wwPDB EM Validation Summary Report (i)

Nov 21, 2022 – 02:14 AM EST

PDB ID	:	7UIZ
EMDB ID	:	EMD-26558
Title	:	ClpAP complex bound to ClpS N-terminal extension, class IIc
Authors	:	Kim, S.; Fei, X.; Sauer, R.T.; Baker, T.A.
Deposited on	:	2022-03-29
Resolution	:	3.24 Å(reported)

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

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

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

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

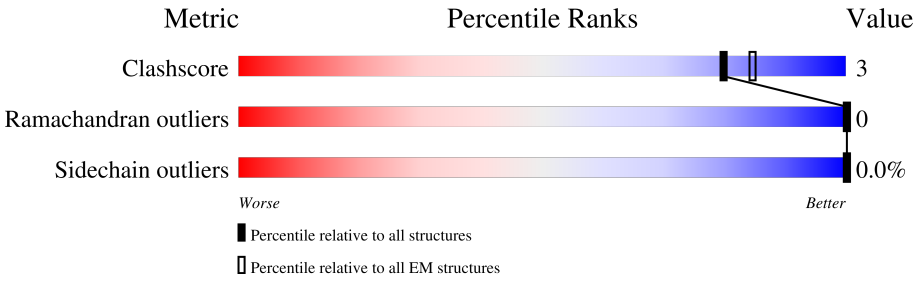
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.24 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	758	20% 72% · 24%
1	B	758	5% 70% 6% 23%
1	C	758	· 72% · 23%
1	D	758	· 70% 6% 23%
1	E	758	10% 70% 6% 23%
1	F	758	38% 70% 6% 24%
2	S	106	13% 21% · 76%
3	H	201	14% 91% · 5%

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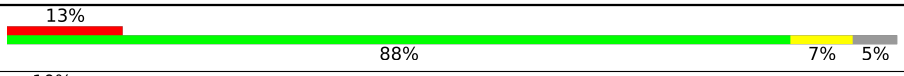
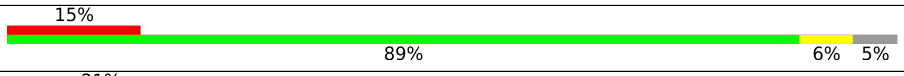
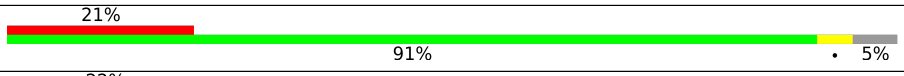
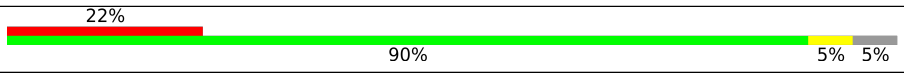
Mol	Chain	Length	Quality of chain
3	I	201	
3	J	201	
3	K	201	
3	L	201	
3	M	201	
3	N	201	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 76665 atoms, of which 38534 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent Clp protease ATP-binding subunit ClpA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	577	Total	C	H	N	O	S	0	0
			9098	2835	4598	804	848	13		
1	B	580	Total	C	H	N	O	S	0	0
			9141	2847	4619	808	854	13		
1	C	581	Total	C	H	N	O	S	0	0
			9152	2851	4623	809	856	13		
1	D	580	Total	C	H	N	O	S	0	0
			9144	2848	4620	808	855	13		
1	E	580	Total	C	H	N	O	S	0	0
			9138	2848	4614	808	855	13		
1	F	579	Total	C	H	N	O	S	0	0
			9122	2844	4605	807	853	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	THR	MET	conflict	UNP A0A836NDF2
B	169	THR	MET	conflict	UNP A0A836NDF2
C	169	THR	MET	conflict	UNP A0A836NDF2
D	169	THR	MET	conflict	UNP A0A836NDF2
E	169	THR	MET	conflict	UNP A0A836NDF2
F	169	THR	MET	conflict	UNP A0A836NDF2

- Molecule 2 is a protein called ATP-dependent Clp protease adapter protein ClpS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	25	Total	C	H	N	O	0	0
			396	127	194	34	41		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	191	Total	C	H	N	O	S	0	0
			3001	943	1506	259	281	12		
3	I	191	Total	C	H	N	O	S	0	0
			3001	943	1506	259	281	12		
3	J	191	Total	C	H	N	O	S	0	0
			3001	943	1506	259	281	12		
3	K	191	Total	C	H	N	O	S	0	0
			3001	943	1506	259	281	12		
3	L	191	Total	C	H	N	O	S	0	0
			3001	943	1506	259	281	12		
3	M	190	Total	C	H	N	O	S	0	0
			2977	937	1493	255	280	12		
3	N	190	Total	C	H	N	O	S	0	0
			2978	937	1494	255	280	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	194	ARG	-	expression tag	UNP A0A0K4NM46
H	195	SER	-	expression tag	UNP A0A0K4NM46
H	196	HIS	-	expression tag	UNP A0A0K4NM46
H	197	HIS	-	expression tag	UNP A0A0K4NM46
H	198	HIS	-	expression tag	UNP A0A0K4NM46
H	199	HIS	-	expression tag	UNP A0A0K4NM46
H	200	HIS	-	expression tag	UNP A0A0K4NM46
H	201	HIS	-	expression tag	UNP A0A0K4NM46
I	194	ARG	-	expression tag	UNP A0A0K4NM46
I	195	SER	-	expression tag	UNP A0A0K4NM46
I	196	HIS	-	expression tag	UNP A0A0K4NM46
I	197	HIS	-	expression tag	UNP A0A0K4NM46
I	198	HIS	-	expression tag	UNP A0A0K4NM46
I	199	HIS	-	expression tag	UNP A0A0K4NM46
I	200	HIS	-	expression tag	UNP A0A0K4NM46
I	201	HIS	-	expression tag	UNP A0A0K4NM46
J	194	ARG	-	expression tag	UNP A0A0K4NM46
J	195	SER	-	expression tag	UNP A0A0K4NM46
J	196	HIS	-	expression tag	UNP A0A0K4NM46
J	197	HIS	-	expression tag	UNP A0A0K4NM46
J	198	HIS	-	expression tag	UNP A0A0K4NM46
J	199	HIS	-	expression tag	UNP A0A0K4NM46
J	200	HIS	-	expression tag	UNP A0A0K4NM46
J	201	HIS	-	expression tag	UNP A0A0K4NM46
K	194	ARG	-	expression tag	UNP A0A0K4NM46
K	195	SER	-	expression tag	UNP A0A0K4NM46

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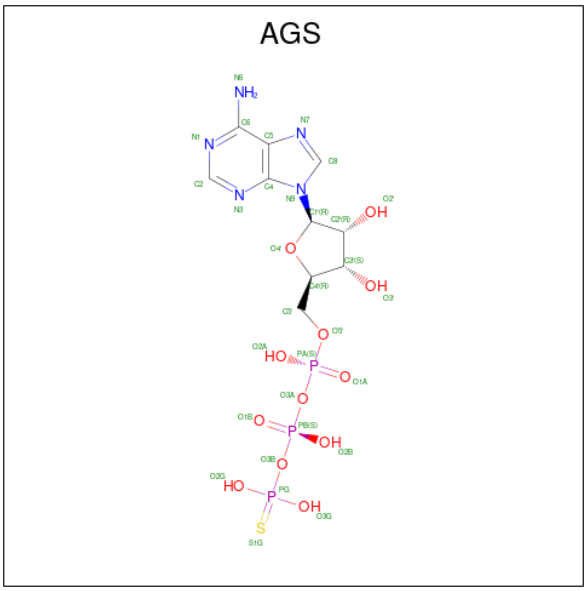
Chain	Residue	Modelled	Actual	Comment	Reference
K	196	HIS	-	expression tag	UNP A0A0K4NM46
K	197	HIS	-	expression tag	UNP A0A0K4NM46
K	198	HIS	-	expression tag	UNP A0A0K4NM46
K	199	HIS	-	expression tag	UNP A0A0K4NM46
K	200	HIS	-	expression tag	UNP A0A0K4NM46
K	201	HIS	-	expression tag	UNP A0A0K4NM46
L	194	ARG	-	expression tag	UNP A0A0K4NM46
L	195	SER	-	expression tag	UNP A0A0K4NM46
L	196	HIS	-	expression tag	UNP A0A0K4NM46
L	197	HIS	-	expression tag	UNP A0A0K4NM46
L	198	HIS	-	expression tag	UNP A0A0K4NM46
L	199	HIS	-	expression tag	UNP A0A0K4NM46
L	200	HIS	-	expression tag	UNP A0A0K4NM46
L	201	HIS	-	expression tag	UNP A0A0K4NM46
M	194	ARG	-	expression tag	UNP A0A0K4NM46
M	195	SER	-	expression tag	UNP A0A0K4NM46
M	196	HIS	-	expression tag	UNP A0A0K4NM46
M	197	HIS	-	expression tag	UNP A0A0K4NM46
M	198	HIS	-	expression tag	UNP A0A0K4NM46
M	199	HIS	-	expression tag	UNP A0A0K4NM46
M	200	HIS	-	expression tag	UNP A0A0K4NM46
M	201	HIS	-	expression tag	UNP A0A0K4NM46
N	194	ARG	-	expression tag	UNP A0A0K4NM46
N	195	SER	-	expression tag	UNP A0A0K4NM46
N	196	HIS	-	expression tag	UNP A0A0K4NM46
N	197	HIS	-	expression tag	UNP A0A0K4NM46
N	198	HIS	-	expression tag	UNP A0A0K4NM46
N	199	HIS	-	expression tag	UNP A0A0K4NM46
N	200	HIS	-	expression tag	UNP A0A0K4NM46
N	201	HIS	-	expression tag	UNP A0A0K4NM46

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	A	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	B	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	B	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	C	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	C	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	D	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	D	1	Total	C	H	N	O	P	S	0
			86	20	24	10	24	6	2	
4	F	1	Total	C	H	N	O	P	S	0
			43	10	12	5	12	3	1	

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

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

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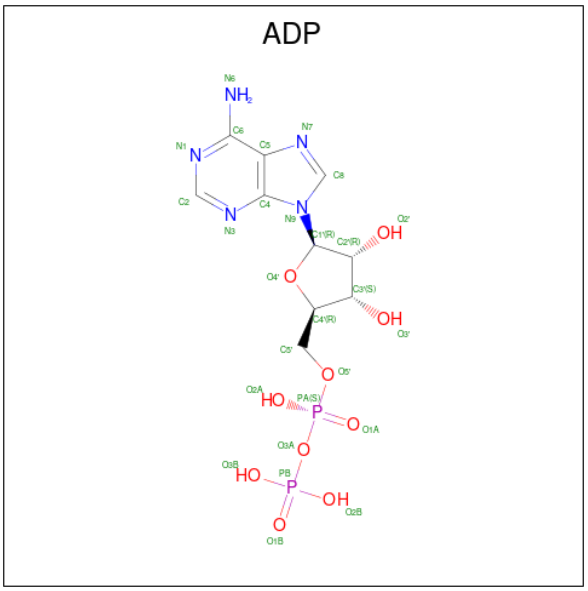
Mol	Chain	Residues	Atoms	AltConf
5	C	2	Total Mg 2 2	0
5	D	2	Total Mg 2 2	0
5	E	1	Total Mg 1 1	0
5	F	1	Total Mg 1 1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



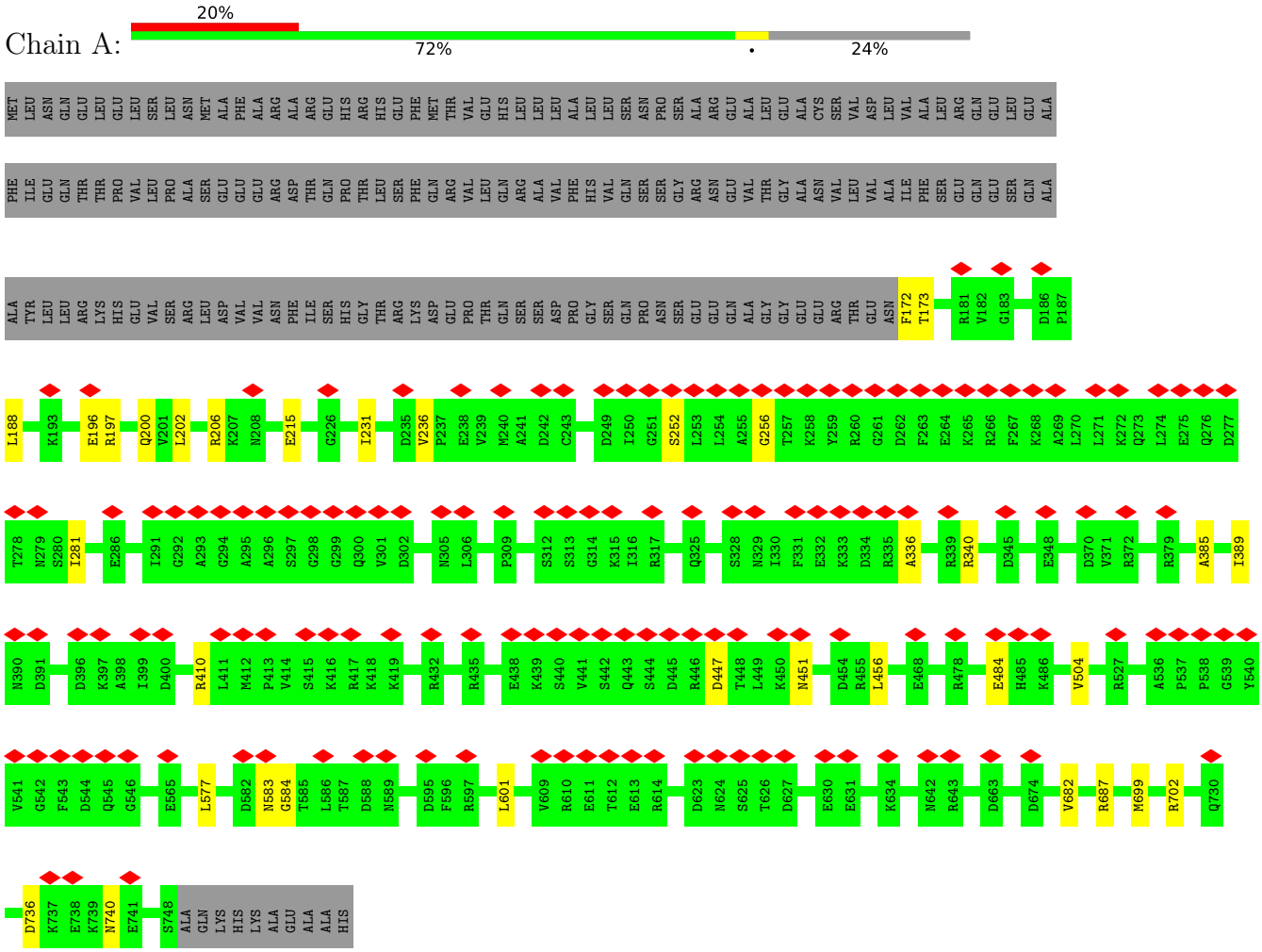
Mol	Chain	Residues	Atoms	AltConf
6	E	1	Total C H N O P 78 20 24 10 20 4	0
6	E	1	Total C H N O P 78 20 24 10 20 4	0
6	F	1	Total C H N O P 39 10 12 5 10 2	0

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.

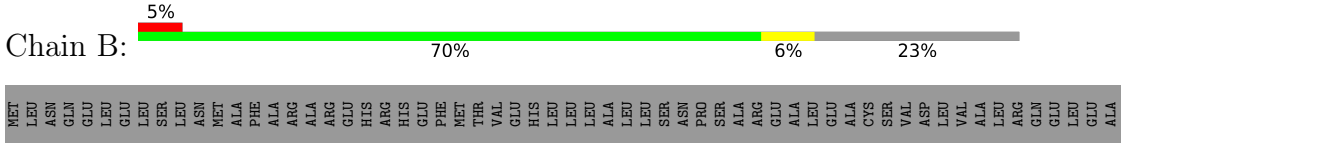
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

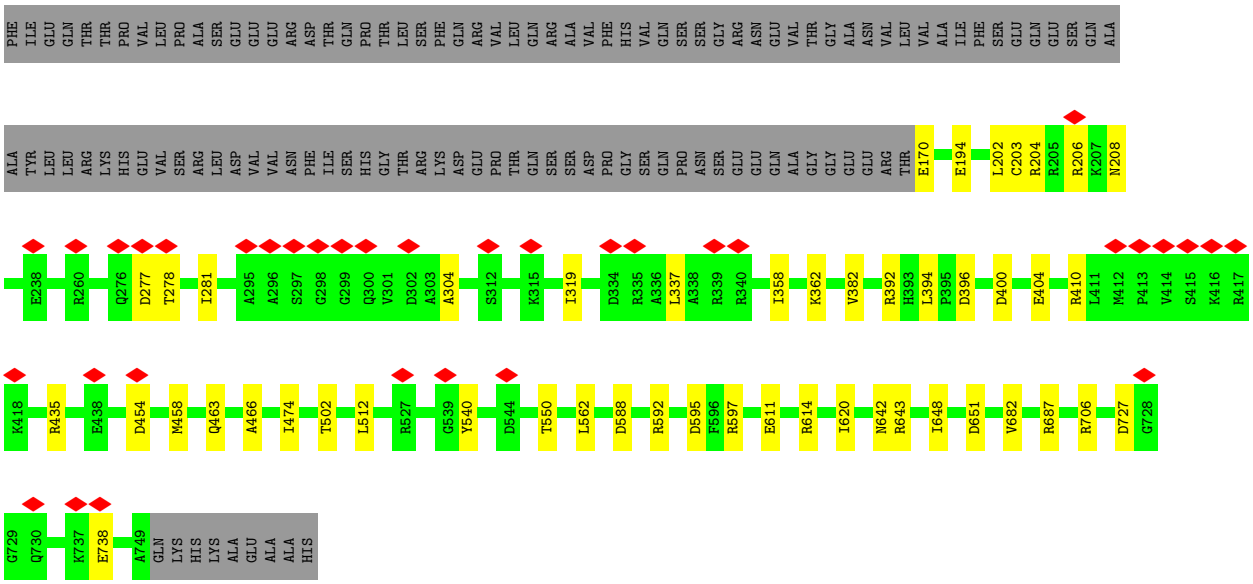
Chain A:



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

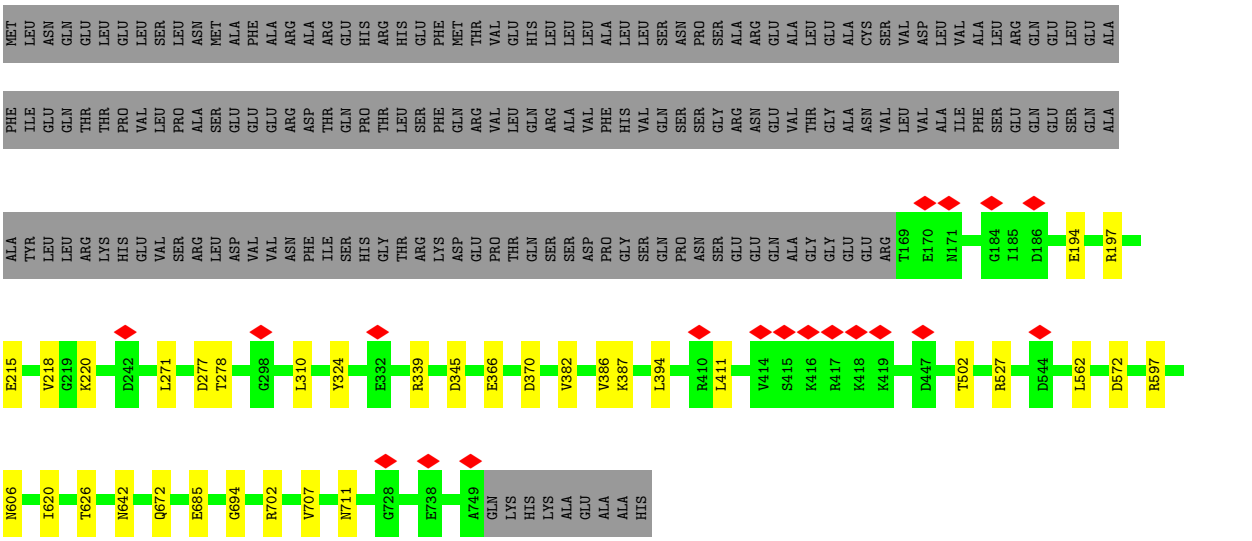
Chain B:





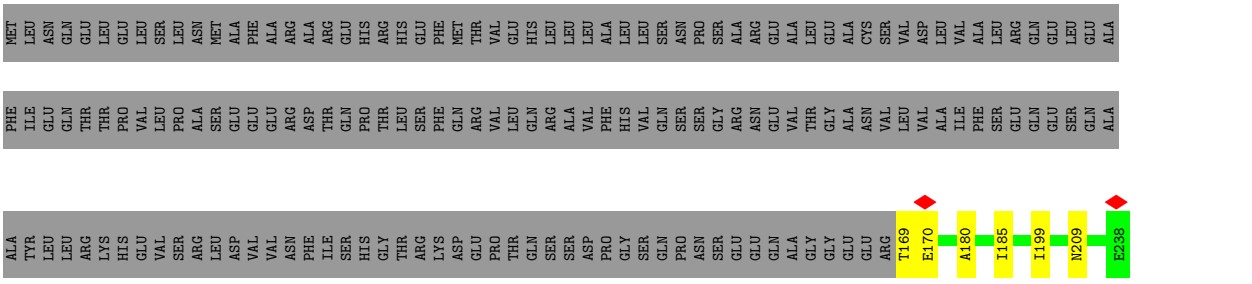
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

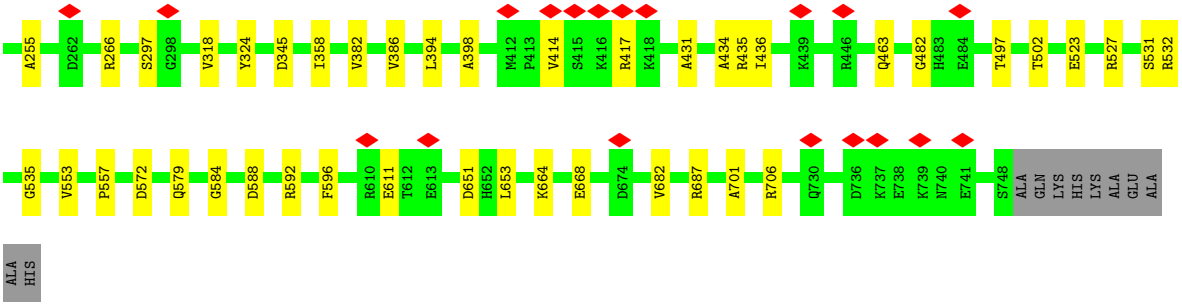
Chain C:



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

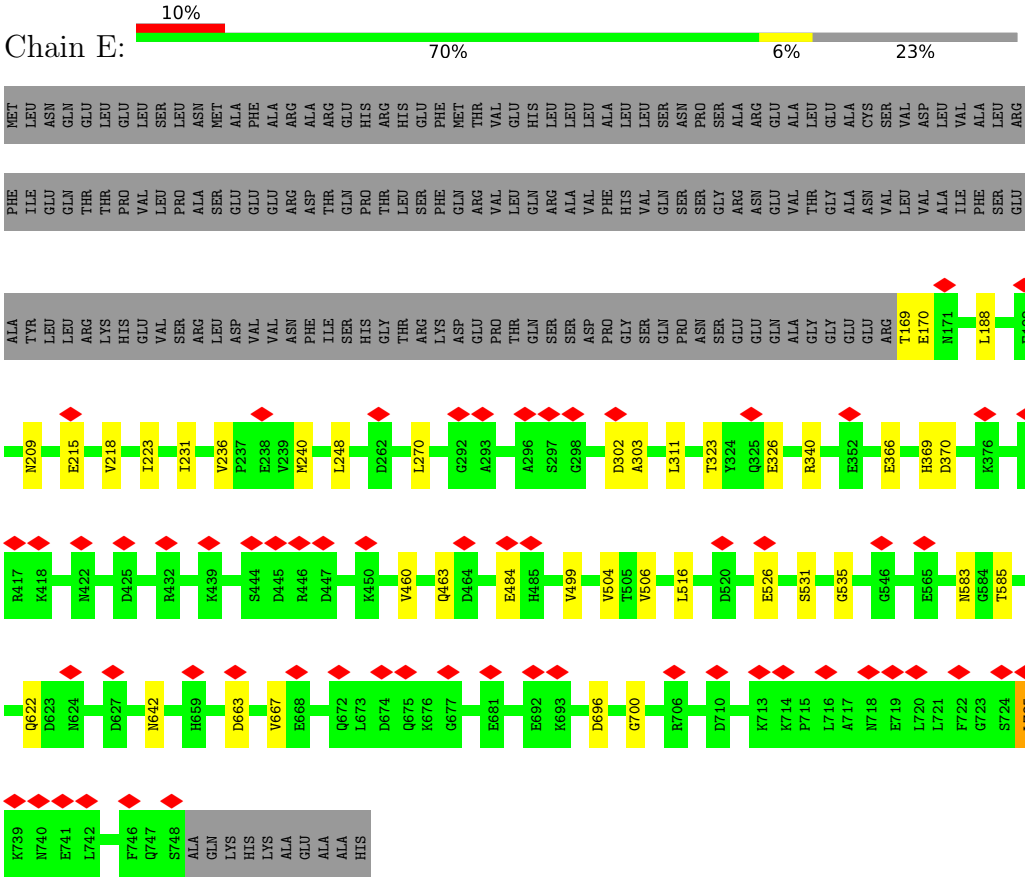
Chain D:





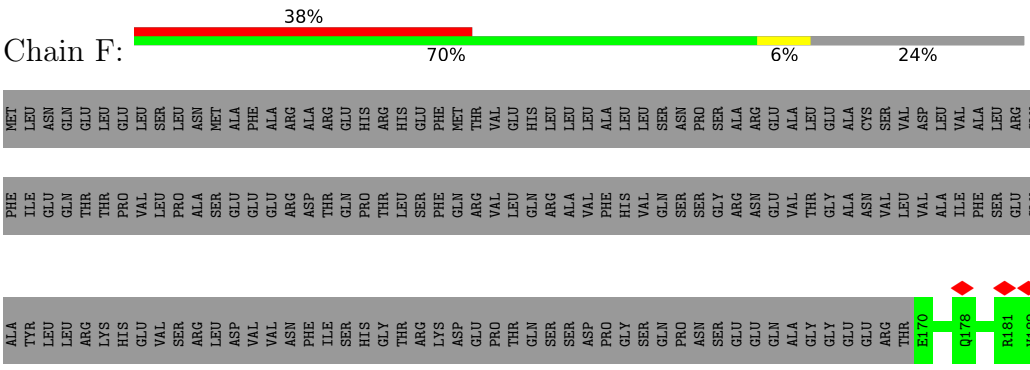
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpA

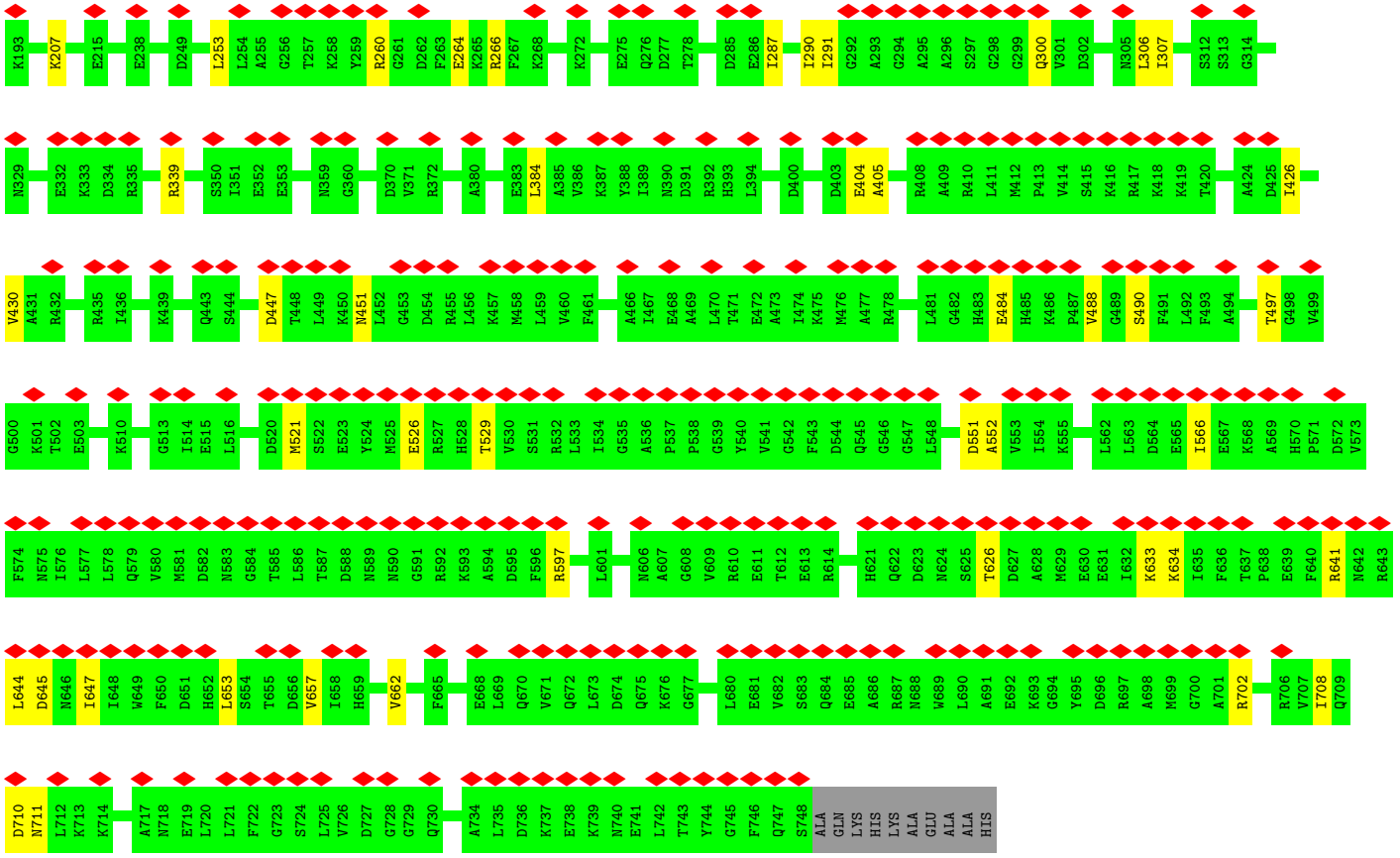
Chain E:



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

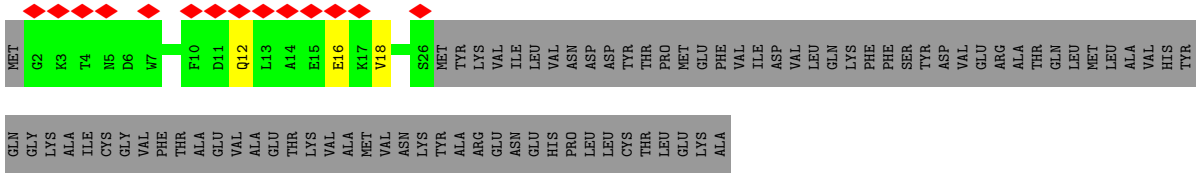
Chain F:





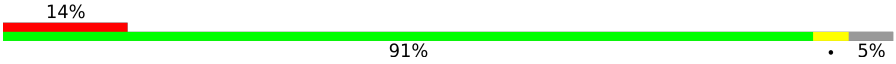
• Molecule 2: ATP-dependent Clp protease adapter protein ClpS

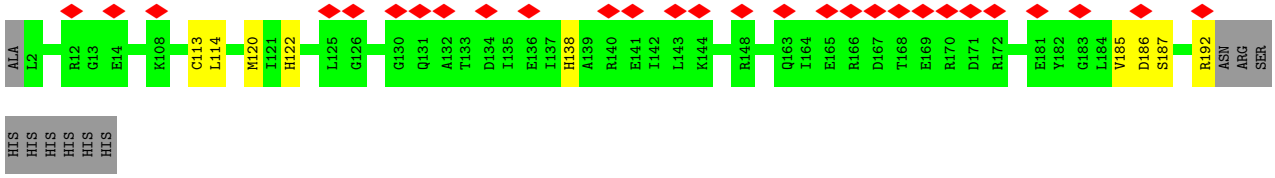
Chain S:



• Molecule 3: ATP-dependent Clp protease proteolytic subunit

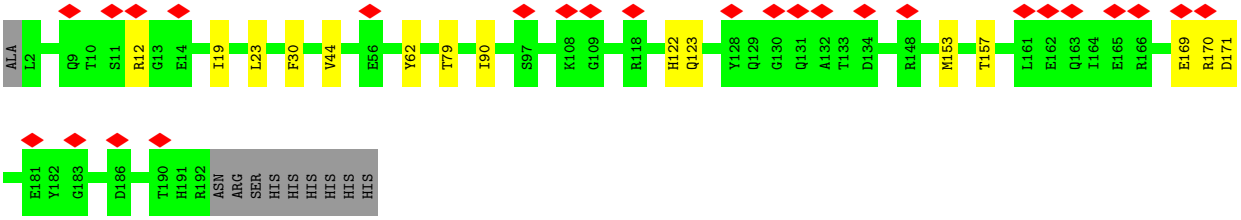
Chain H:



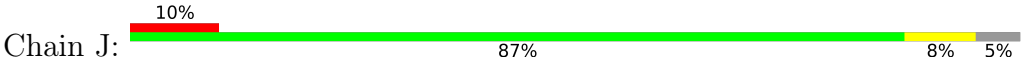


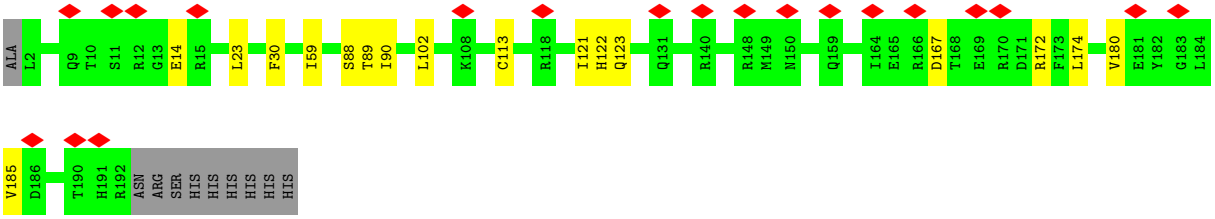
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain I:

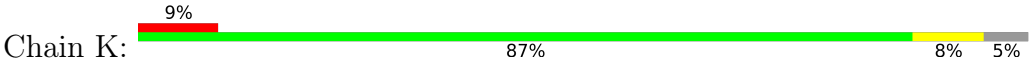


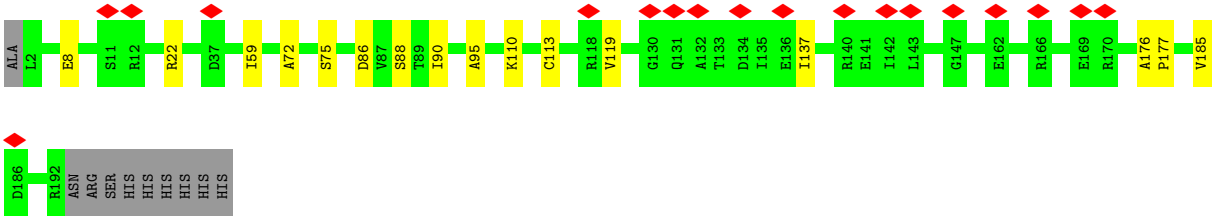
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



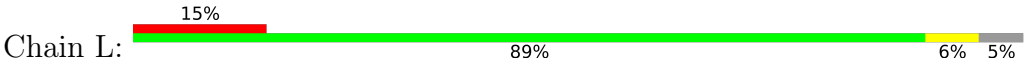


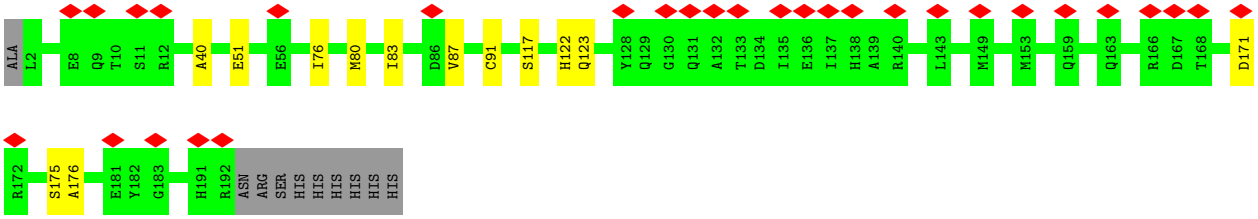
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



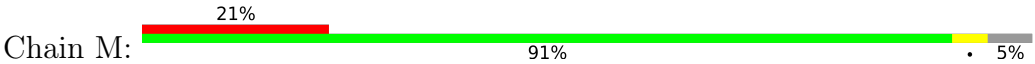


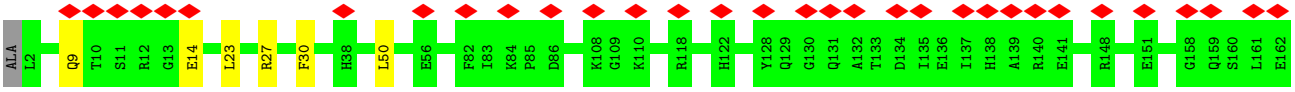
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

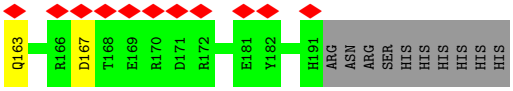




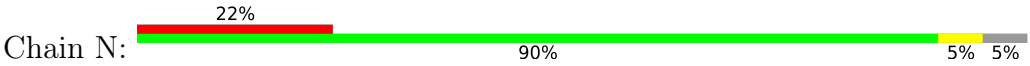
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

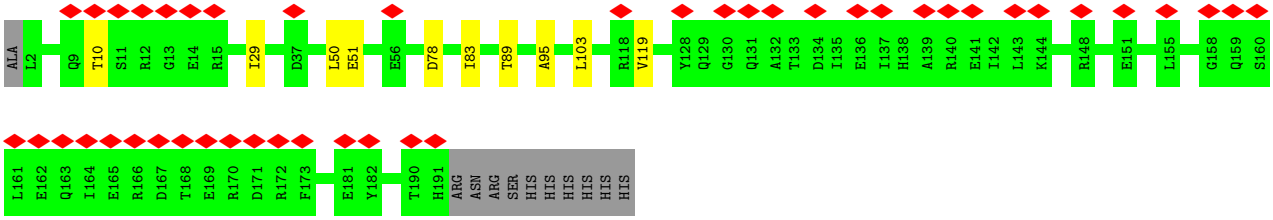






• Molecule 3: ATP-dependent Clp protease proteolytic subunit





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38131	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.779	Depositor
Minimum map value	-7.668	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.66	Depositor
Map size (Å)	149.64, 148.77, 188.79001	wwPDB
Map dimensions	217, 171, 172	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87000006	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/4566	0.51	0/6162
1	B	0.25	0/4588	0.50	0/6192
1	C	0.25	0/4595	0.50	0/6202
1	D	0.25	0/4590	0.50	0/6195
1	E	0.25	0/4590	0.51	2/6195 (0.0%)
1	F	0.26	0/4583	0.51	0/6185
2	S	0.29	0/206	0.49	0/278
3	H	0.26	0/1519	0.48	0/2047
3	I	0.25	0/1519	0.50	0/2047
3	J	0.26	0/1519	0.51	0/2047
3	K	0.26	0/1519	0.51	0/2047
3	L	0.26	0/1519	0.48	0/2047
3	M	0.27	0/1508	0.50	0/2033
3	N	0.26	0/1508	0.48	0/2033
All	All	0.26	0/38329	0.50	2/51710 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	725	LEU	CB-CG-CD2	5.65	120.60	111.00
1	E	725	LEU	CB-CG-CD1	5.42	120.22	111.00

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	4500	4598	4600	21	0
1	B	4522	4619	4617	32	0
1	C	4529	4623	4623	27	0
1	D	4524	4620	4619	30	0
1	E	4524	4614	4620	32	0
1	F	4517	4605	4613	27	0
2	S	202	194	193	3	0
3	H	1495	1506	1507	6	0
3	I	1495	1506	1507	11	0
3	J	1495	1506	1507	11	0
3	K	1495	1506	1507	9	0
3	L	1495	1506	1507	8	0
3	M	1484	1493	1494	5	0
3	N	1484	1494	1494	7	0
4	A	62	24	24	3	0
4	B	62	24	24	1	0
4	C	62	24	24	3	0
4	D	62	24	24	2	0
4	F	31	12	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	E	54	24	24	0	0
6	F	27	12	12	0	0
All	All	38131	38534	38552	208	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 3.

The worst 5 of 208 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ARG:NH1	4:C:802:AGS:O3G	2.22	0.71
1:F:447:ASP:O	1:F:451:ASN:ND2	2.26	0.69
4:D:801:AGS:O2G	1:E:340:ARG:NH1	2.26	0.68
1:A:699:MET:SD	1:B:642:ASN:ND2	2.68	0.67
1:B:396:ASP:OD2	1:C:339:ARG:NH1	2.28	0.67

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	575/758 (76%)	575 (100%)	0	0	100	100
1	B	578/758 (76%)	578 (100%)	0	0	100	100
1	C	579/758 (76%)	575 (99%)	4 (1%)	0	100	100
1	D	578/758 (76%)	577 (100%)	1 (0%)	0	100	100
1	E	578/758 (76%)	577 (100%)	1 (0%)	0	100	100
1	F	577/758 (76%)	577 (100%)	0	0	100	100
2	S	23/106 (22%)	23 (100%)	0	0	100	100
3	H	189/201 (94%)	189 (100%)	0	0	100	100
3	I	189/201 (94%)	189 (100%)	0	0	100	100
3	J	189/201 (94%)	189 (100%)	0	0	100	100
3	K	189/201 (94%)	189 (100%)	0	0	100	100
3	L	189/201 (94%)	189 (100%)	0	0	100	100
3	M	188/201 (94%)	188 (100%)	0	0	100	100
3	N	188/201 (94%)	188 (100%)	0	0	100	100
All	All	4809/6061 (79%)	4803 (100%)	6 (0%)	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	484/639 (76%)	484 (100%)	0	100 100
1	B	486/639 (76%)	485 (100%)	1 (0%)	93 97
1	C	487/639 (76%)	487 (100%)	0	100 100
1	D	487/639 (76%)	487 (100%)	0	100 100
1	E	487/639 (76%)	487 (100%)	0	100 100
1	F	486/639 (76%)	486 (100%)	0	100 100
2	S	22/93 (24%)	22 (100%)	0	100 100
3	H	162/171 (95%)	161 (99%)	1 (1%)	86 93
3	I	162/171 (95%)	162 (100%)	0	100 100
3	J	162/171 (95%)	162 (100%)	0	100 100
3	K	162/171 (95%)	162 (100%)	0	100 100
3	L	162/171 (95%)	162 (100%)	0	100 100
3	M	161/171 (94%)	161 (100%)	0	100 100
3	N	161/171 (94%)	161 (100%)	0	100 100
All	All	4071/5124 (79%)	4069 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	410	ARG
3	H	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	41	ASN
3	I	163	GLN
3	M	116	ASN
3	K	116	ASN

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Mol	Chain	Res	Type
3	L	41	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
4	AGS	B	802	5	26,33,33	0.82	1 (3%)	26,52,52	0.79	1 (3%)
4	AGS	B	801	5	26,33,33	0.81	1 (3%)	26,52,52	0.85	1 (3%)
4	AGS	C	802	5	26,33,33	0.81	1 (3%)	26,52,52	0.89	1 (3%)
4	AGS	F	801	-	26,33,33	0.80	1 (3%)	26,52,52	0.81	1 (3%)
6	ADP	E	801	5	24,29,29	0.65	0	29,45,45	0.75	1 (3%)
4	AGS	D	802	5	26,33,33	0.81	1 (3%)	26,52,52	0.76	1 (3%)
4	AGS	C	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.88	1 (3%)
4	AGS	A	801	5	26,33,33	0.80	1 (3%)	26,52,52	0.84	1 (3%)
6	ADP	E	802	-	24,29,29	0.68	0	29,45,45	0.76	1 (3%)
6	ADP	F	802	5	24,29,29	0.66	0	29,45,45	0.81	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	AGS	D	801	5	26,33,33	0.82	1 (3%)	26,52,52	0.91	2 (7%)
4	AGS	A	802	5	26,33,33	0.82	1 (3%)	26,52,52	0.80	1 (3%)

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
4	AGS	B	802	5	-	1/17/38/38	0/3/3/3
4	AGS	B	801	5	-	3/17/38/38	0/3/3/3
4	AGS	C	802	5	-	0/17/38/38	0/3/3/3
4	AGS	F	801	-	-	2/17/38/38	0/3/3/3
6	ADP	E	801	5	-	4/12/32/32	0/3/3/3
4	AGS	D	802	5	-	0/17/38/38	0/3/3/3
4	AGS	C	801	5	-	6/17/38/38	0/3/3/3
4	AGS	A	801	5	-	2/17/38/38	0/3/3/3
6	ADP	E	802	-	-	0/12/32/32	0/3/3/3
6	ADP	F	802	5	-	3/12/32/32	0/3/3/3
4	AGS	D	801	5	-	0/17/38/38	0/3/3/3
4	AGS	A	802	5	-	3/17/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	AGS	PG-S1G	2.15	1.95	1.90
4	F	801	AGS	PG-S1G	2.11	1.95	1.90
4	A	801	AGS	PG-S1G	2.10	1.95	1.90
4	B	802	AGS	PG-S1G	2.09	1.95	1.90
4	C	801	AGS	PG-S1G	2.08	1.95	1.90

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	AGS	C5-C6-N6	2.31	123.86	120.35
4	D	801	AGS	O4'-C1'-C2'	-2.28	103.60	106.93
4	B	801	AGS	C5-C6-N6	2.27	123.80	120.35
6	F	802	ADP	C5-C6-N6	2.22	123.73	120.35
4	D	801	AGS	C5-C6-N6	2.22	123.72	120.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	AGS	C4'-C5'-O5'-PA
4	B	801	AGS	O4'-C4'-C5'-O5'
4	C	801	AGS	C5'-O5'-PA-O1A
6	E	801	ADP	C5'-O5'-PA-O1A
6	E	801	ADP	C5'-O5'-PA-O3A

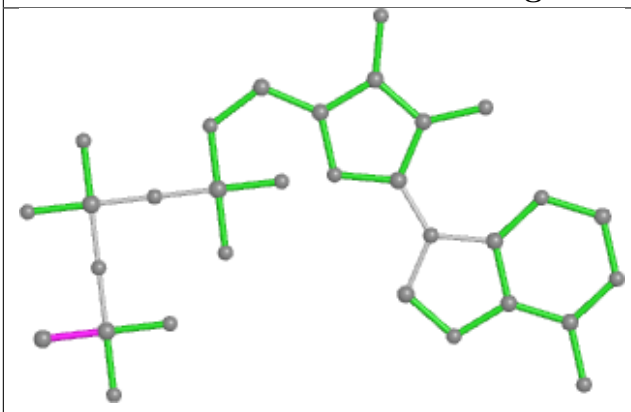
There are no ring outliers.

7 monomers are involved in 9 short contacts:

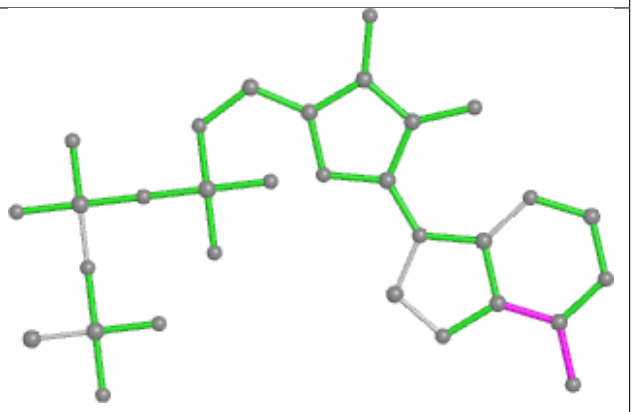
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	AGS	1	0
4	C	802	AGS	2	0
4	D	802	AGS	1	0
4	C	801	AGS	1	0
4	A	801	AGS	1	0
4	D	801	AGS	1	0
4	A	802	AGS	2	0

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

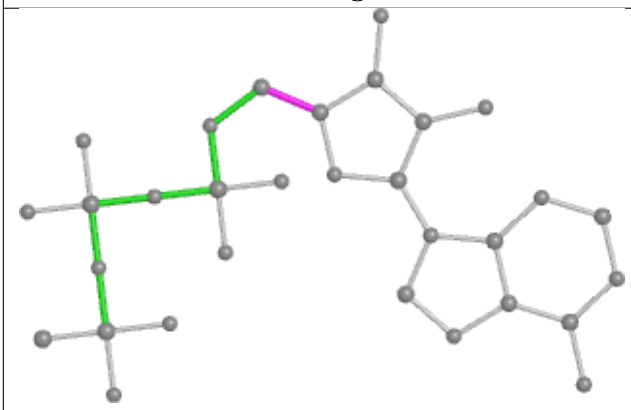
Ligand AGS B 802



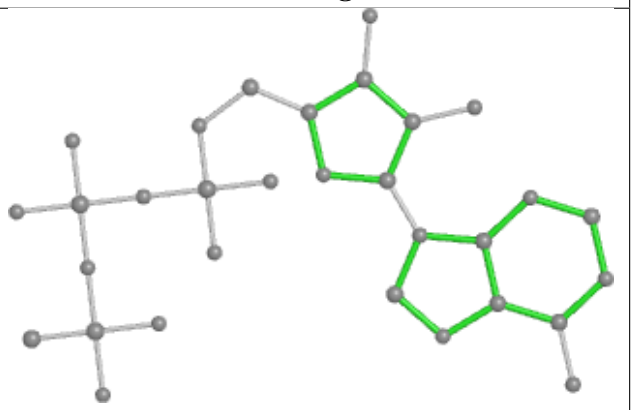
Bond lengths



Bond angles

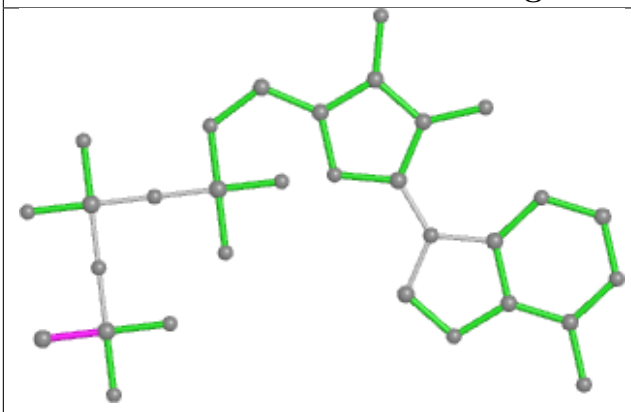


Torsions

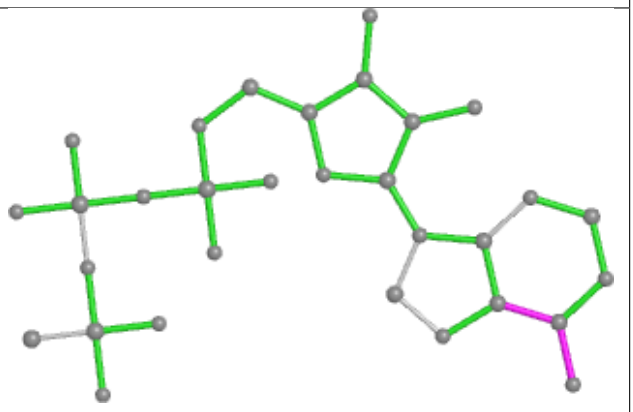


Rings

Ligand AGS B 801



Bond lengths



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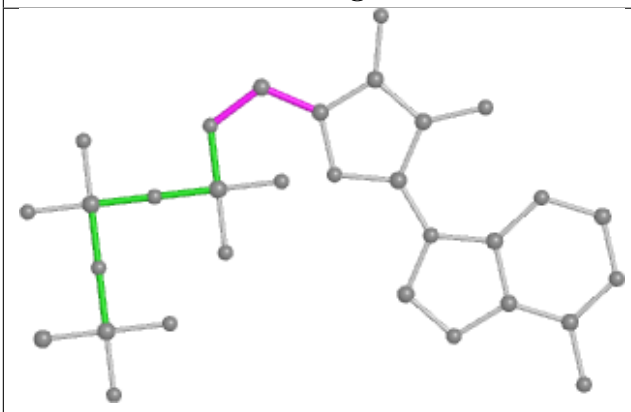

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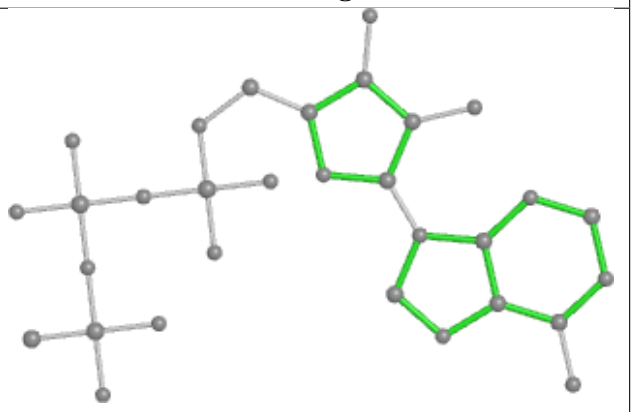
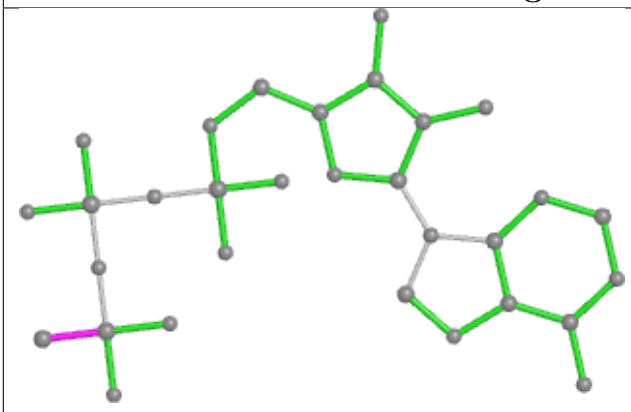
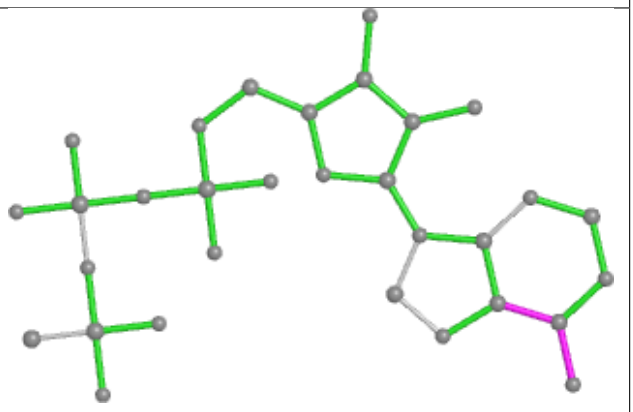


Rings

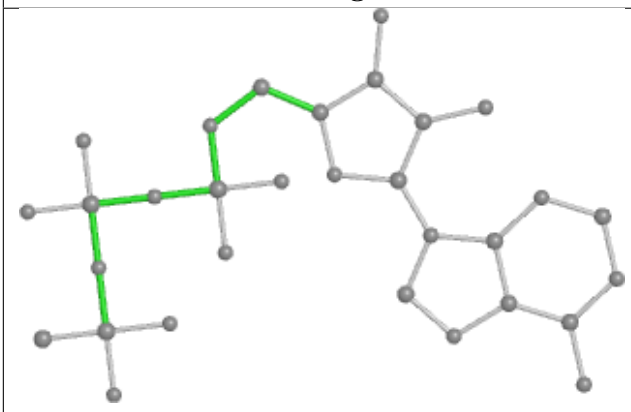
Ligand AGS C 802



Bond lengths



Bond angles



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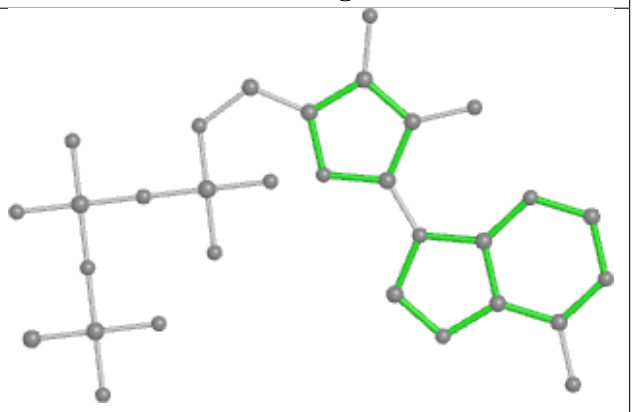
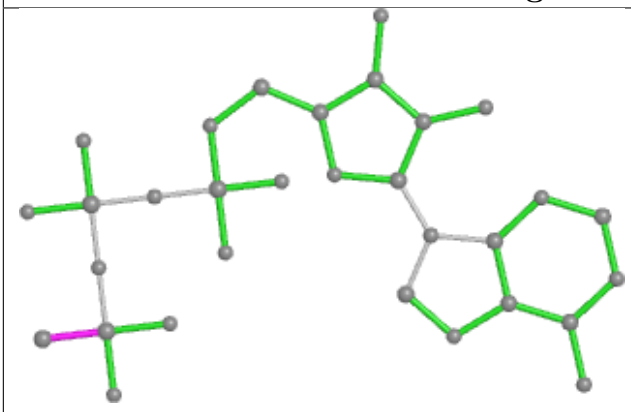
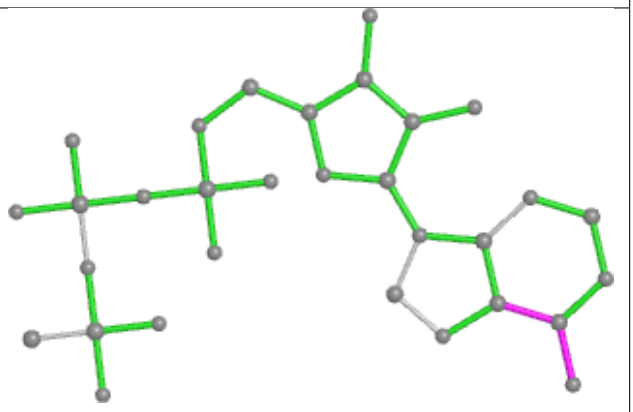


Rings

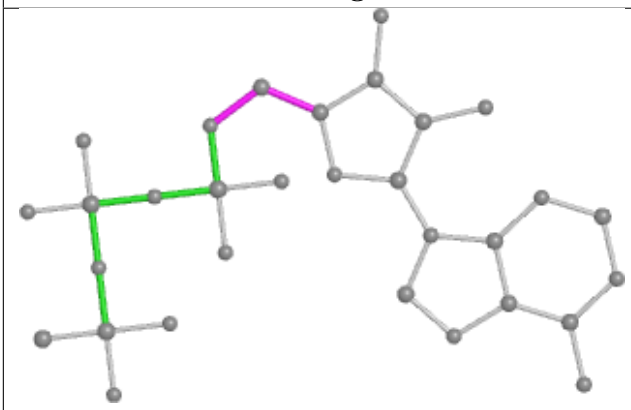
Ligand AGS F 801



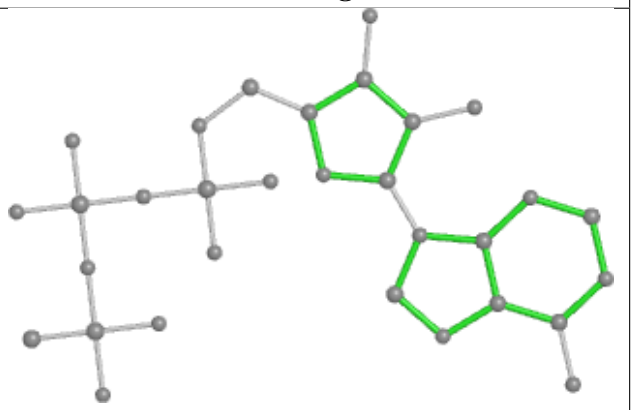
Bond lengths



Bond angles

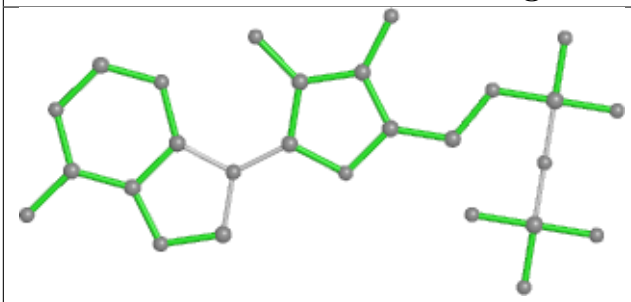


Torsions

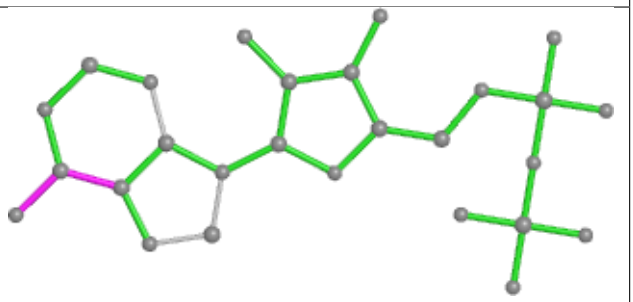


Rings

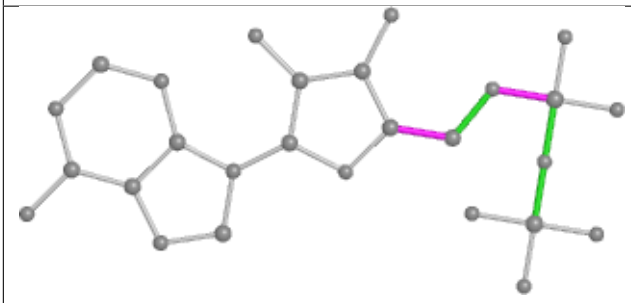
Ligand ADP E 801



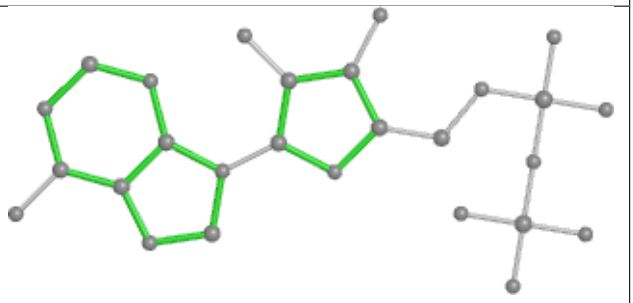
Bond lengths



Bond angles

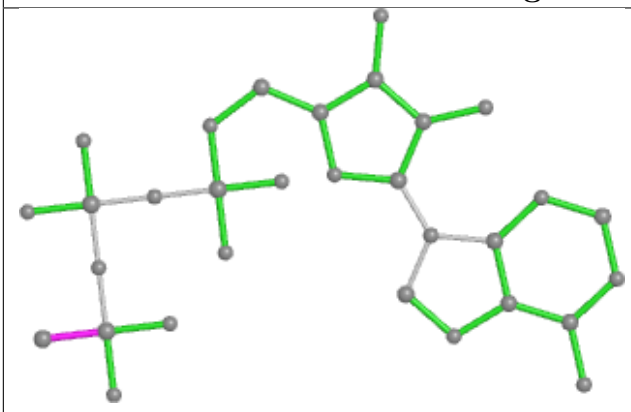


Torsions

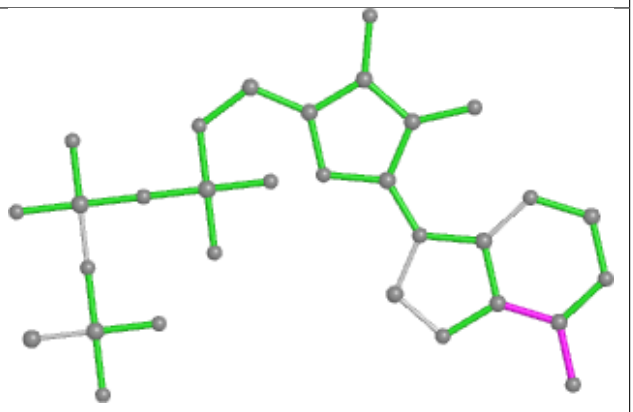


Rings

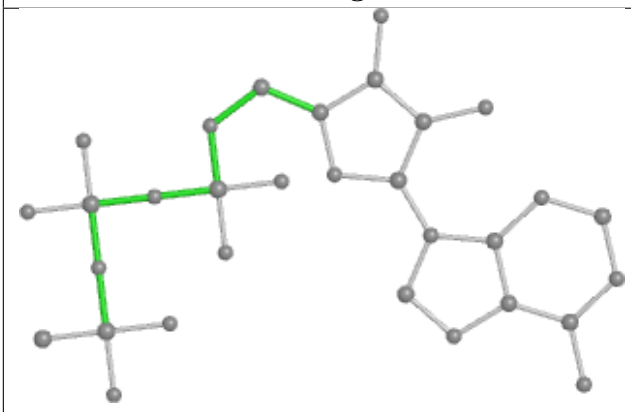
Ligand AGS D 802



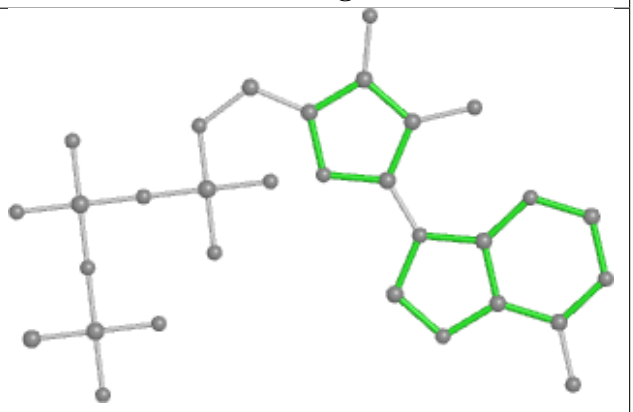
Bond lengths



Bond angles

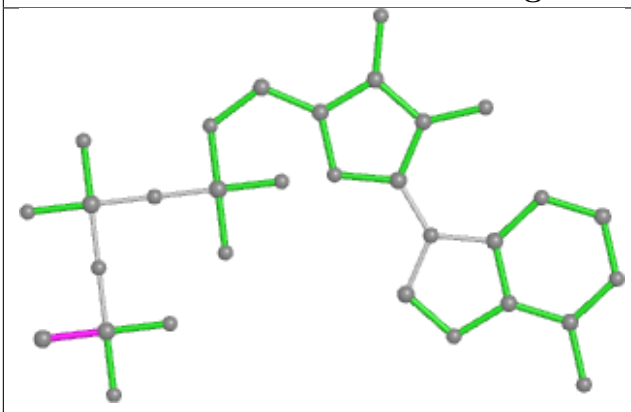


Torsions

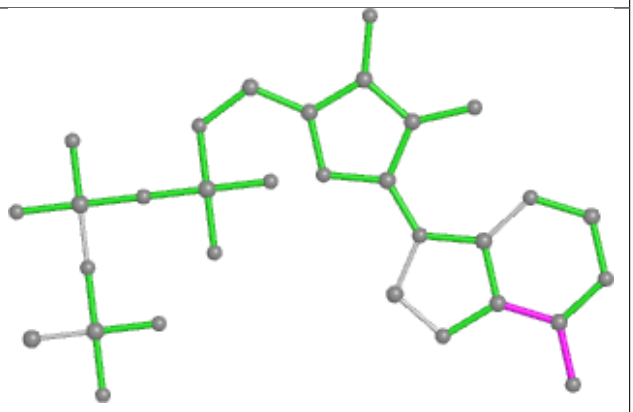


Rings

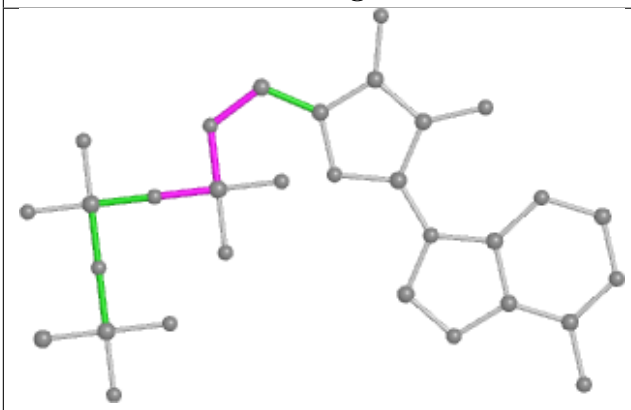
Ligand AGS C 801



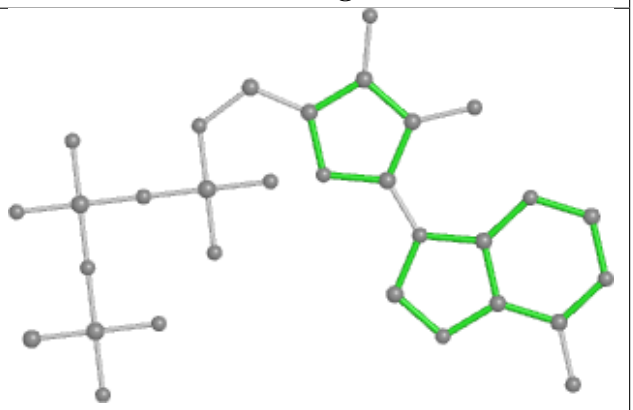
Bond lengths



Bond angles

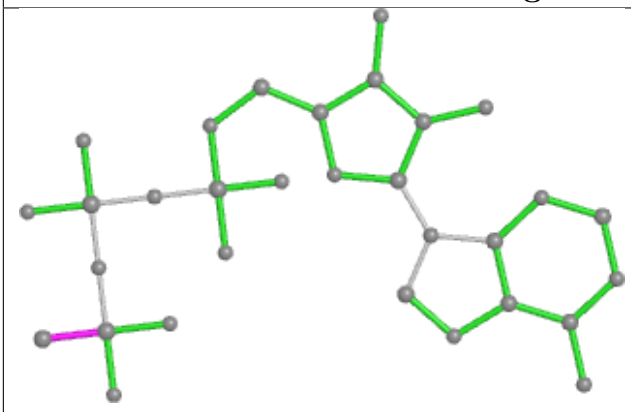


Torsions

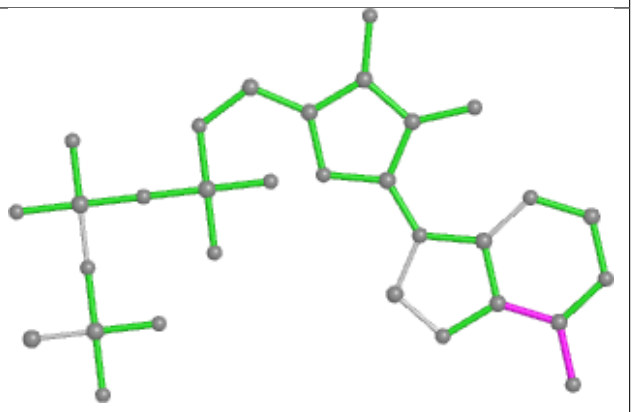


Rings

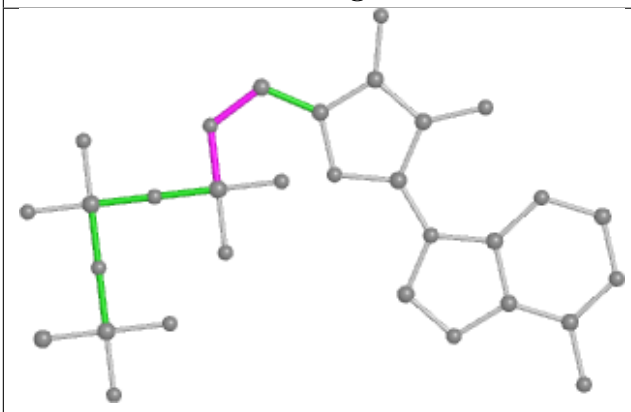
Ligand AGS A 801



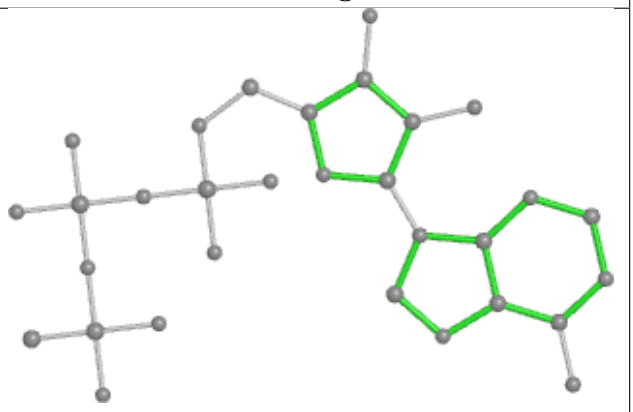
Bond lengths



Bond angles

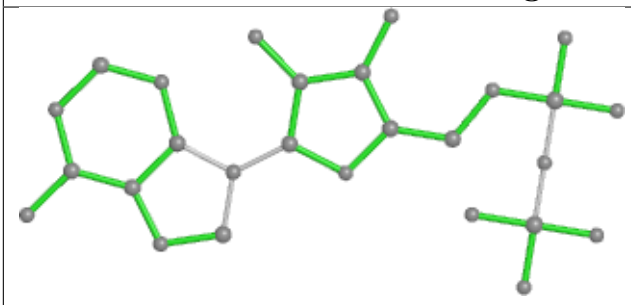


Torsions

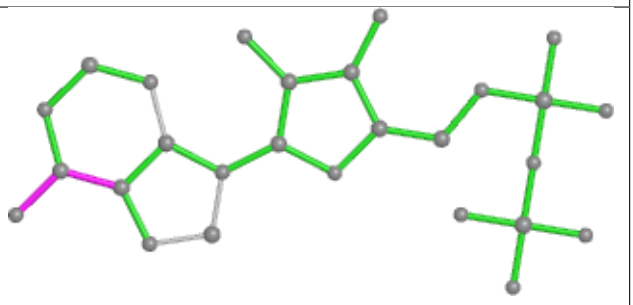


Rings

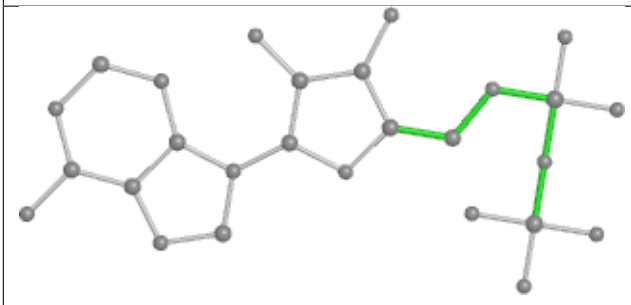
Ligand ADP E 802



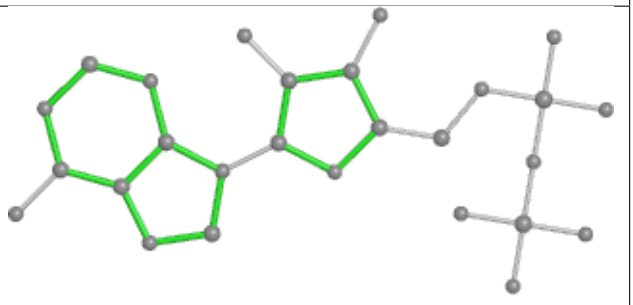
Bond lengths



Bond angles

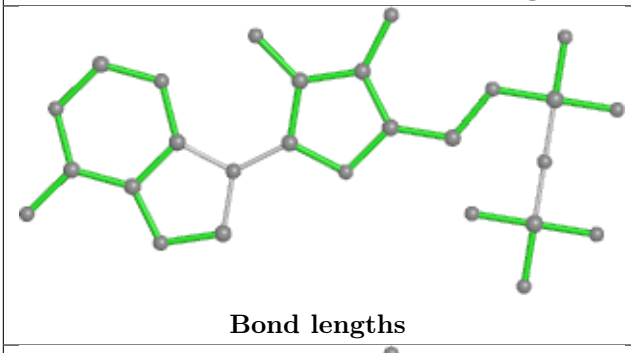


Torsions

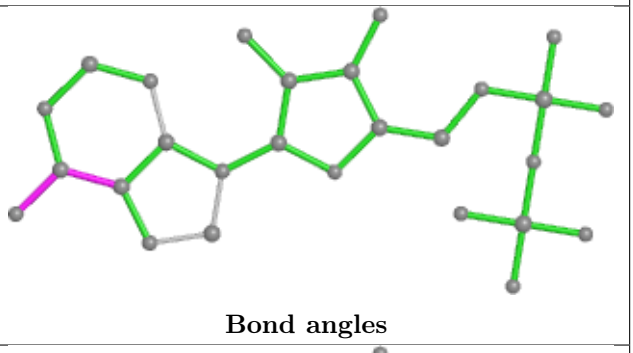


Rings

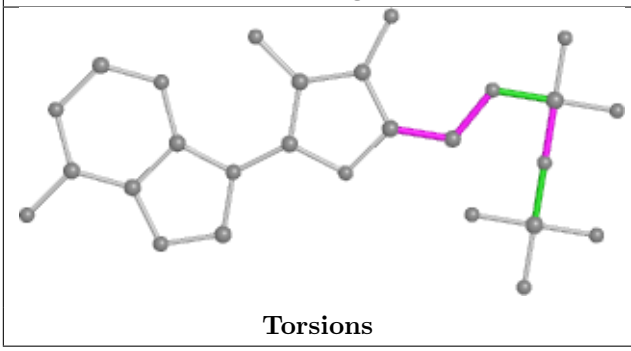
Ligand ADP F 802



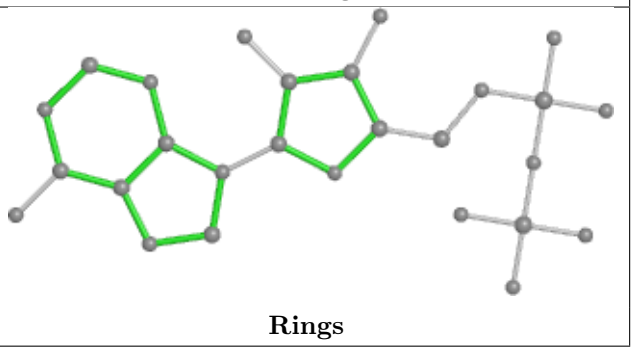
Bond lengths



Bond angles

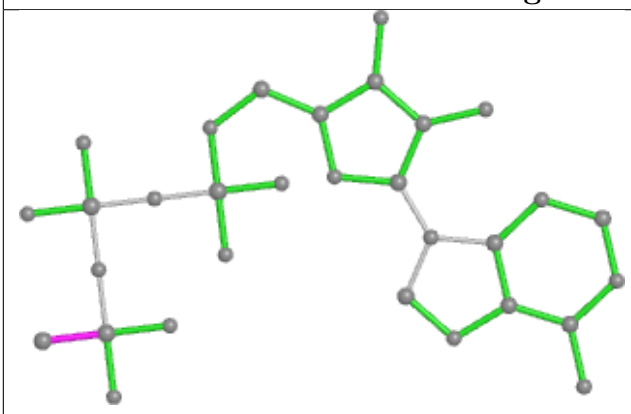


Torsions

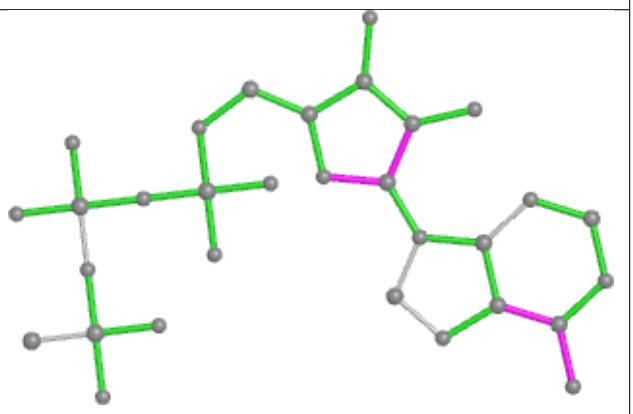


Rings

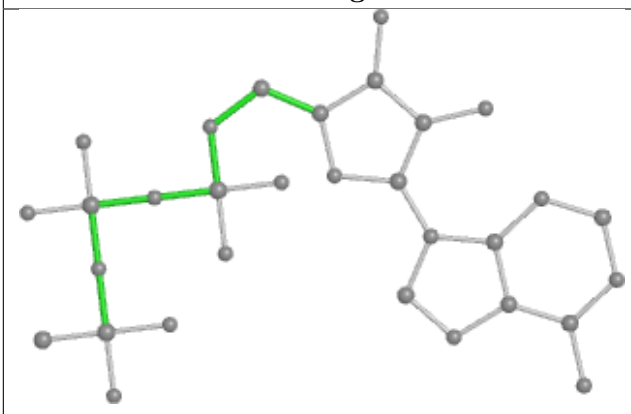
Ligand AGS D 801



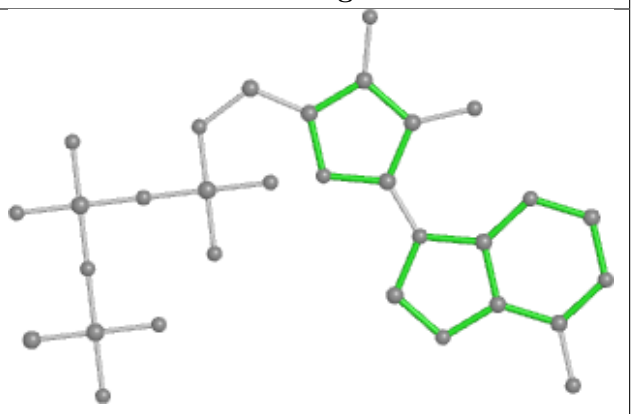
Bond lengths



Bond angles

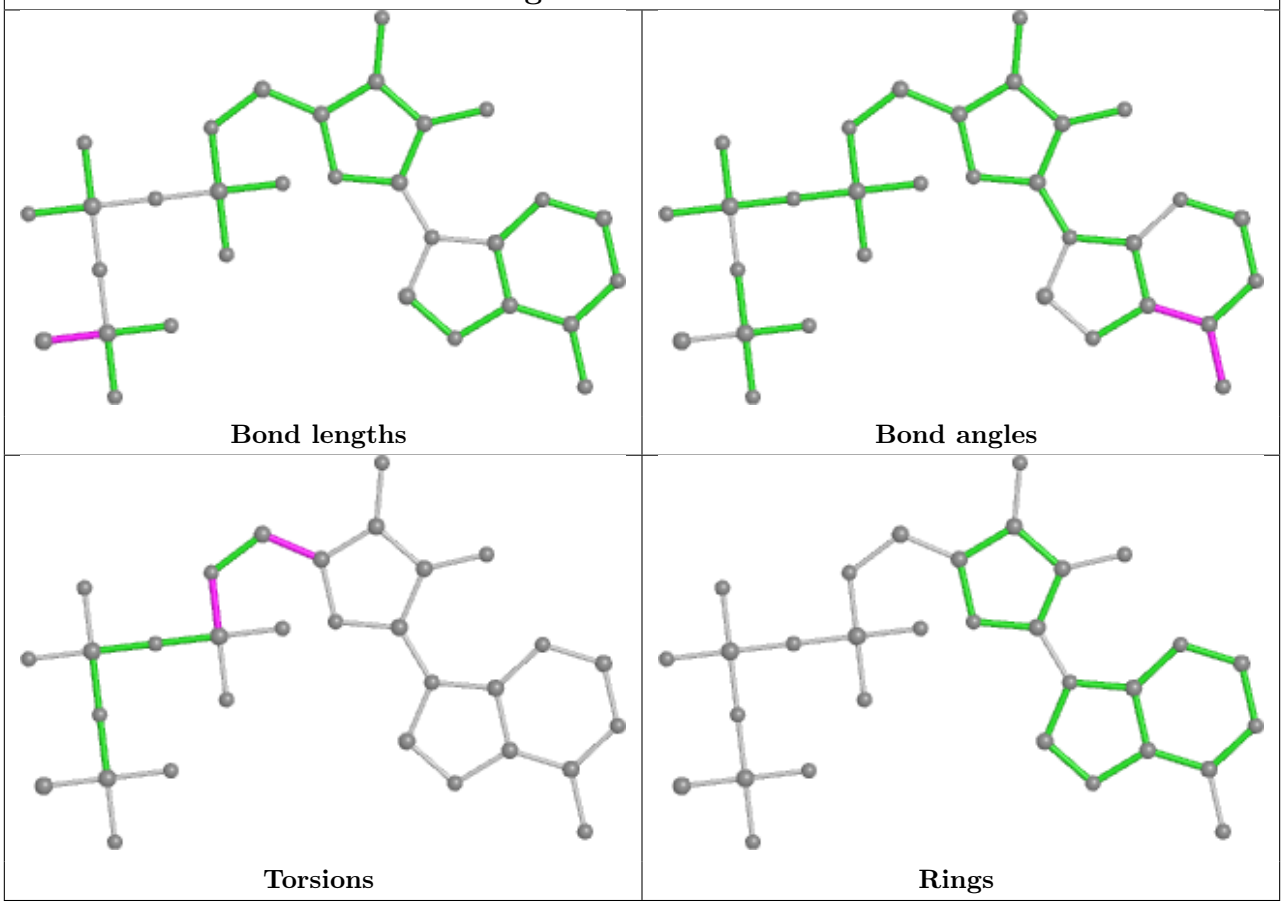


Torsions



Rings

Ligand AGS A 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

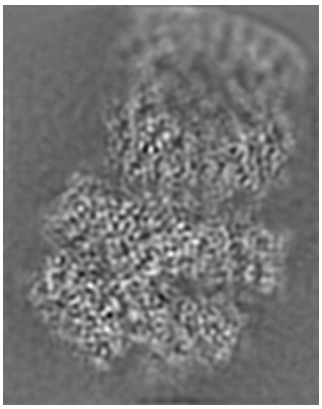
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26558. These allow visual inspection of the internal detail of the map and identification of artifacts.

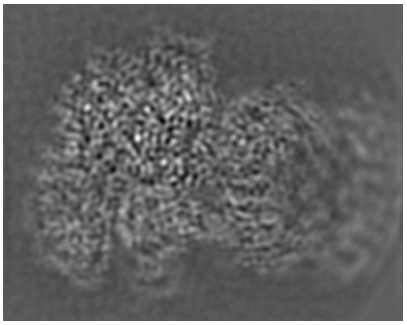
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

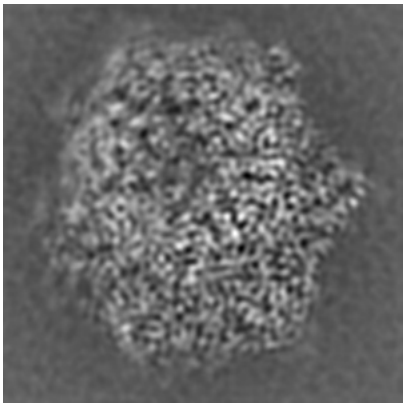
6.1.1 Primary map



X



Y

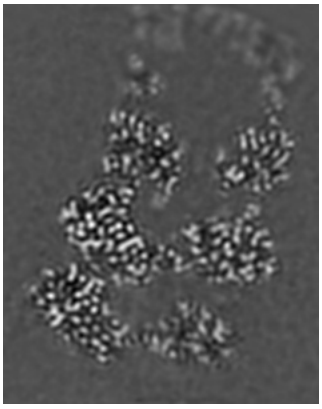


Z

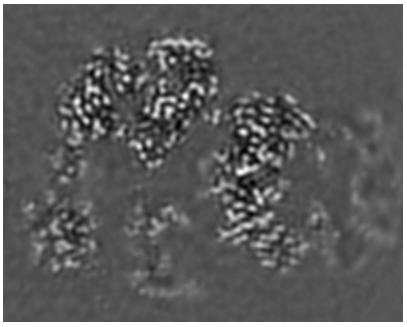
The images above show the map projected in three orthogonal directions.

6.2 Central slices

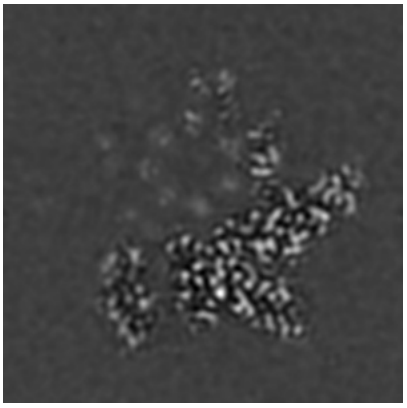
6.2.1 Primary map



X Index: 86



Y Index: 85

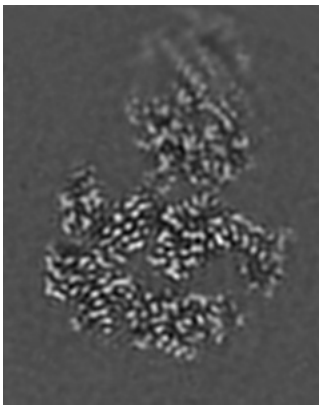


Z Index: 108

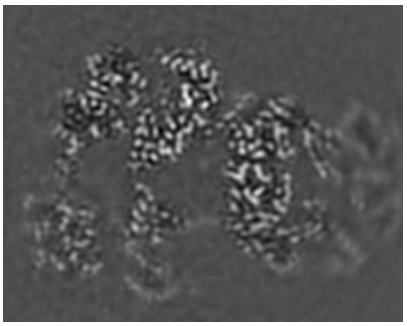
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

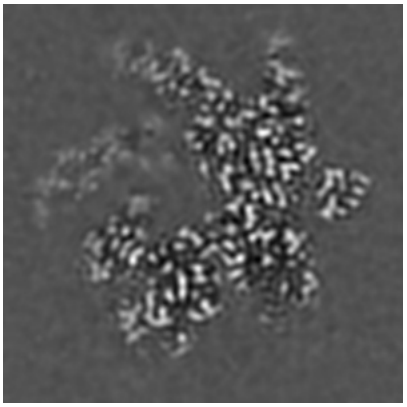
6.3.1 Primary map



X Index: 114



Y Index: 80

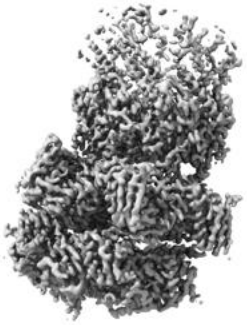


Z Index: 92

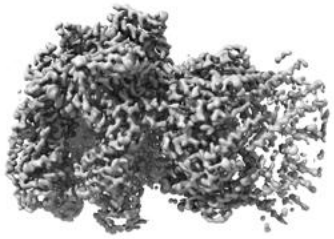
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

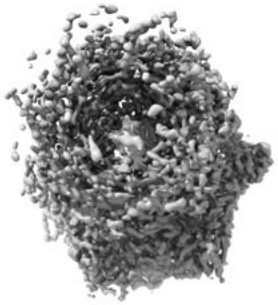
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

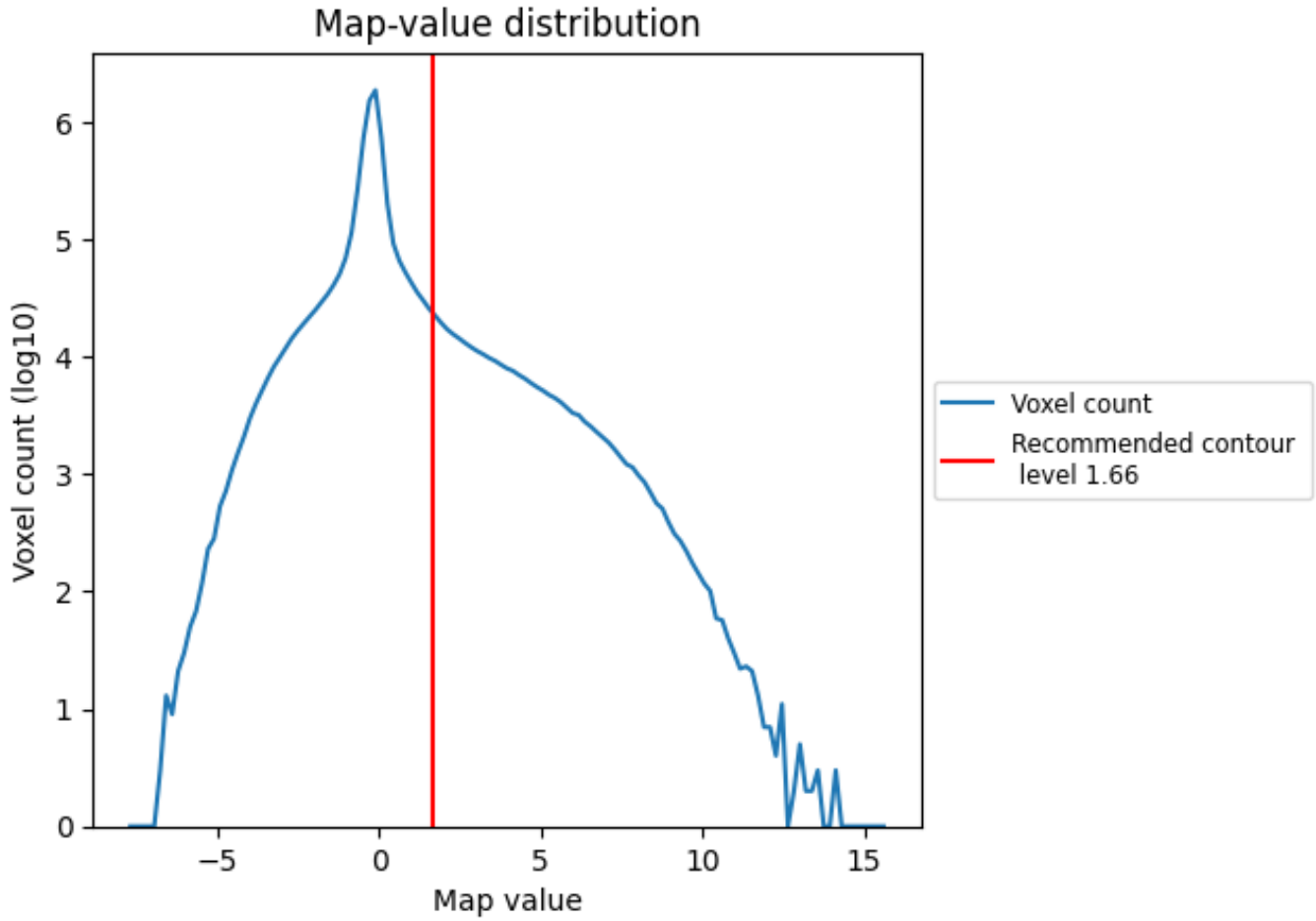
6.5 Mask visualisation (i)

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

7 Map analysis

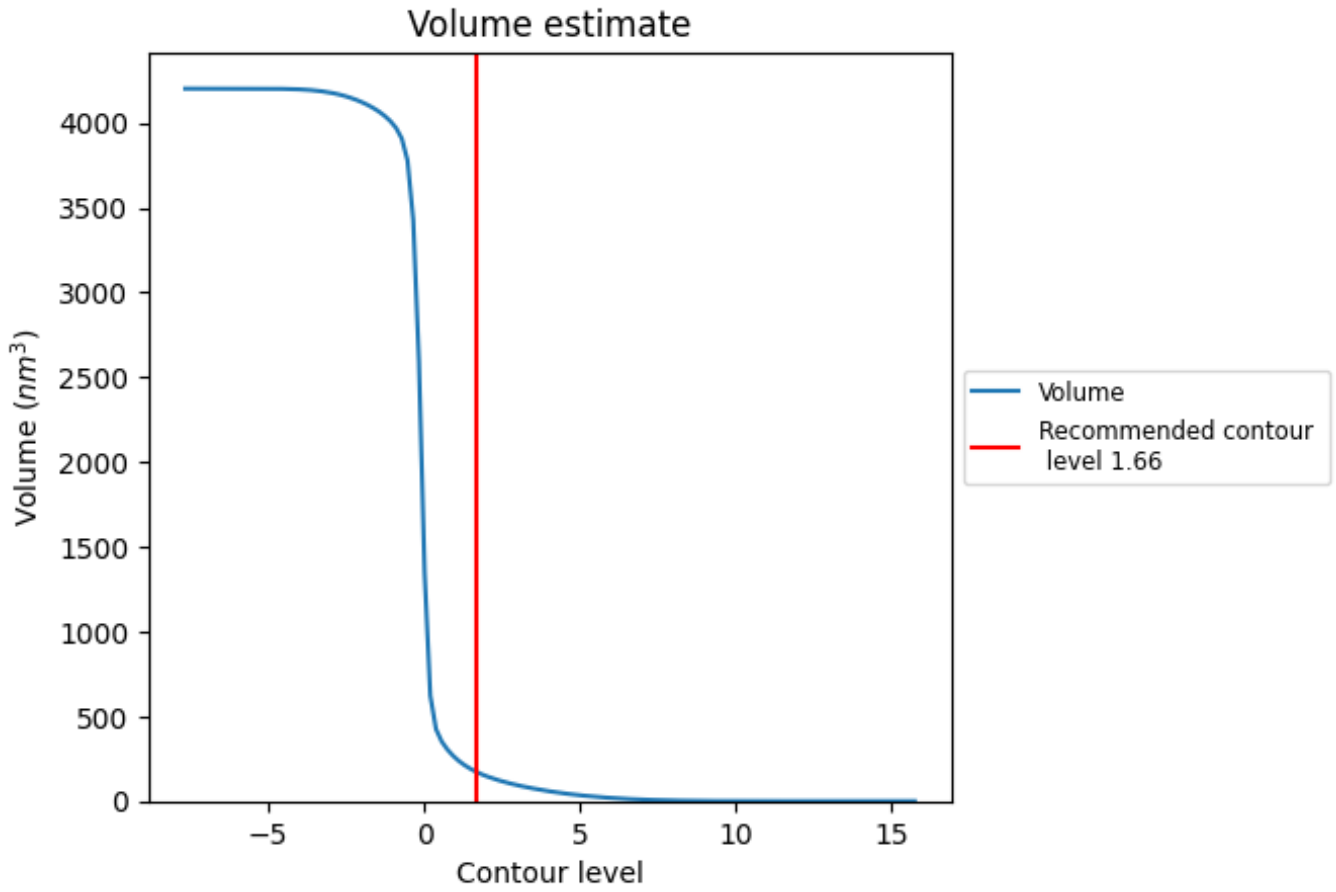
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 175 nm^3; this corresponds to an approximate mass of 158 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

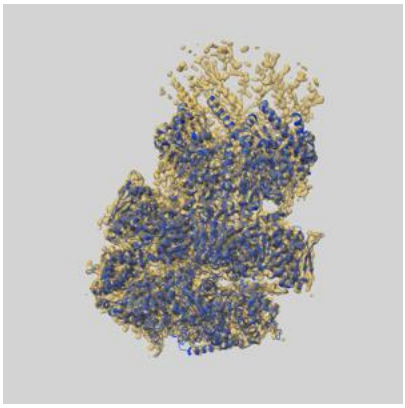
8 Fourier-Shell correlation (i)

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

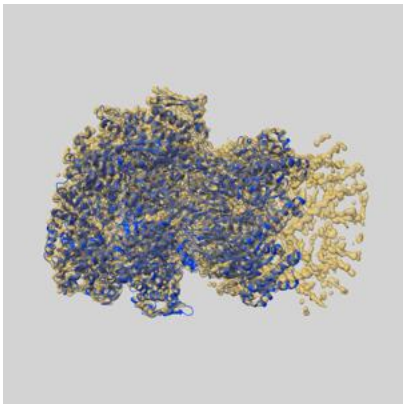
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26558 and PDB model 7UIZ. Per-residue inclusion information can be found in section 3 on page 9.

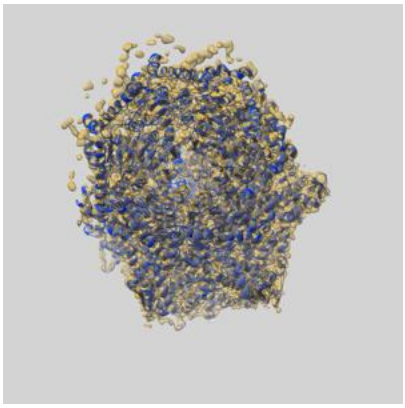
9.1 Map-model overlay



X



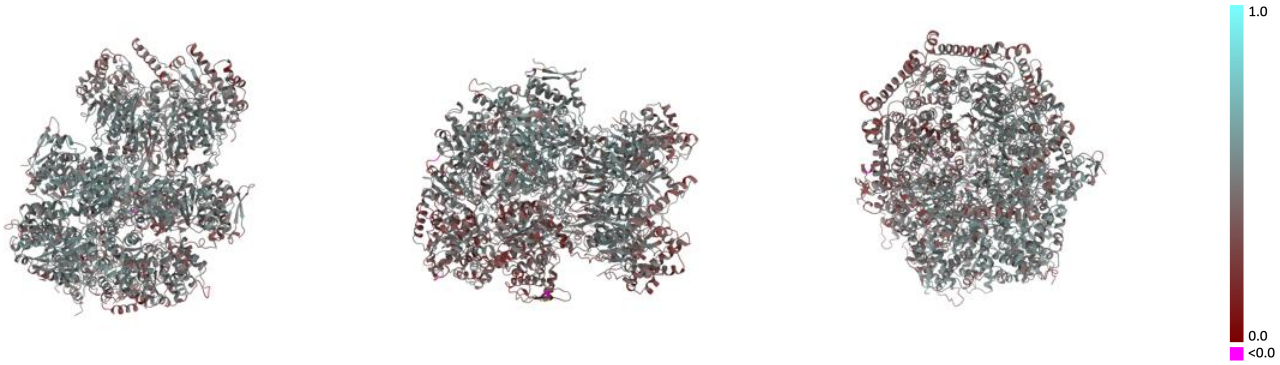
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.66 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.

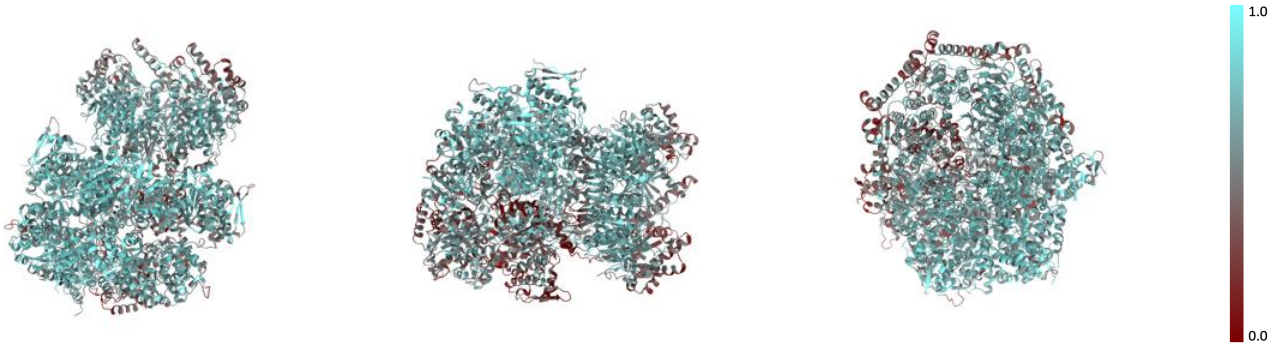
9.2 Q-score mapped to coordinate model (i)



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.

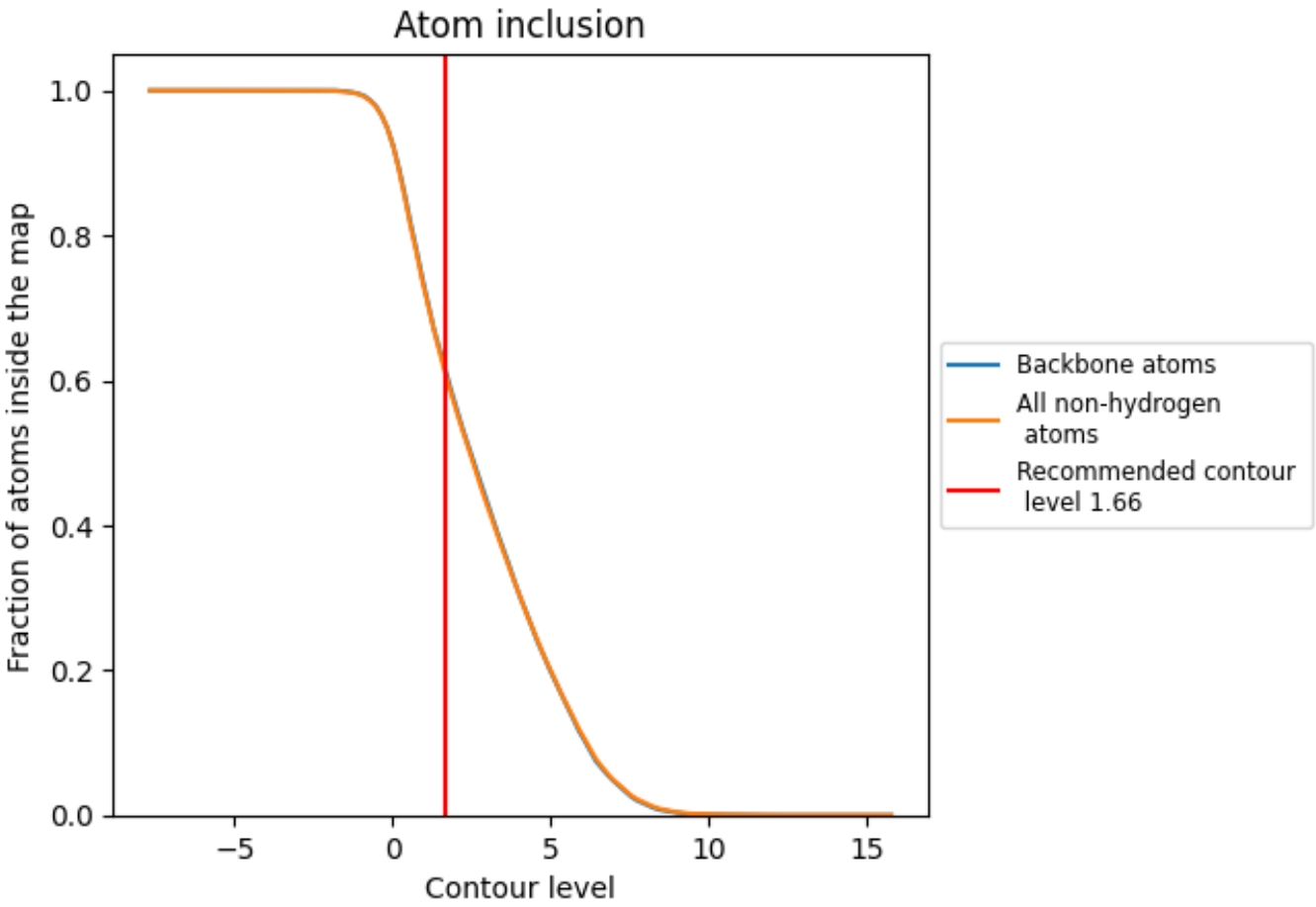
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.66).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (1.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6109	0.4530
A	0.5443	0.4180
B	0.7104	0.4870
C	0.7479	0.5110
D	0.7352	0.5010
E	0.6509	0.4580
F	0.4061	0.3590
H	0.6218	0.4530
I	0.6259	0.4630
J	0.6416	0.4560
K	0.6485	0.4670
L	0.6014	0.4390
M	0.5501	0.4140
N	0.5584	0.4330
S	0.3216	0.3860