 Primary map



X

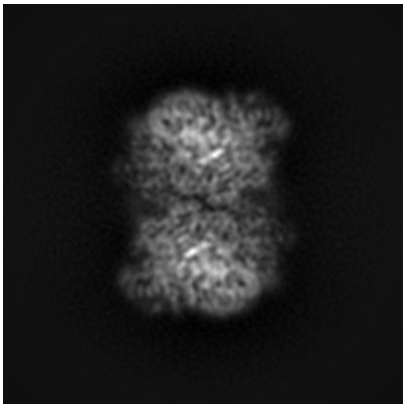


Y

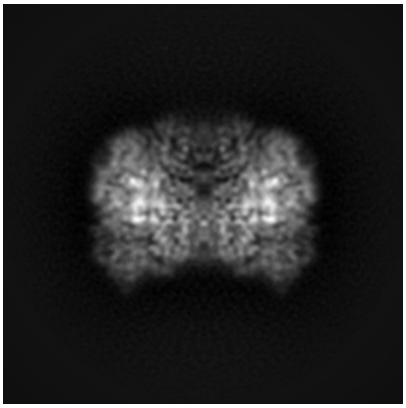


Z

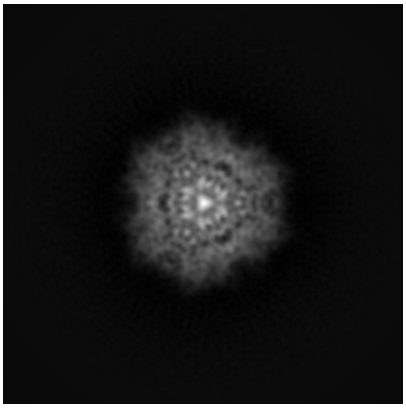
6.1.2 Raw map



X



Y

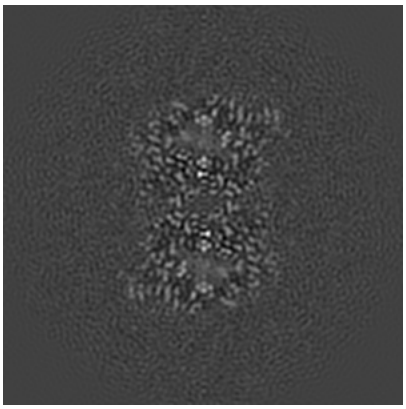


Z

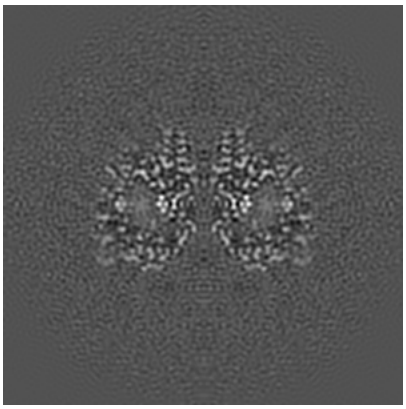
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

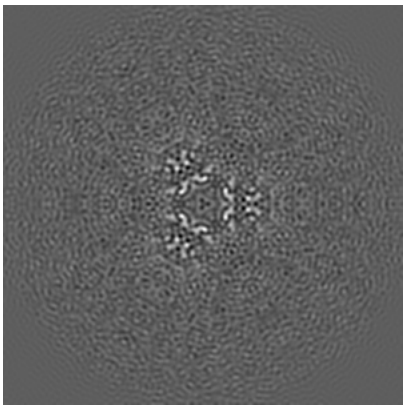
6.2.1 Primary map



X Index: 100

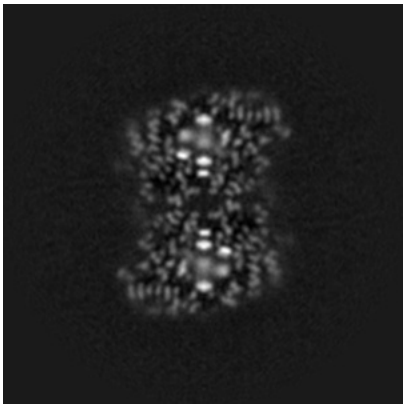


Y Index: 100

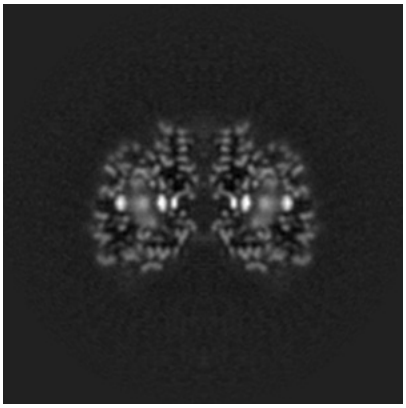


Z Index: 100

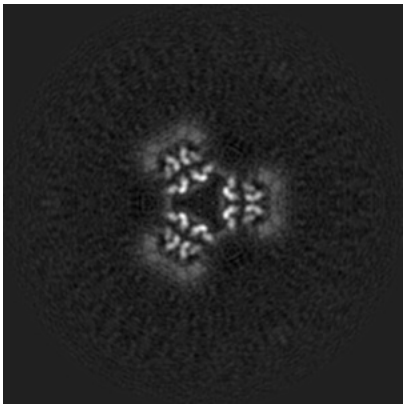
6.2.2 Raw map



X Index: 100



Y Index: 100

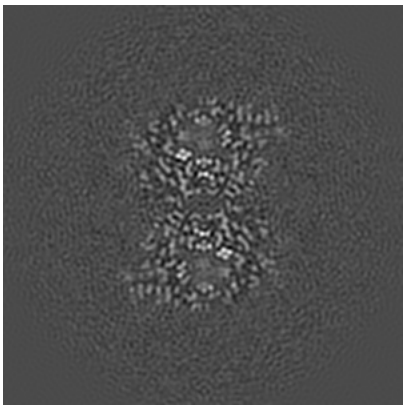


Z Index: 100

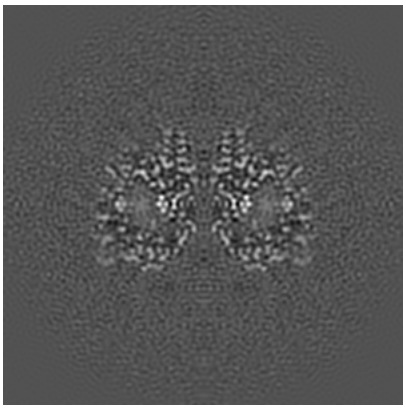
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

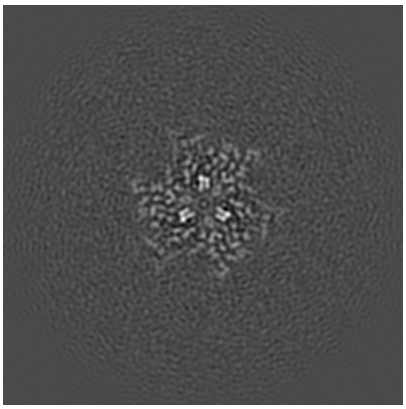
6.3.1 Primary map



X Index: 99

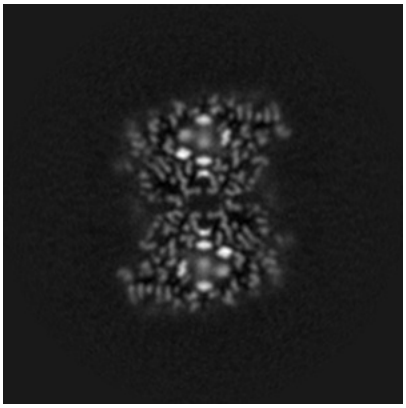


Y Index: 100

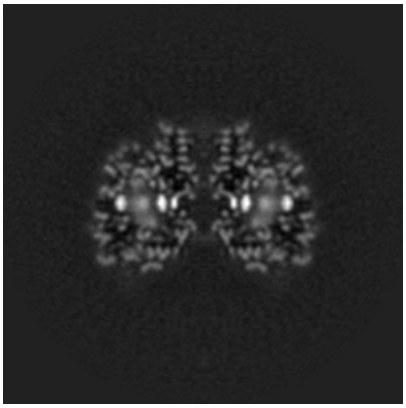


Z Index: 76

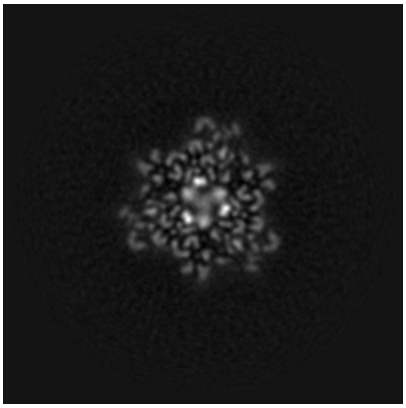
6.3.2 Raw map



X Index: 99



Y Index: 100

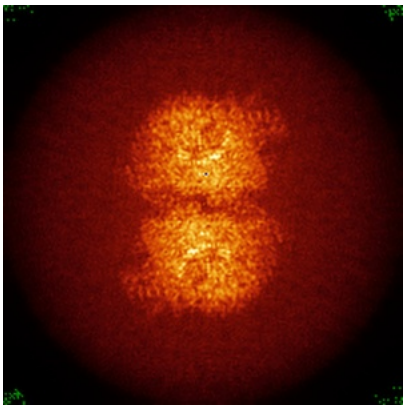


Z Index: 134

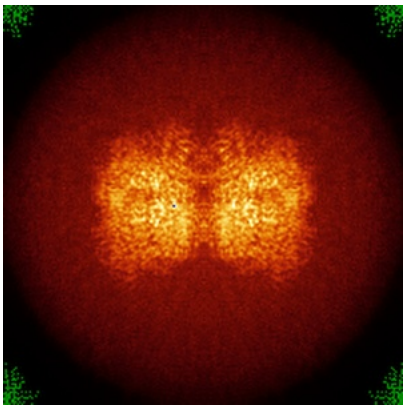
The images above show the largest variance slices of the map in three orthogonal directions.

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

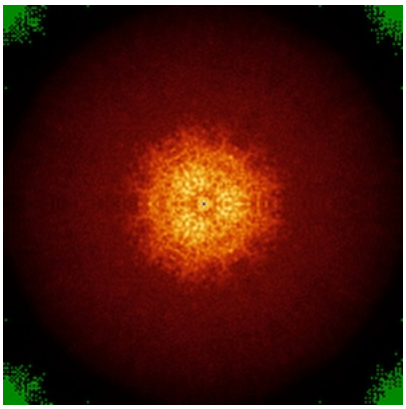
6.4.1 Primary map



X

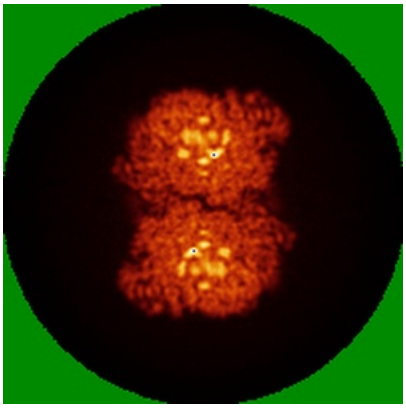


Y

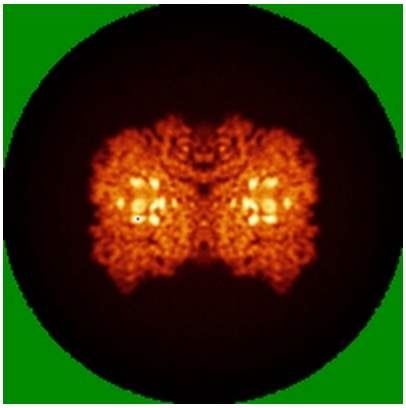


Z

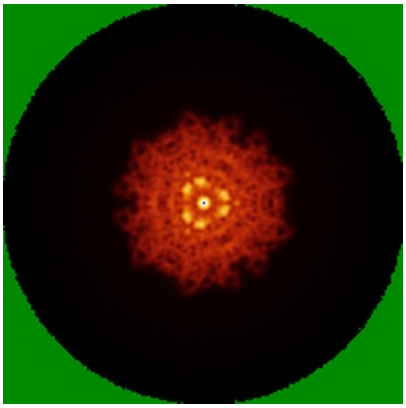
6.4.2 Raw map



X



Y

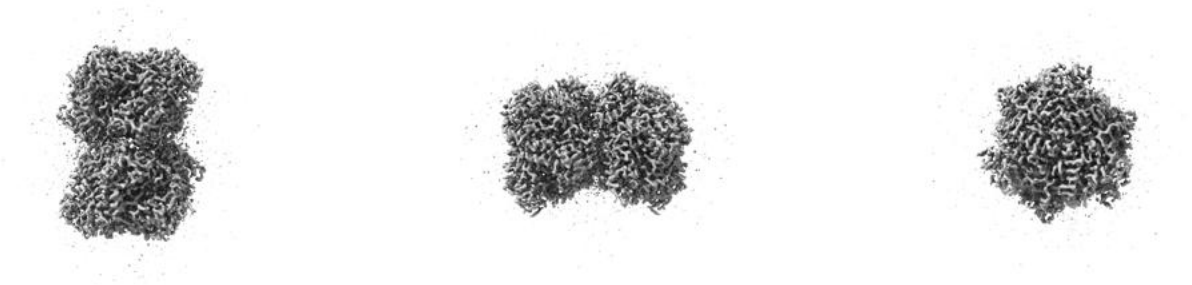


Z

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.

6.5.2 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.

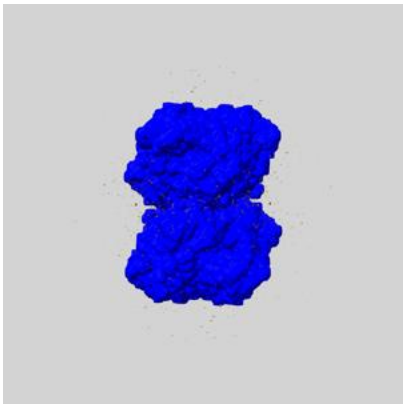
6.6 Mask visualisation (i)

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

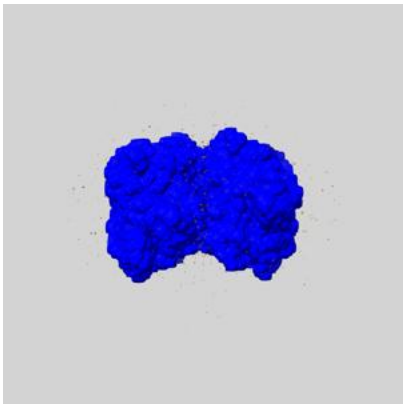
A mask typically either:

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

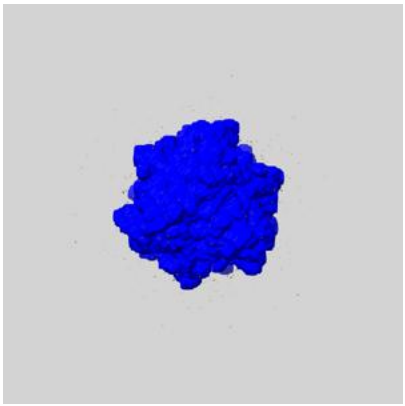
6.6.1 emd_4907_msk_1.map (i)



X



Y

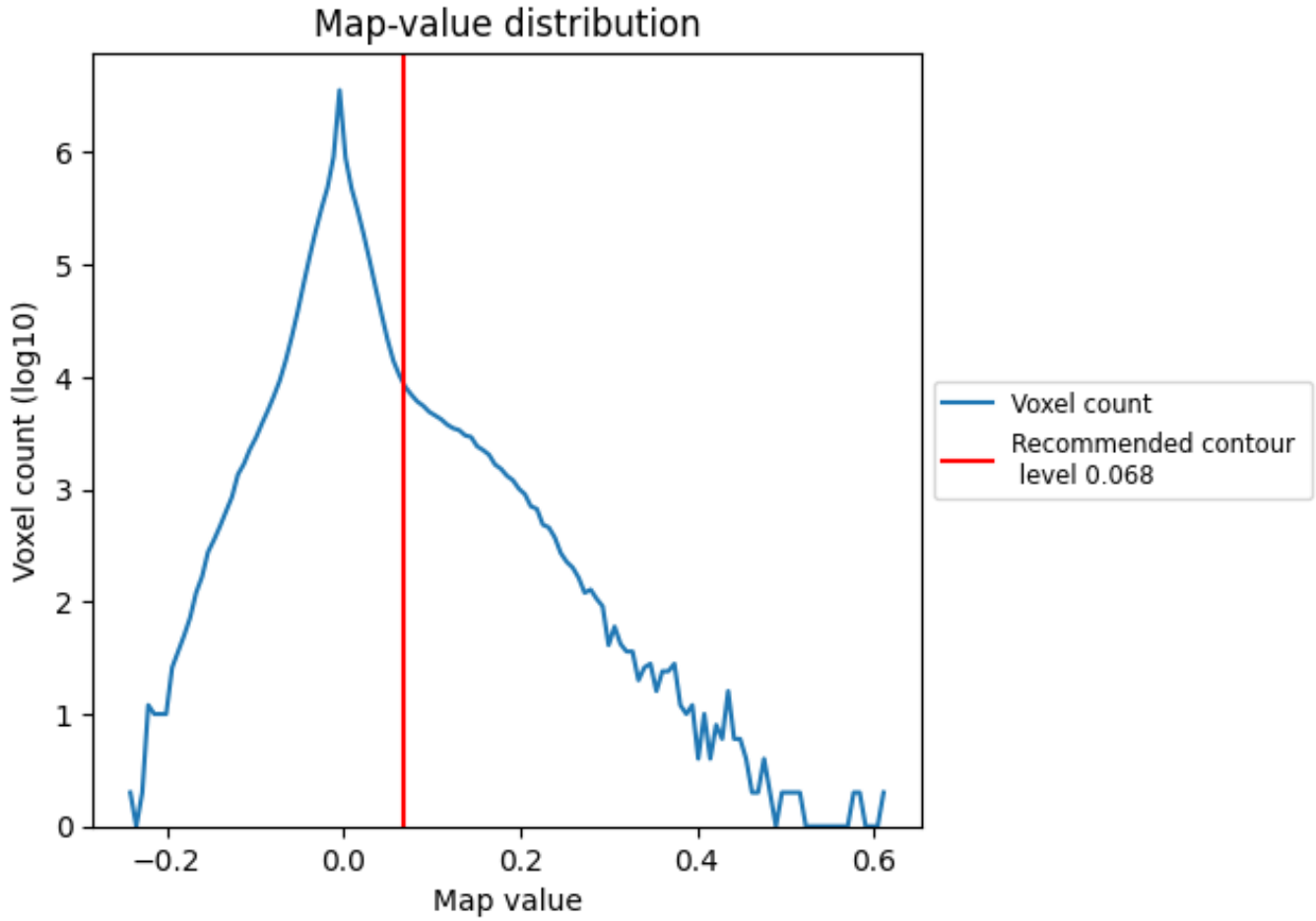


Z

7 Map analysis

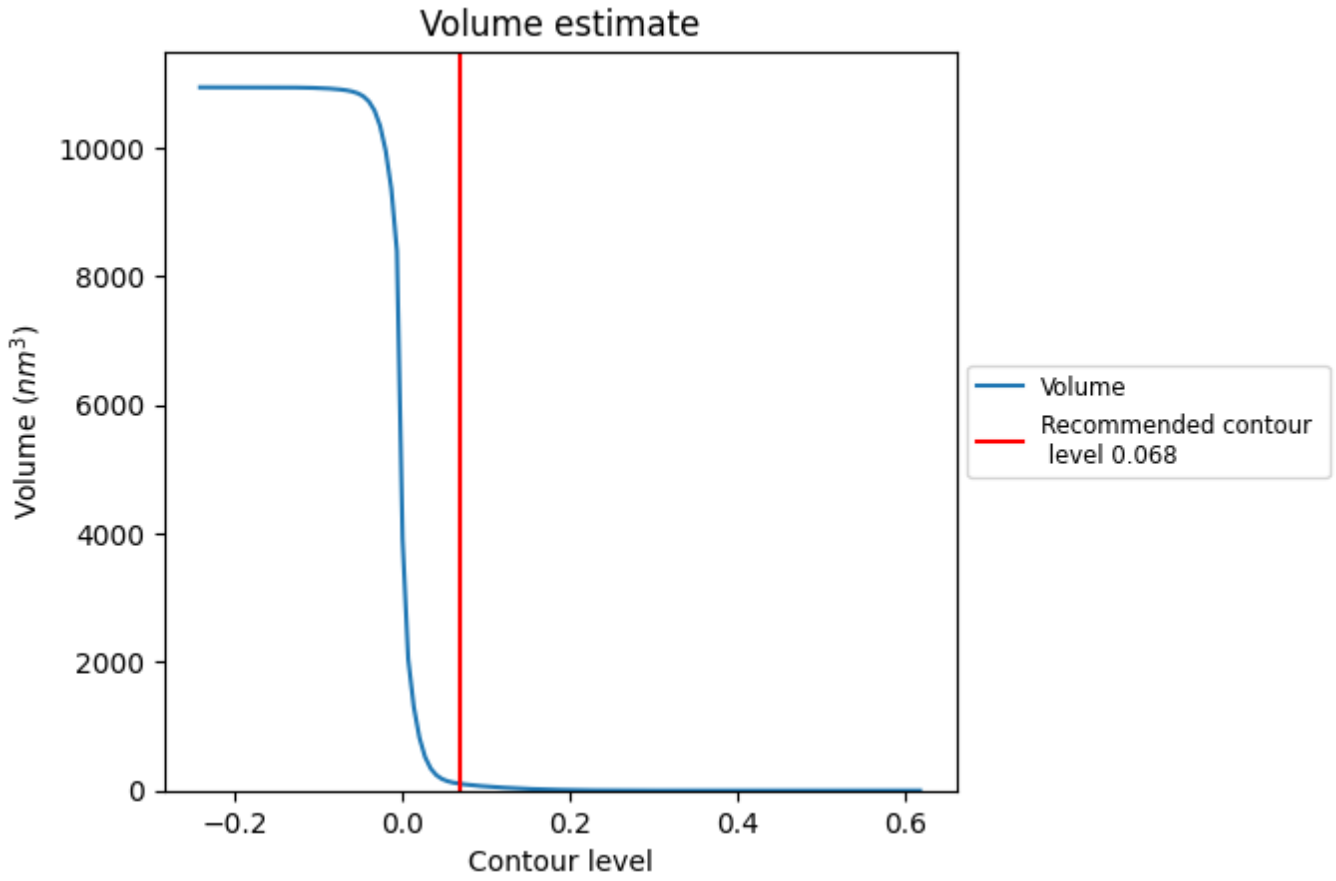
This section contains the results of statistical analysis of the map.

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.

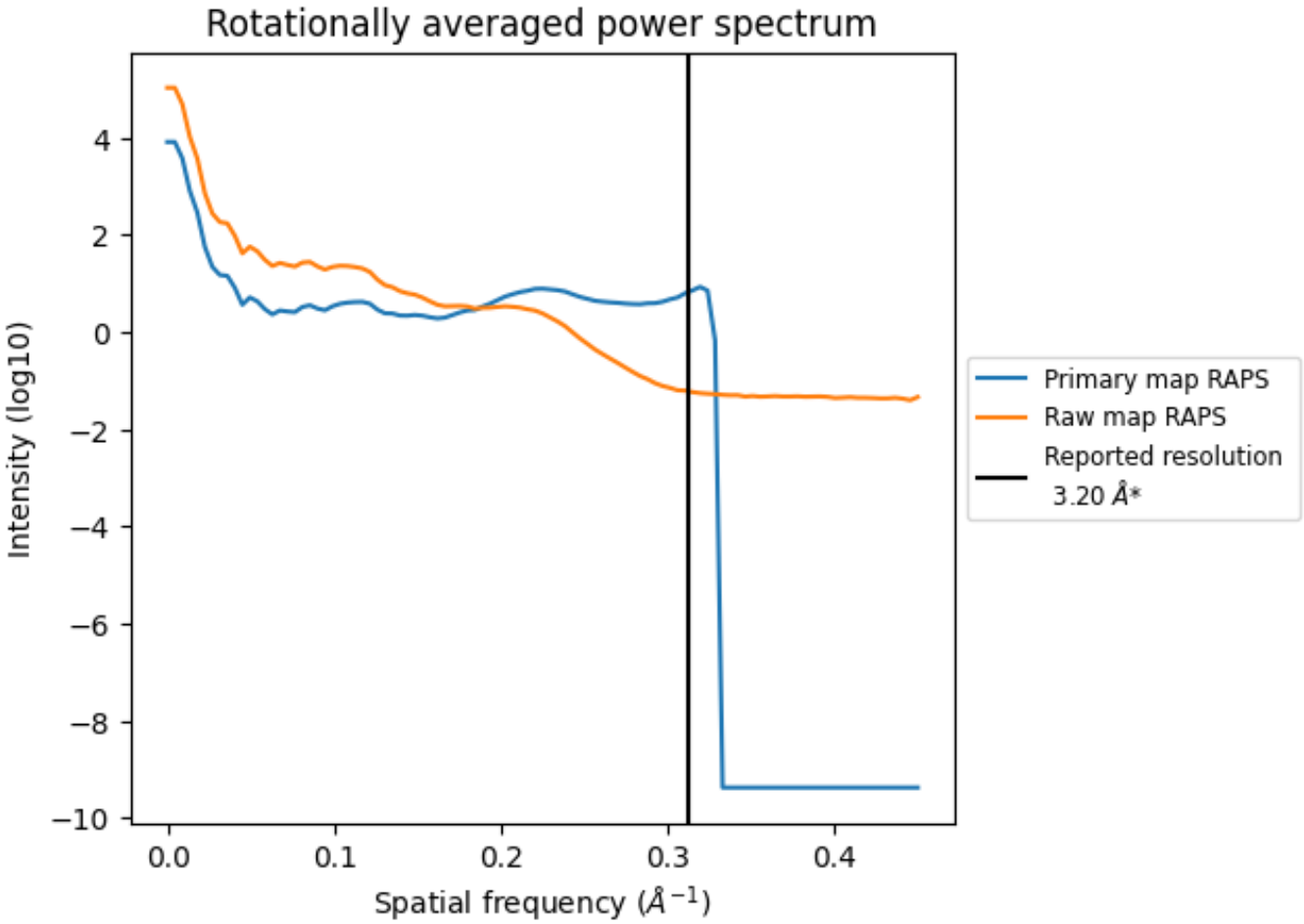
7.2 Volume estimate



The volume at the recommended contour level is 108 nm^3; 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 (i)

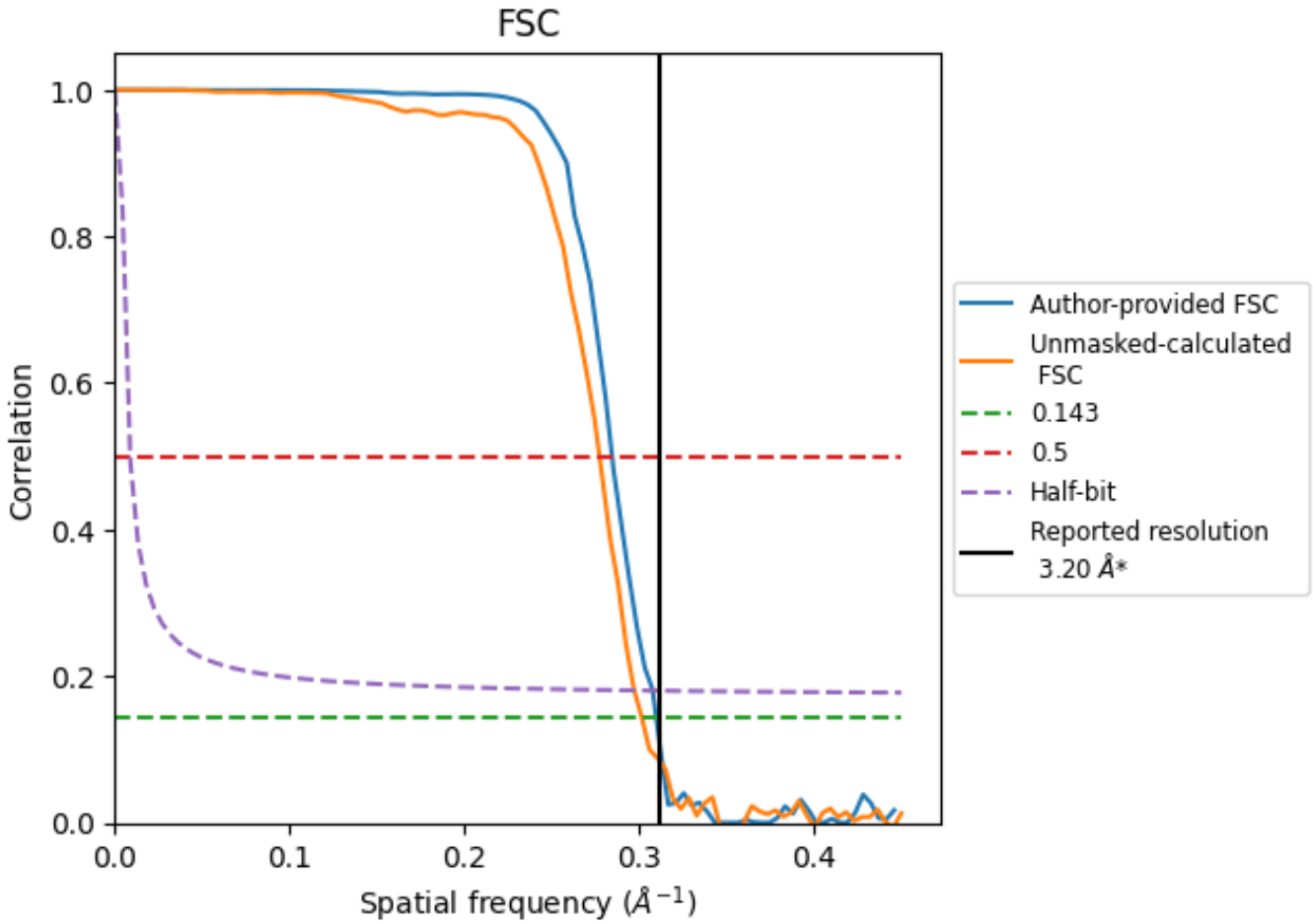


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

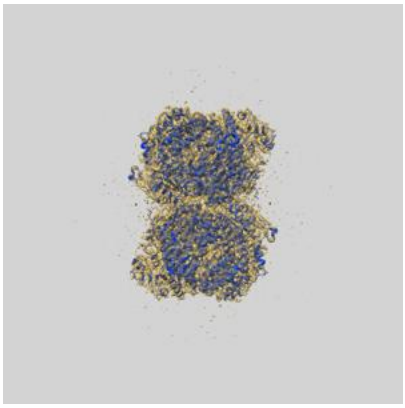
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.51	3.25
Unmasked-calculated*	3.31	3.60	3.36

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

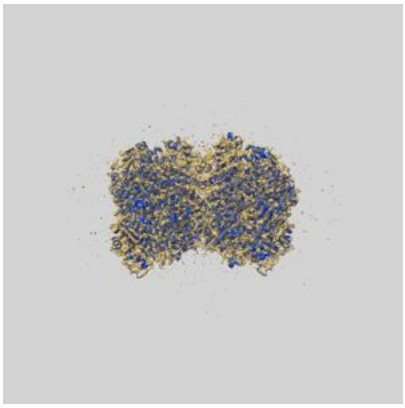
9 Map-model fit

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.

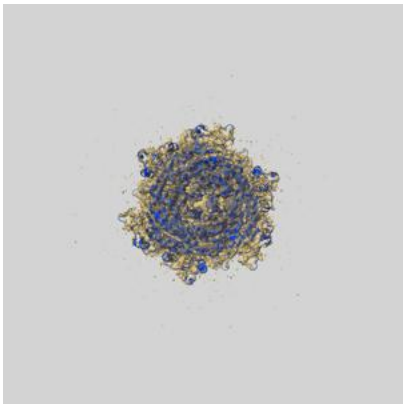
9.1 Map-model overlay



X



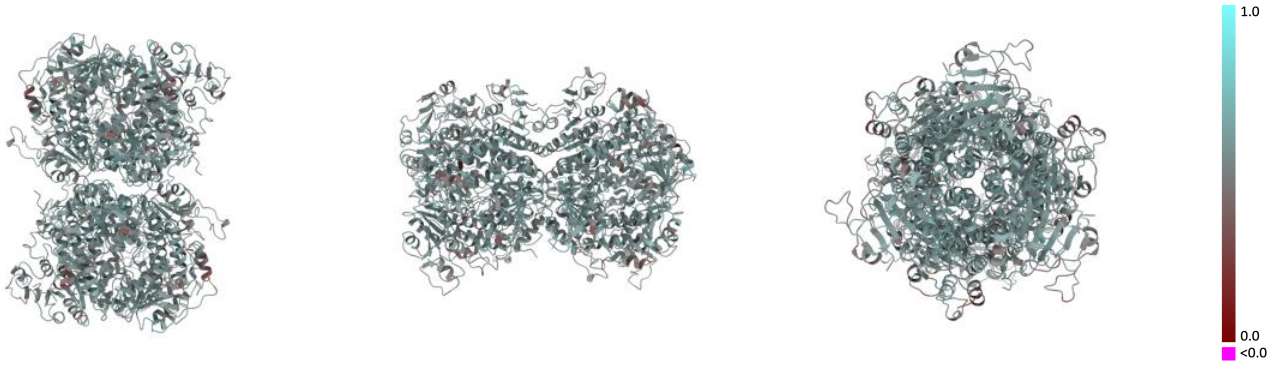
Y



Z

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.

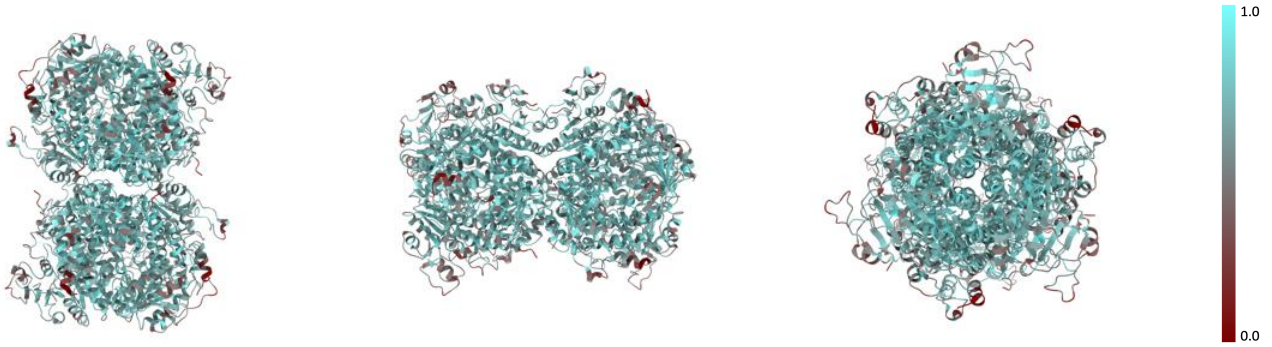
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

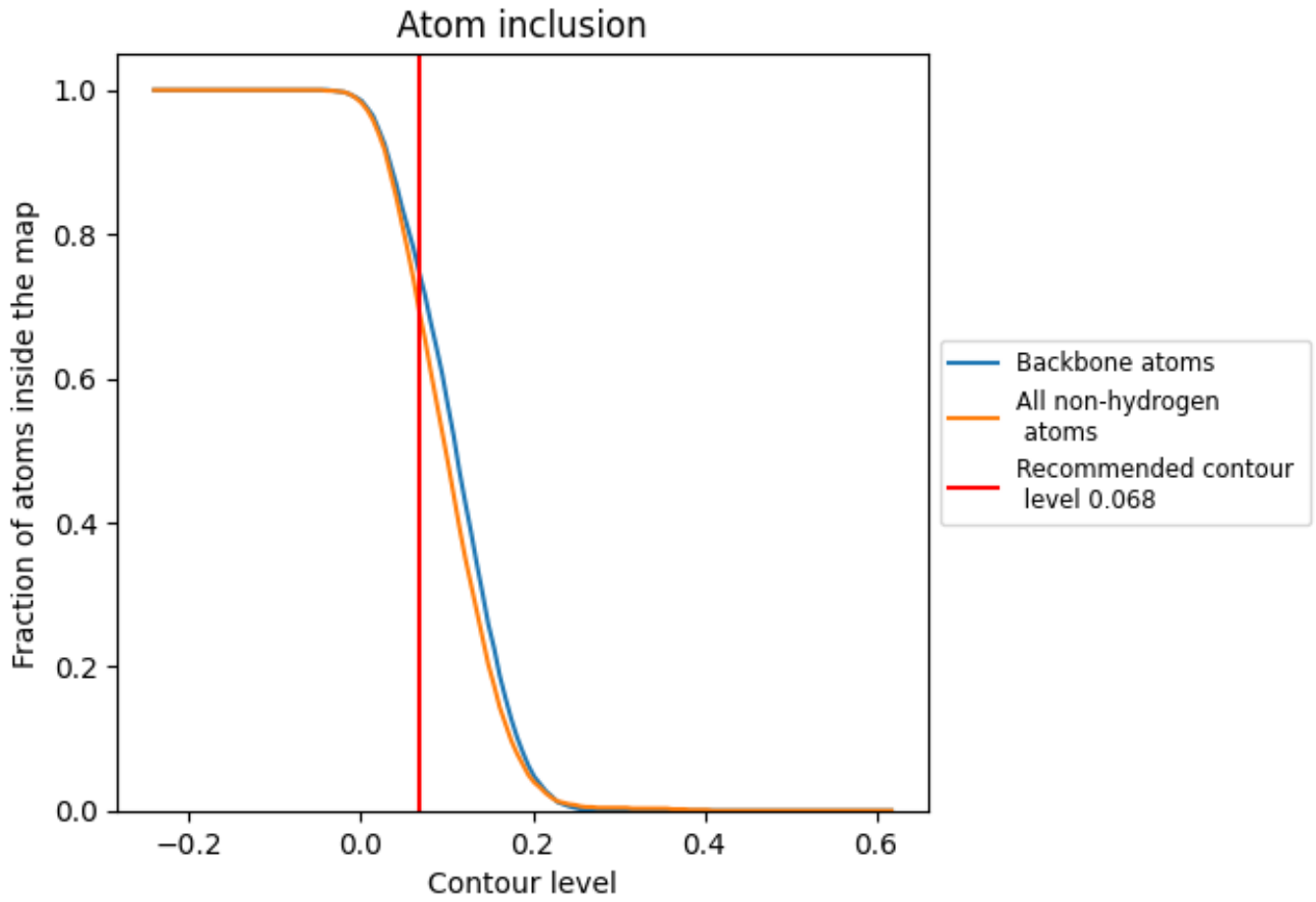
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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