wwPDB EM Validation Summary Report

Nov 8, 2022 – 01:08 AM EST

PDB ID	:	6E11
EMDB ID	:	EMD-8952
Title	:	PTEX Core Complex in the Resetting (Compact) State
Authors	:	Ho, C.; Lai, M.; Zhou, Z.H.
Deposited on	:	2018-07-08
Resolution	:	4.23 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 (1)) were used in the production of this report:

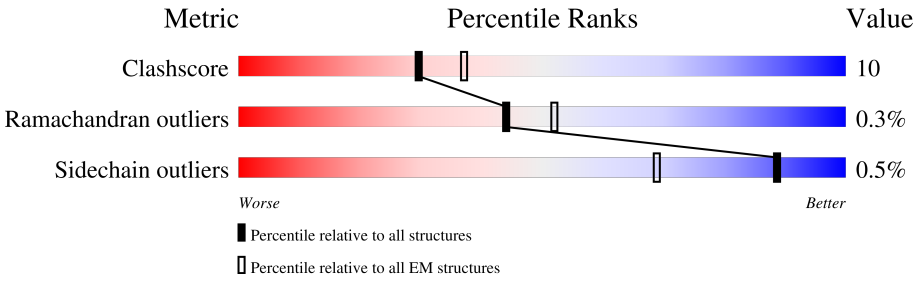
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.23 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%

Mol	Chain	Length	Quality of chain
1	h	60	78% 22%
1	i	60	75% . 23%
1	j	60	92% 8%
1	k	60	100%
1	l	60	88% 12%
1	m	60	97% .
1	n	60	60% 40%
2	1	906	60% 19% . 21%
2	2	906	62% 17% . 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	3	906	60% 19% 21%
2	4	906	59% 19% 21%
2	5	906	60% 19% 21%
2	6	906	65% 13% 21%
3	A	287	54% 13% 33%
3	B	287	57% 15% 27%
3	C	287	60% 13% 27%
3	D	287	59% 14% 27%
3	E	287	57% 16% 27%
3	F	287	59% 13% 27%
3	G	287	56% 11% 33%
4	0	6	83% 17%
5	a	993	16% 84%
5	b	993	16% 84%
5	c	993	16% 84%
5	d	993	16% 84%
5	e	993	16% 84%
5	f	993	16% 84%
5	g	993	16% 84%

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
6	AGS	1	1003	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 57401 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 Unknown (Claw).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	i	46	Total	C	N	O	0	0
			230	138	46	46		
1	j	55	Total	C	N	O	0	0
			275	165	55	55		
1	k	60	Total	C	N	O	0	0
			300	180	60	60		
1	n	36	Total	C	N	O	0	0
			180	108	36	36		
1	h	47	Total	C	N	O	0	0
			235	141	47	47		
1	l	53	Total	C	N	O	0	0
			265	159	53	53		
1	m	58	Total	C	N	O	0	0
			290	174	58	58		

- Molecule 2 is a protein called Heat shock protein 101.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	2	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	3	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	4	717	Total	C	N	O	S	0	0
			5752	3687	964	1086	15		
2	5	716	Total	C	N	O	S	0	0
			5744	3681	963	1085	15		
2	6	716	Total	C	N	O	S	0	0
			5744	3681	963	1085	15		

- Molecule 3 is a protein called Exported protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	D	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	E	210	Total	C	N	O	S	0	0
			1724	1112	294	312	6		
3	B	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
3	A	191	Total	C	N	O	S	0	0
			1571	1019	271	275	6		
3	G	191	Total	C	N	O	S	0	0
			1571	1019	271	275	6		
3	F	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		

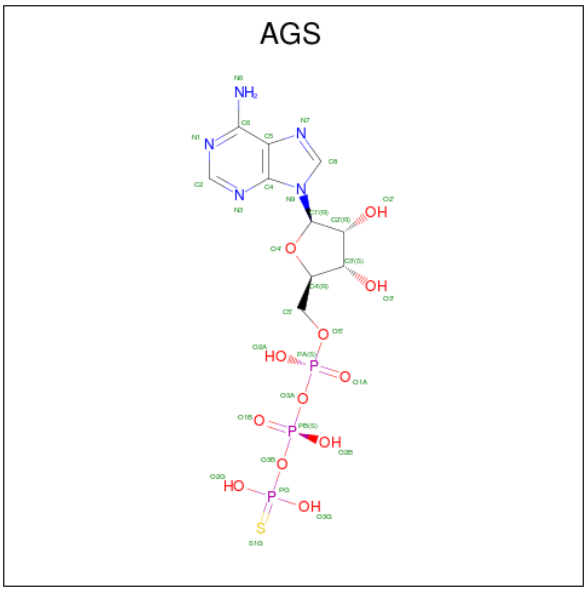
- Molecule 4 is a protein called Endogenous cargo polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	0	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 5 is a protein called Translocon component PTEX150.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	c	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	b	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	a	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	g	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	f	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		
5	e	156	Total	C	N	O	S	0	0
			1286	809	203	273	1		

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
6	1	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	1	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	1	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	3	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	3	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	4	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	4	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	5	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	5	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	6	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	6	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

3 Residue-property plots (i)

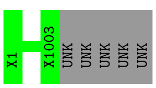
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Unknown (Claw)

Chain i:

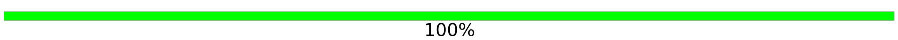
- Molecule 1: Unknown (Claw)

Chain j:



- Molecule 1: Unknown (Claw)

Chain k:



There are no outlier residues recorded for this chain.

- Molecule 1: Unknown (Claw)

Chain n:

- Molecule 1: Unknown (Claw)

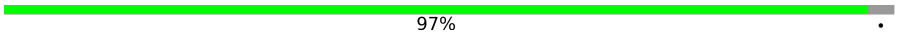
Chain h:

- Molecule 1: Unknown (Claw)

Chain l:

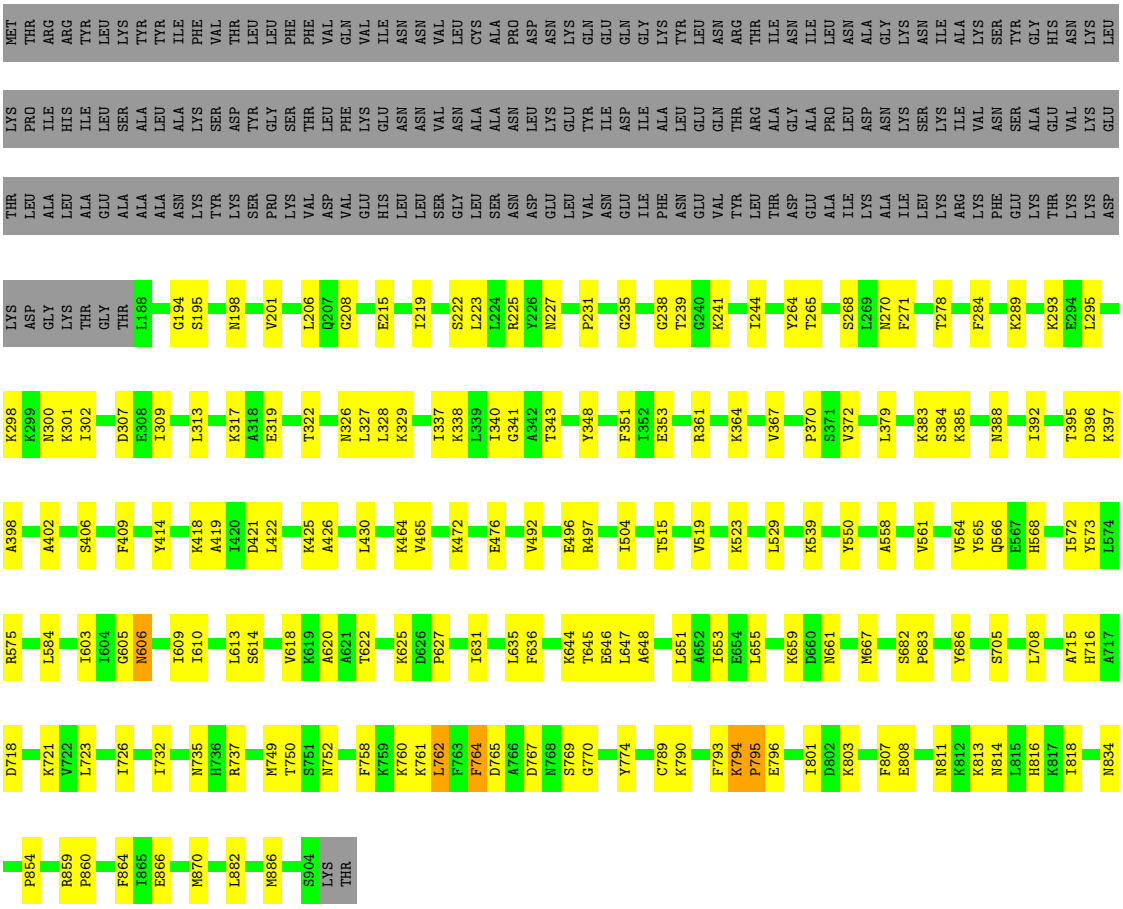
• Molecule 1: Unknown (Claw)

Chain m:



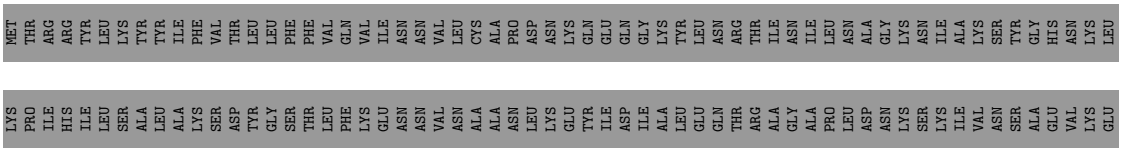
• Molecule 2: Heat shock protein 101

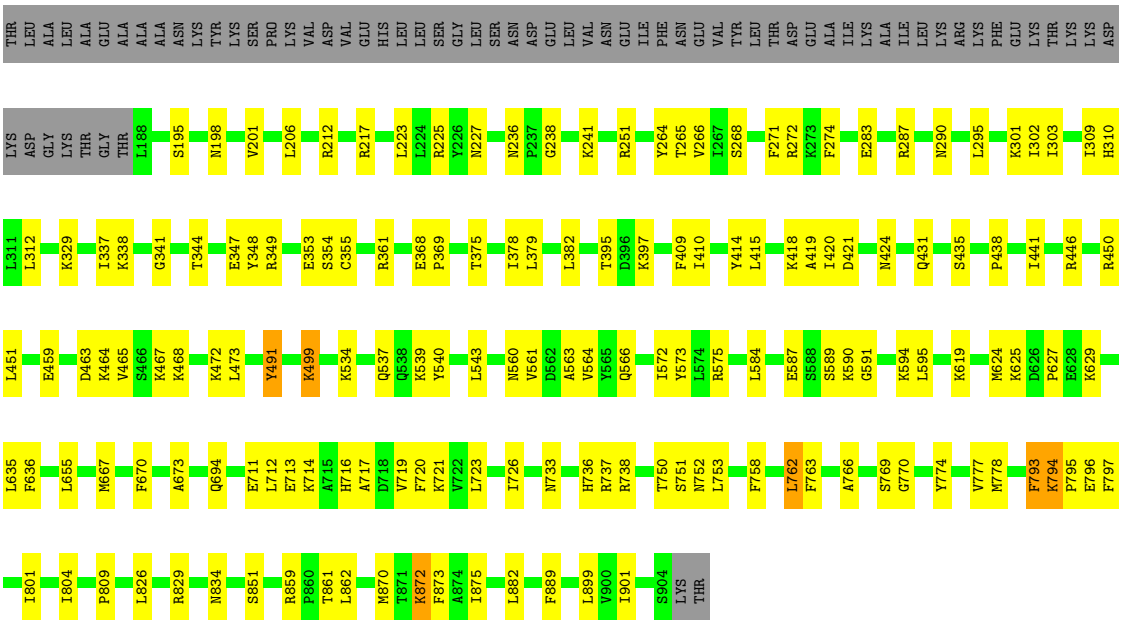
Chain 1:



• Molecule 2: Heat shock protein 101

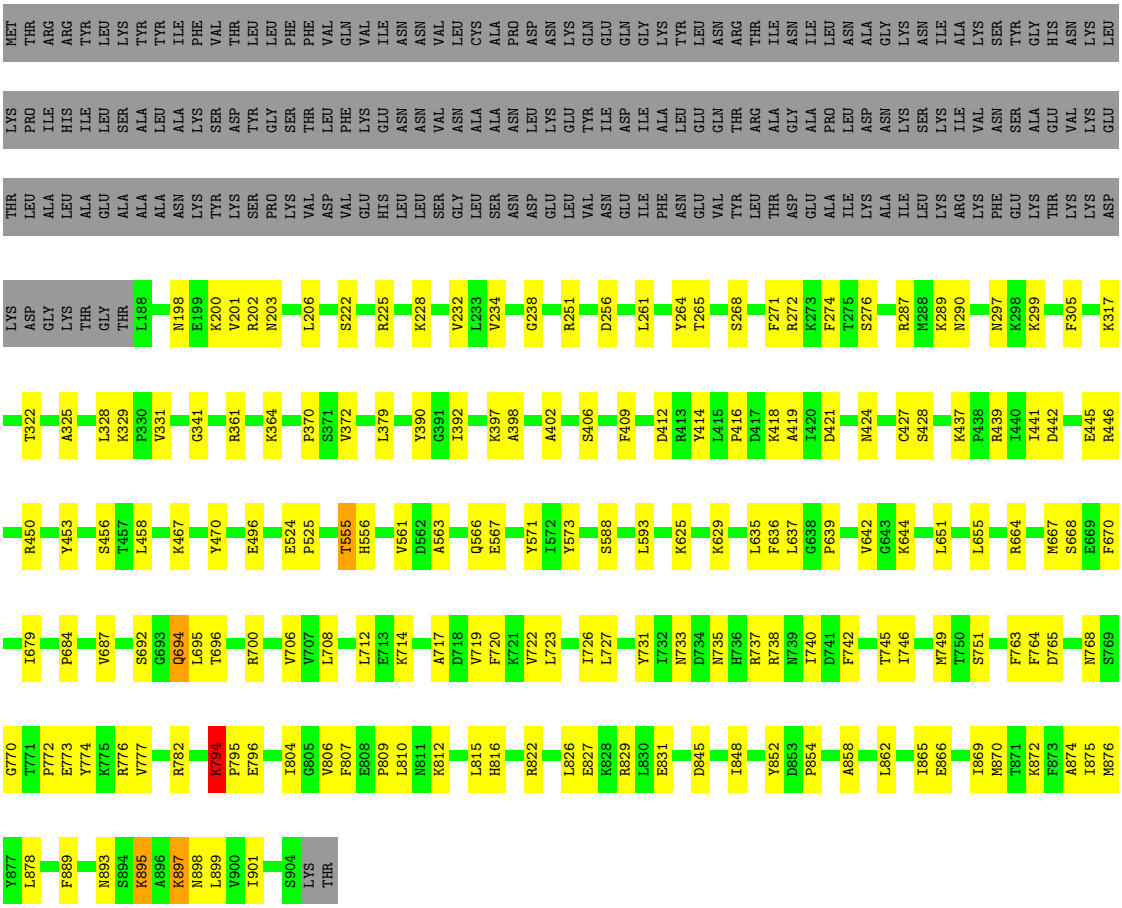
Chain 2:





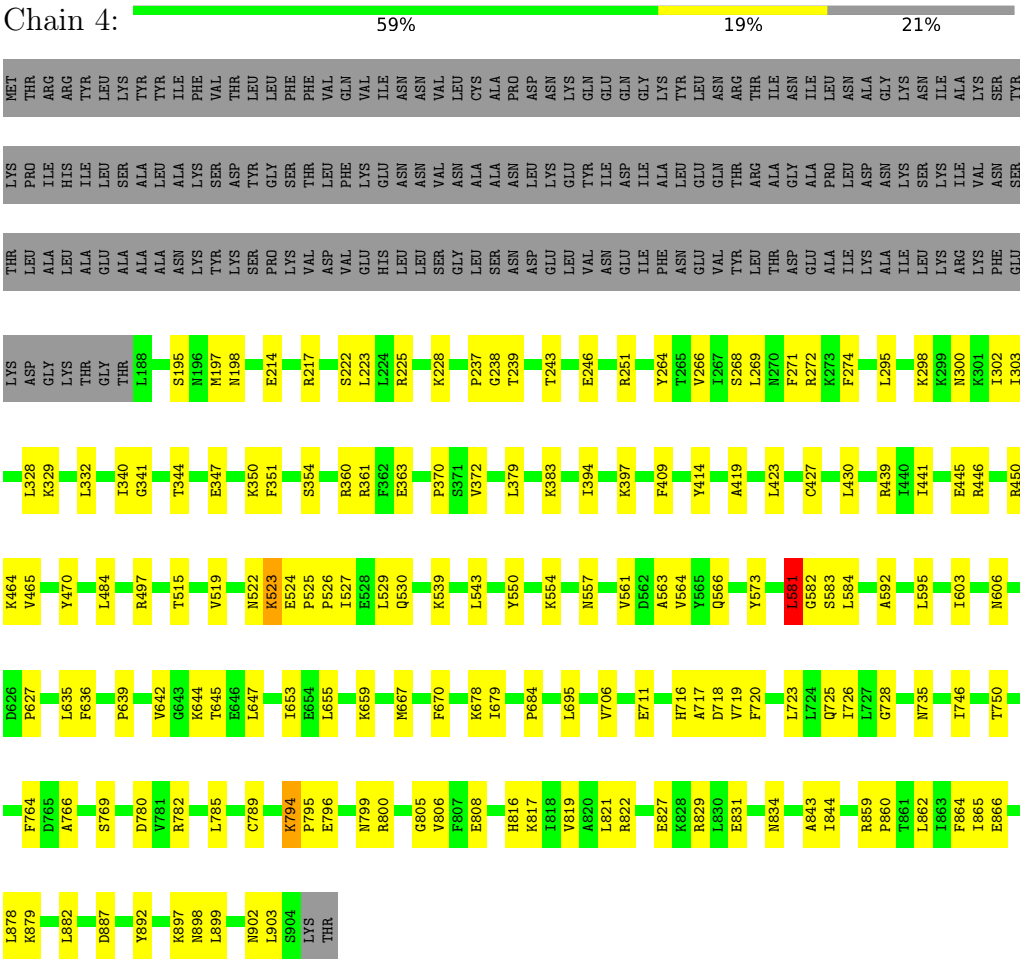
• Molecule 2: Heat shock protein 101

Chain 3:



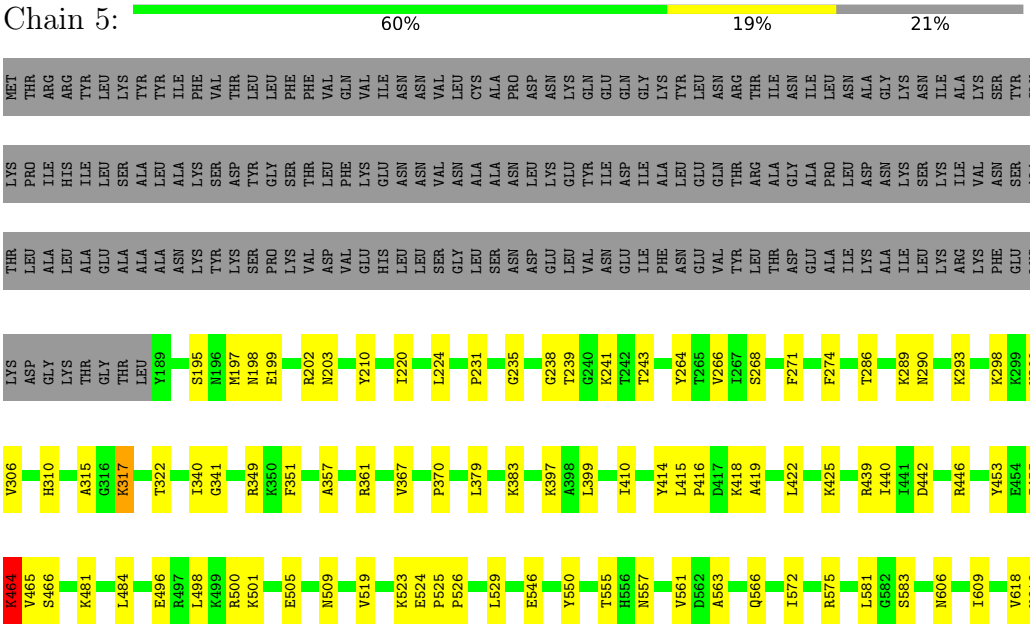
• Molecule 2: Heat shock protein 101

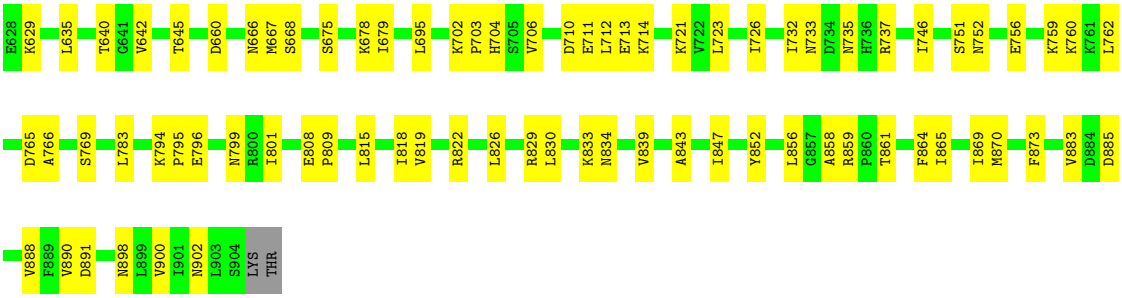
Chain 4:



• Molecule 2: Heat shock protein 101

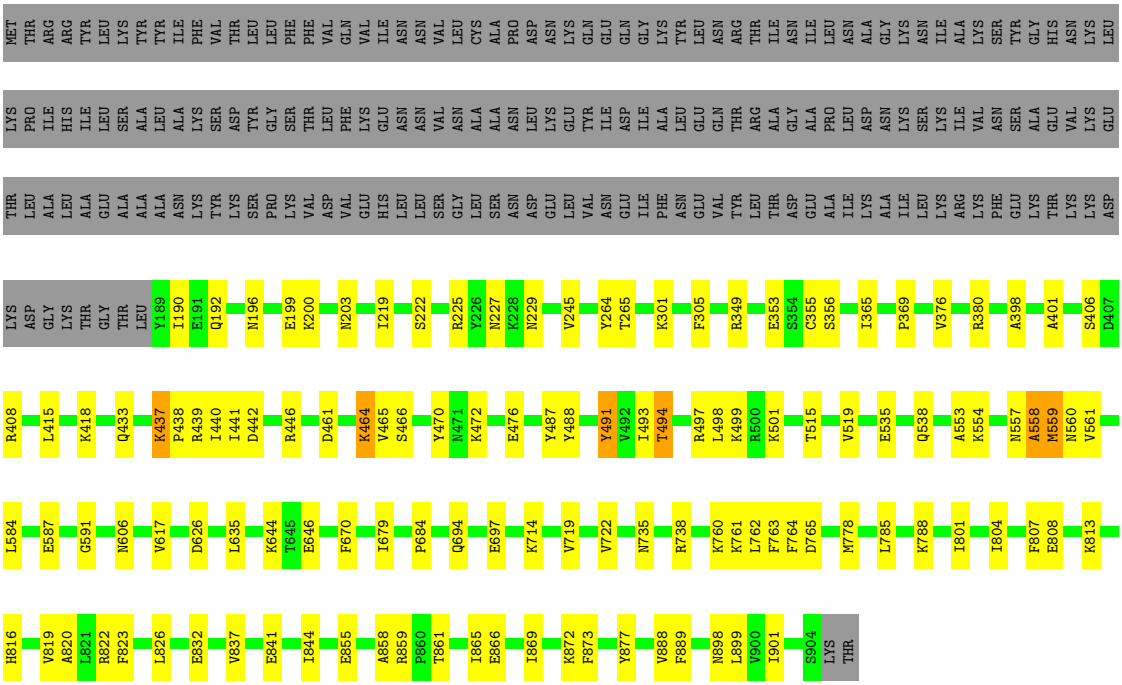
Chain 5:





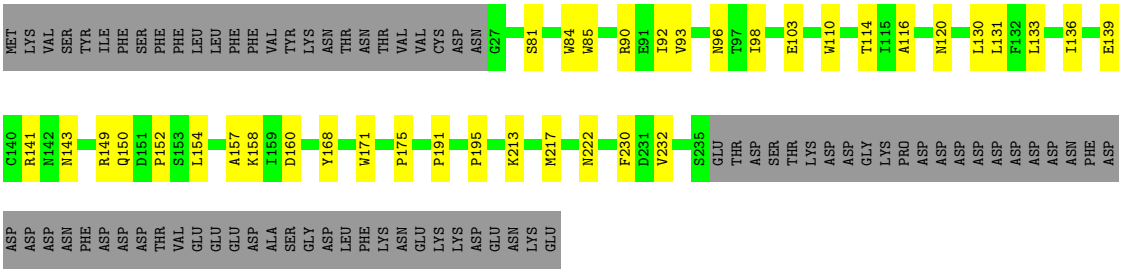
• Molecule 2: Heat shock protein 101

Chain 6:



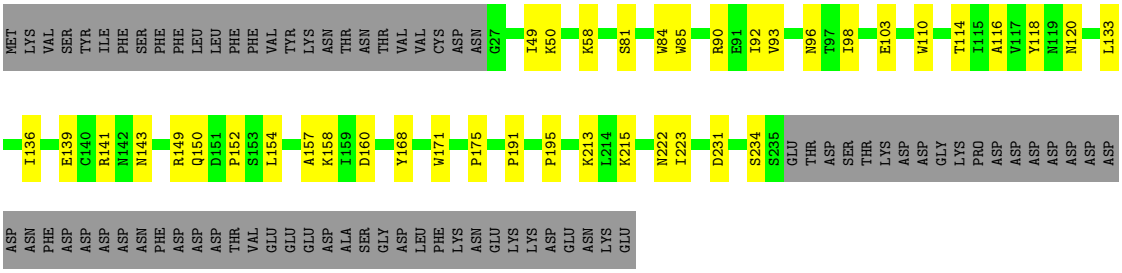
• Molecule 3: Exported protein 2

Chain C:



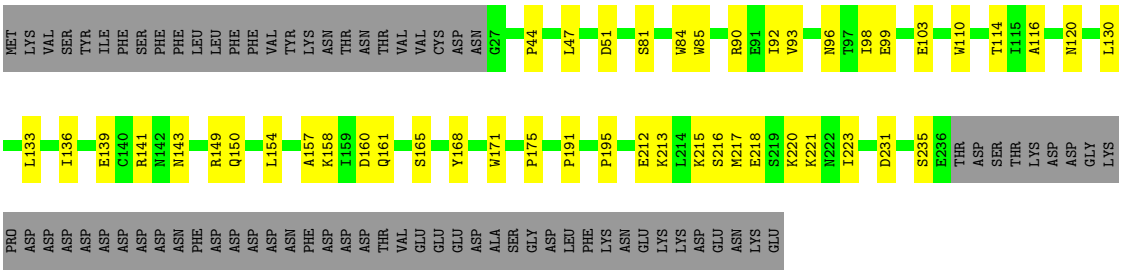
• Molecule 3: Exported protein 2

Chain D:



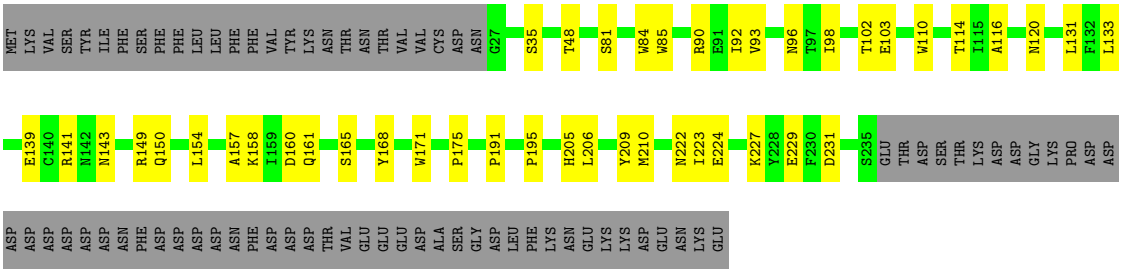
• Molecule 3: Exported protein 2

Chain E:



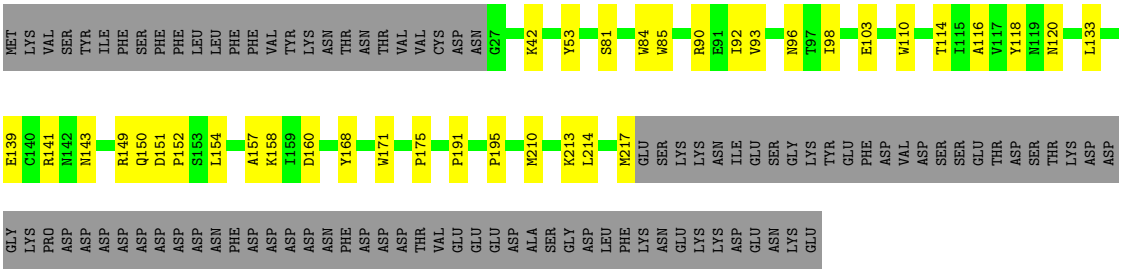
• Molecule 3: Exported protein 2

Chain B:



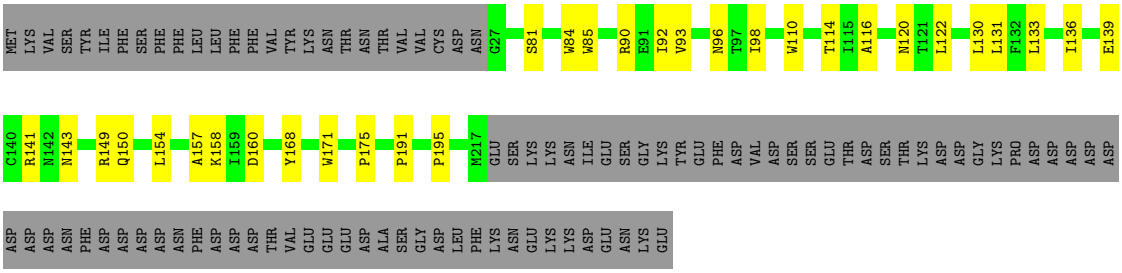
• Molecule 3: Exported protein 2

Chain A:



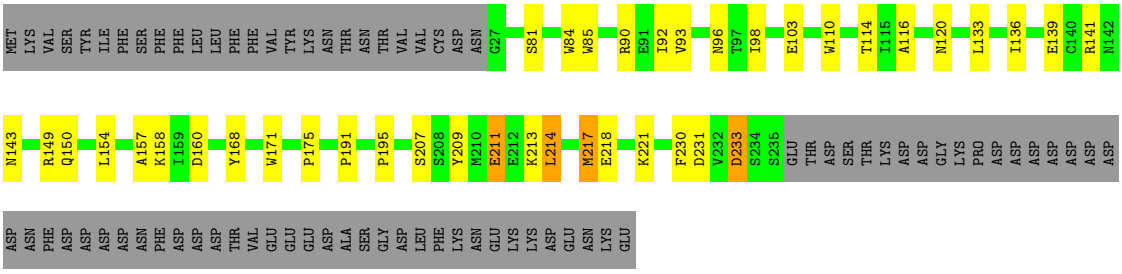
• Molecule 3: Exported protein 2

Chain G:



• Molecule 3: Exported protein 2

Chain F:

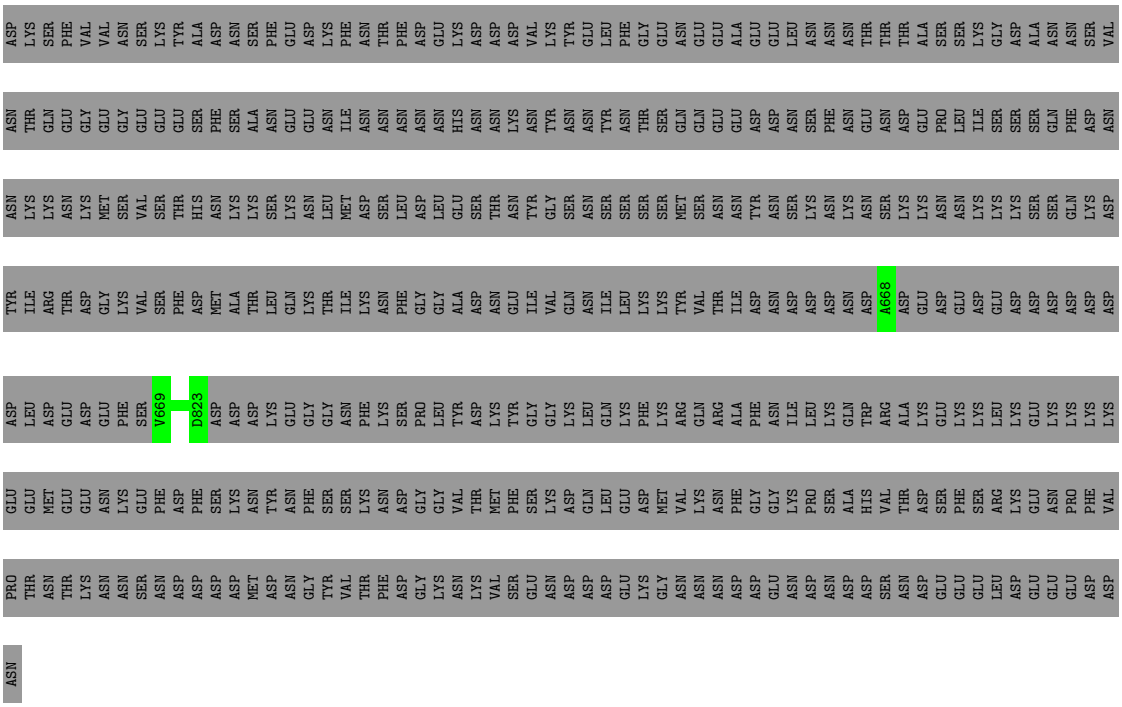


• Molecule 4: Endogenous cargo polypeptide

Chain 0:

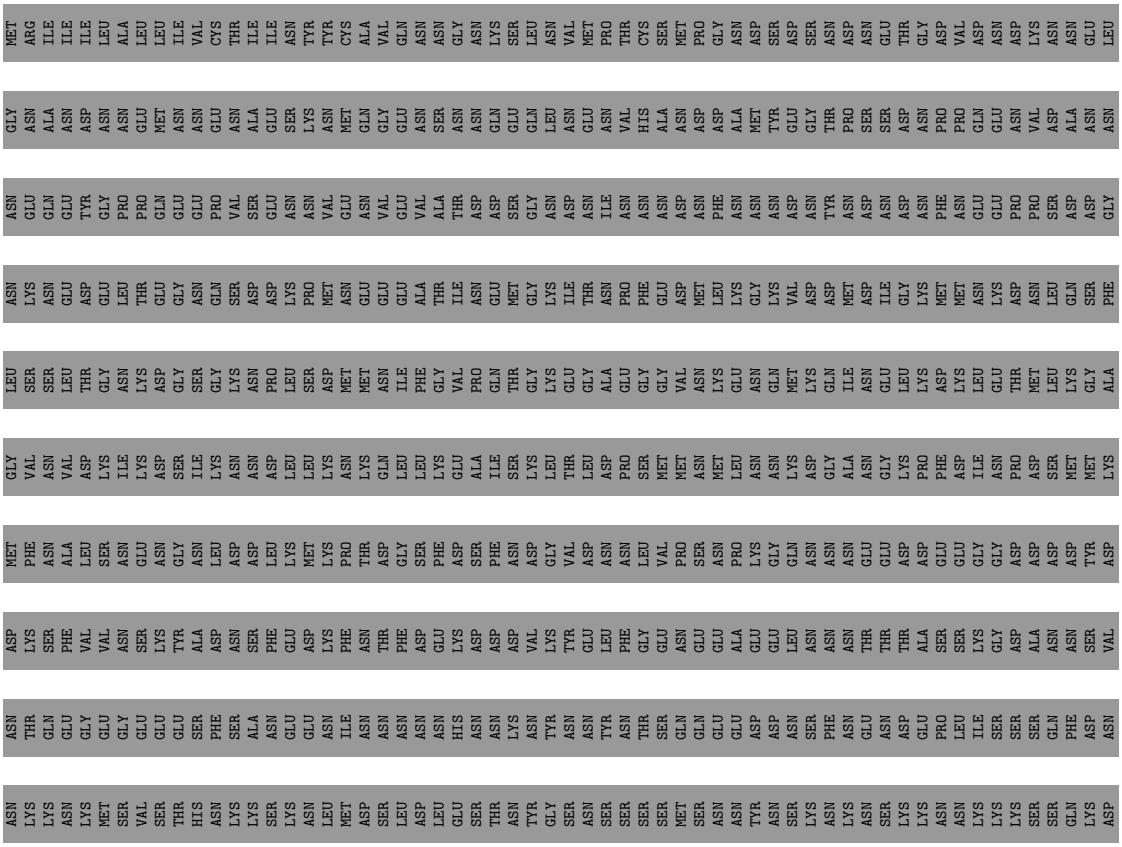
• Molecule 5: Translocon component PTEX150

Chain d:



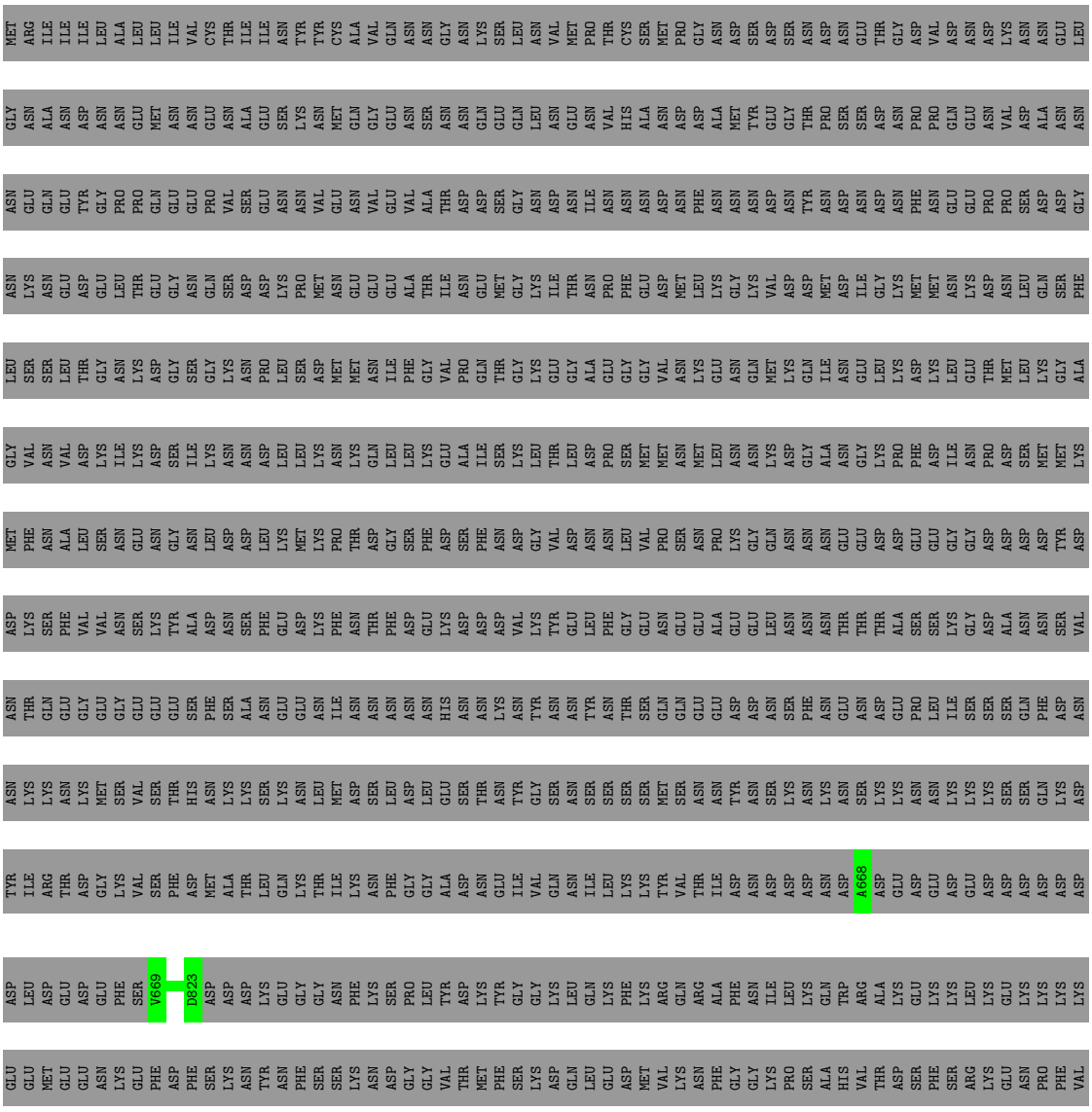
• Molecule 5: Translocon component PTEX150

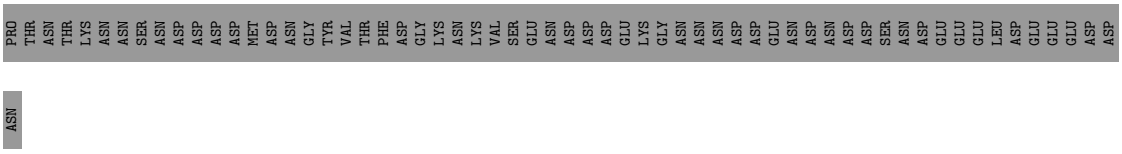
Chain c:



• Molecule 5: Translocon component PTEX150

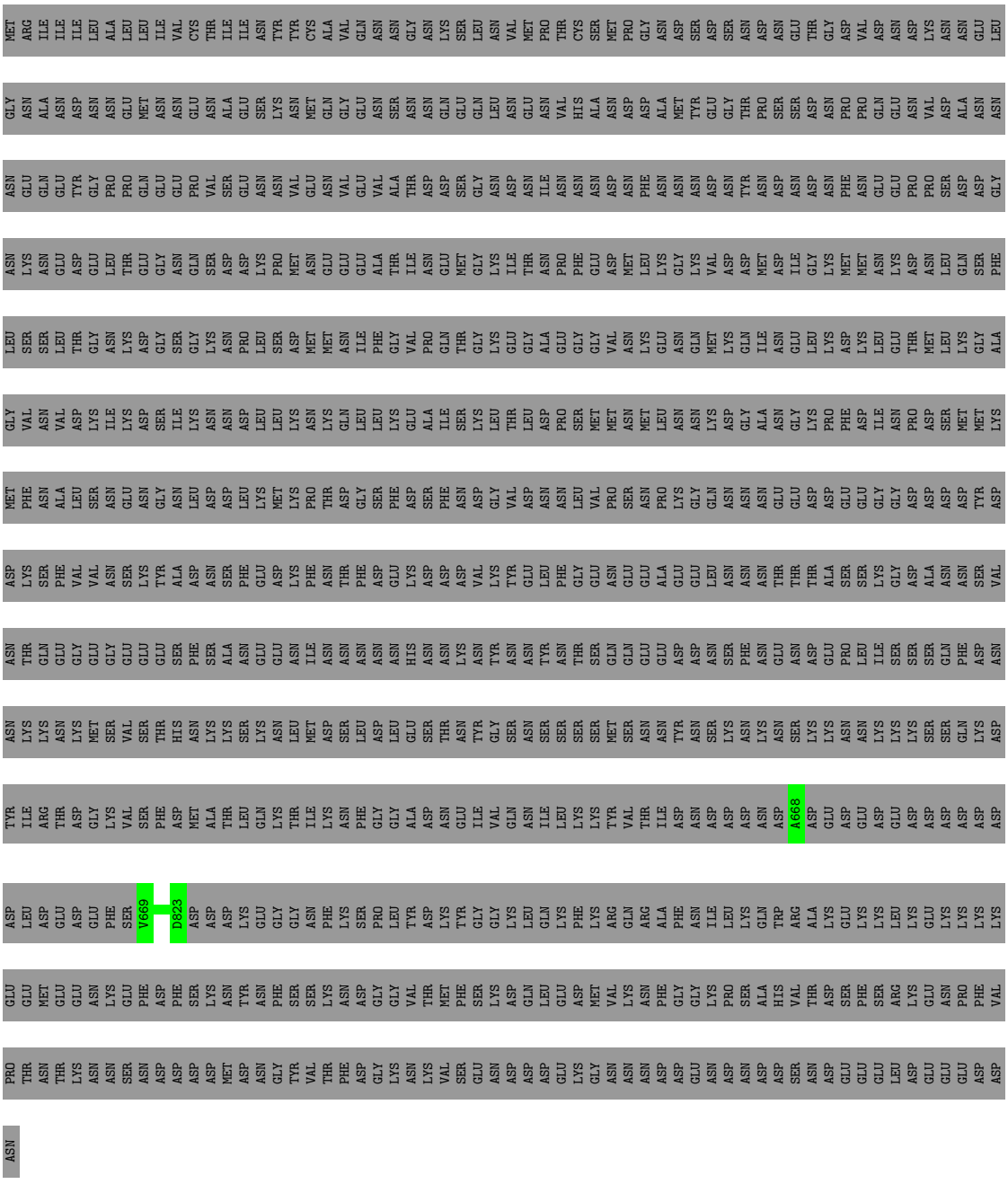
Chain b:





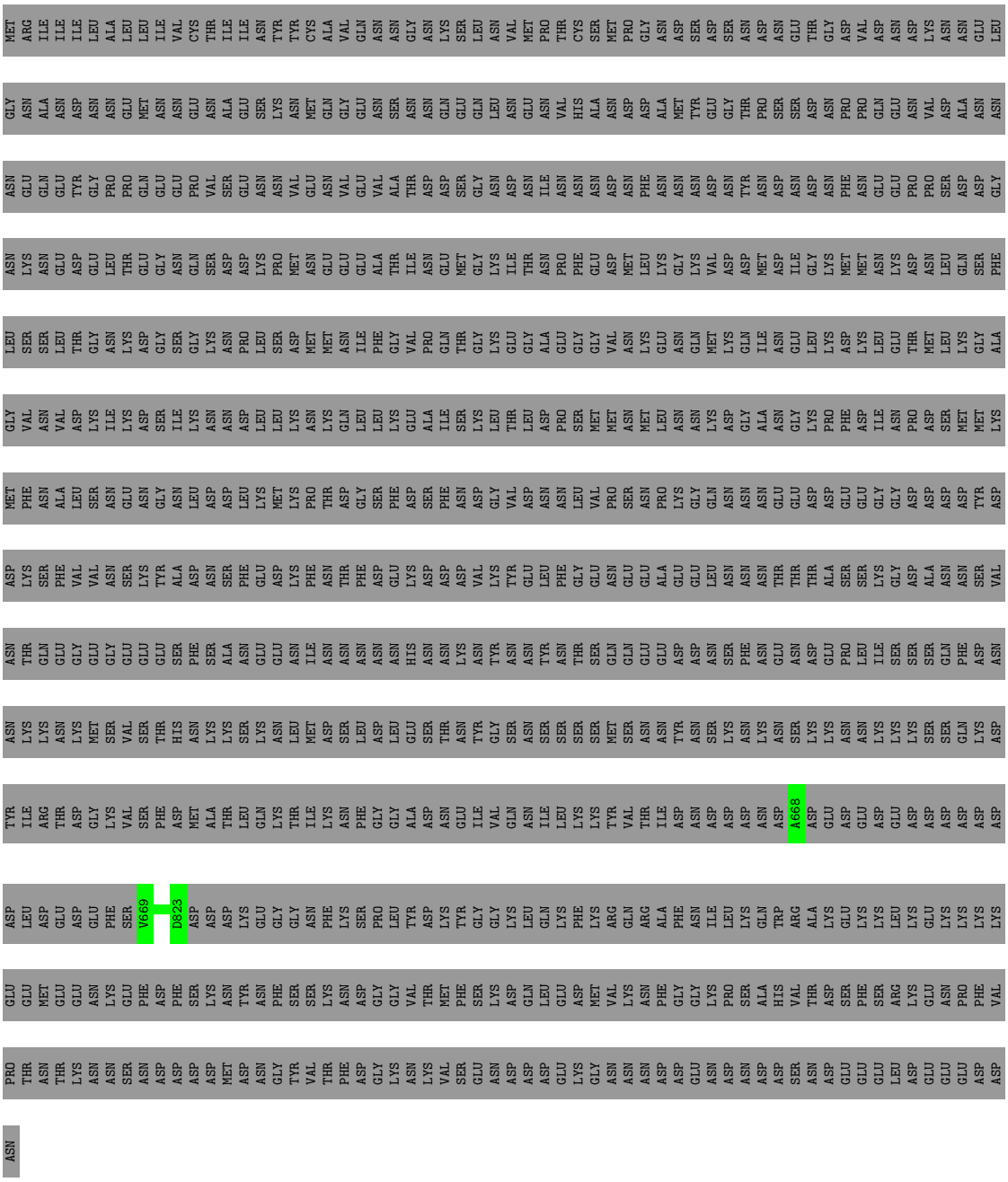
• Molecule 5: Translocon component PTEX150

Chain a:



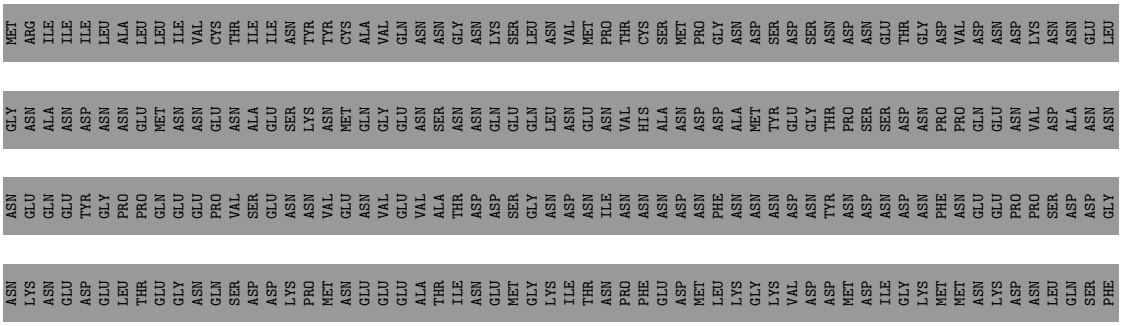
• Molecule 5: Translocon component PTEX150

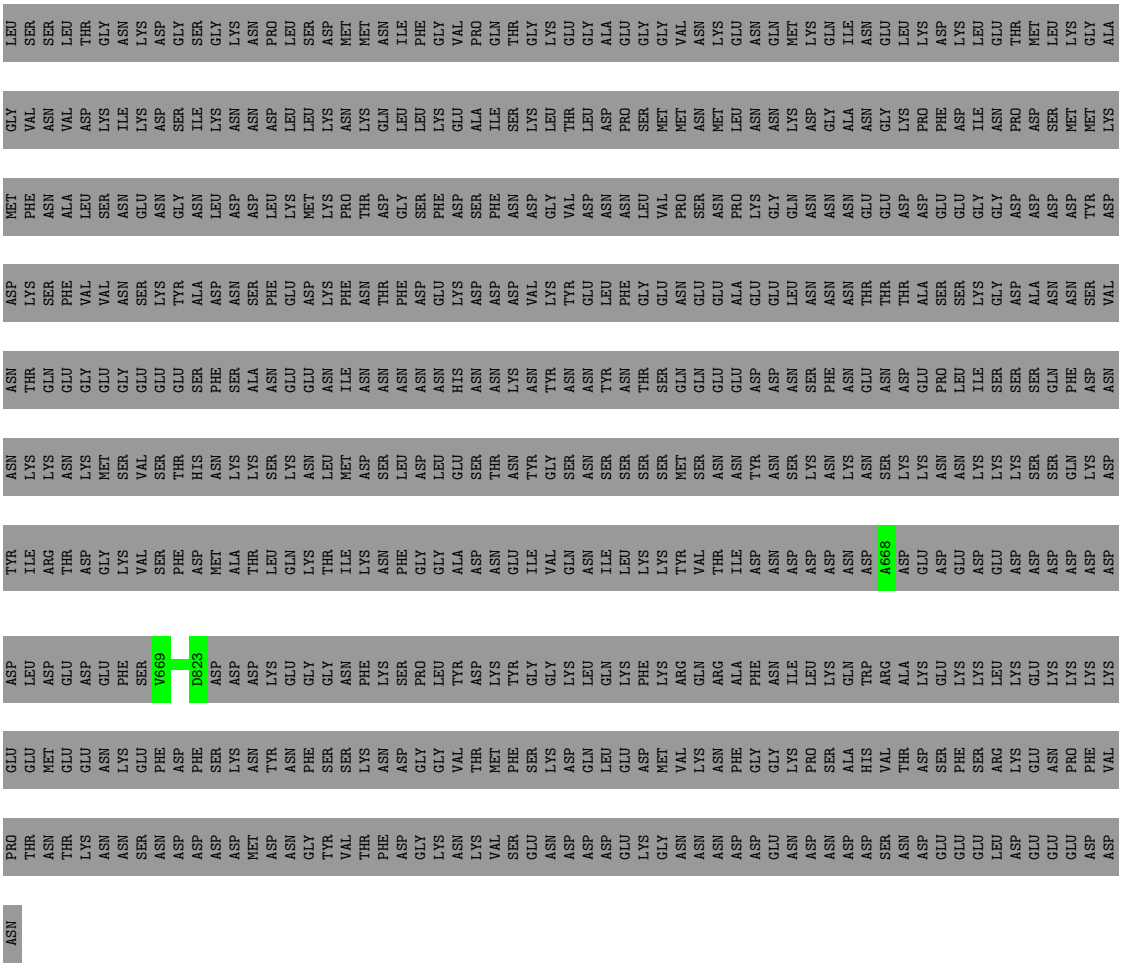
Chain g:



• Molecule 5: Translocon component PTEX150

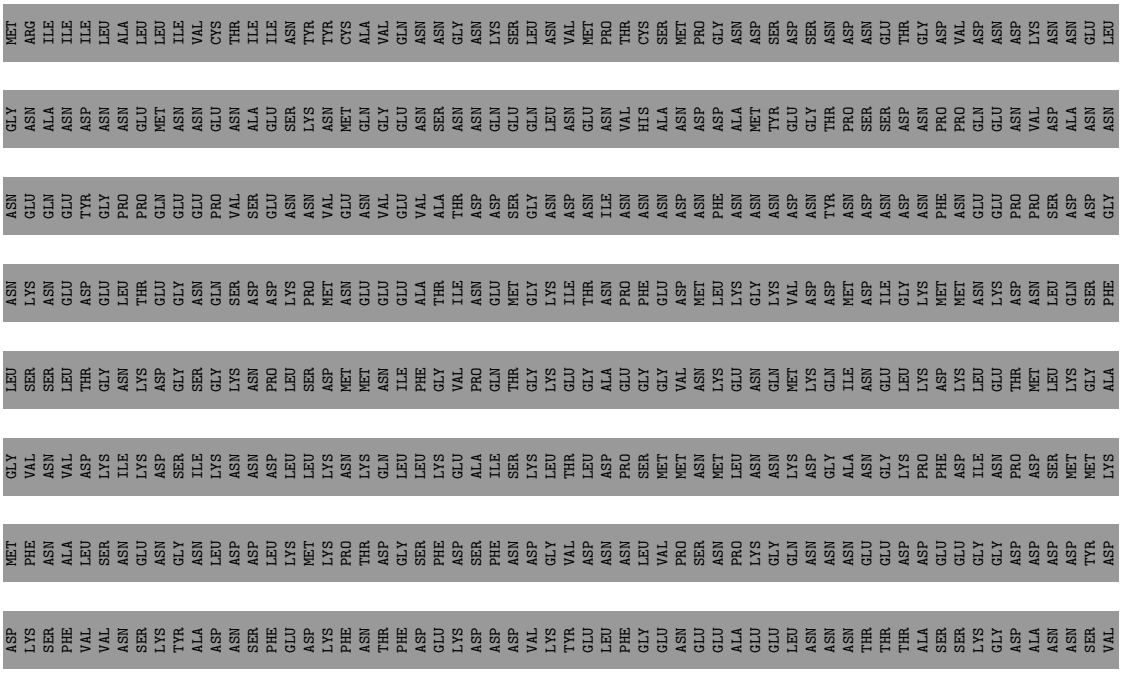
Chain f:





• Molecule 5: Translocon component PTEX150

Chain e:




ASN THR GLN GLU GLY GLU GLY GLU GLU GLU SER PHE SER ALA ASN GLU GLU ASN ILE ASN ASN ASN ASN ASN HIS ASN ASN LYS ASN TYR ASN ASN TYR ASN THR SER GLN GLN GLU GLU ASP ASP ASN SER PHE ASN GLU ASN ASP GLU PRO LEU ILE SER SER SER GLN PHE ASP ASN
ASN LYS LYS ASN LYS MET SER VAL SER THR HIS ASN LYS LYS SER LYS ASN LEU MET ASP SER LEU ASP LEU GLU SER GLY SER ASN SER SER SER SER MET SER ASN ASN TYR ASN SER LYS LYS ASN ASN LYS LYS LYS LYS SER SER SER GLN LYS ASP
TYR ILE ARG THR ASP GLY LYS VAL SER PHE ASP MET ALA THR LEU GLN LYS THR ILE LYS ASN PHE GLY GLY ALA ASP ASN GLU ILE VAL GLN ASN ILE LEU LYS LYS TYR VAL THR ILE ASP ASN ASP ASP ASP ASN A668 ASP GLU ASP GLU ASP GLU ASP ASP ASP ASP ASP ASP
ASP LEU ASP GLU ASP GLU PHE SER V669 D769 D823 ASP ASP ASP LYS GLU GLY GLY ASN PHE LYS SER PRO LEU TYR ASP LYS TYR GLY GLY LYS LEU GLN LYS PHE LYS ARG GLN ARG ALA PHE ASN ILE LEU LYS GLN TRP ARG ALA LYS GLU LYS LYS LEU LYS GLU LYS LYS
LYS LYS GLU GLU MET GLU GLU ASN LYS GLU PHE ASP PHE SER LYS ASN TYR ASN PHE SER SER LYS ASN ASP GLY GLY VAL THR MET PHE SER LYS ASP GLN LEU GLU ASP MET VAL LYS ASN PHE GLY GLY LYS PRO SER ALA HIS VAL THR ASP SER PHE SER ARG LYS GLU ASN PRO
PHE VAL PRO THR ASN THR LYS ASN ASN SER ASN ASP ASP ASP MET ASP ASN GLY TYR VAL THR PHE ASP GLY LYS ASN LYS VAL SER GLU ASN ASP ASP GLU LYS GLY ASN ASN ASN ASP ASP GLU ASN ASP ASN ASP ASP SER ASN ASP GLU GLU GLU LEU ASP GLU GLU GLU
ASP ASP ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78499	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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

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
2	1	0.34	0/5843	0.57	0/7848
2	2	0.40	0/5843	0.61	0/7848
2	3	0.42	0/5843	0.65	0/7848
2	4	0.39	0/5843	0.61	0/7848
2	5	0.36	0/5835	0.58	1/7837 (0.0%)
2	6	0.32	0/5835	0.59	1/7837 (0.0%)
3	A	0.32	0/1607	0.57	0/2175
3	B	0.35	0/1753	0.60	0/2369
3	C	0.32	0/1753	0.57	0/2369
3	D	0.33	0/1753	0.56	0/2369
3	E	0.33	0/1762	0.59	0/2381
3	F	0.33	0/1753	0.61	0/2369
3	G	0.32	0/1607	0.56	0/2175
5	a	0.29	0/1309	0.52	0/1760
5	b	0.29	0/1309	0.52	0/1760
5	c	0.29	0/1309	0.52	0/1760
5	d	0.29	0/1309	0.52	0/1760
5	e	0.28	0/1309	0.52	0/1760
5	f	0.28	0/1309	0.51	0/1760
5	g	0.29	0/1309	0.53	0/1760
All	All	0.35	0/56193	0.58	2/75593 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	i	0	1
2	1	0	3
2	2	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	3	0	7
2	4	0	4
2	5	0	3
3	A	0	1
3	B	0	3
3	C	0	1
3	D	0	1
3	E	0	2
3	F	0	3
3	G	0	1
All	All	0	33

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	765	ASP	N-CA-CB	6.78	122.80	110.60
2	5	317	LYS	O-C-N	-6.19	112.80	122.70

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	464	LYS	Peptide
2	1	758	PHE	Peptide
2	1	794	LYS	Peptide
2	2	793	PHE	Peptide
1	i	22	UNK	Mainchain

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	h	235	0	53	0	0
1	i	230	0	50	0	0
1	j	275	0	63	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	k	300	0	67	0	0
1	l	265	0	57	0	0
1	m	290	0	62	0	0
1	n	180	0	38	0	0
2	1	5752	0	5955	130	0
2	2	5752	0	5956	131	0
2	3	5752	0	5957	130	0
2	4	5752	0	5957	127	0
2	5	5744	0	5945	113	0
2	6	5744	0	5946	92	0
3	A	1571	0	1635	25	0
3	B	1715	0	1767	29	0
3	C	1715	0	1767	32	0
3	D	1715	0	1767	42	0
3	E	1724	0	1773	37	0
3	F	1715	0	1767	26	0
3	G	1571	0	1635	19	0
4	0	30	0	9	1	0
5	a	1286	0	1212	0	0
5	b	1286	0	1212	0	0
5	c	1286	0	1212	0	0
5	d	1286	0	1212	0	0
5	e	1286	0	1212	0	0
5	f	1286	0	1212	0	0
5	g	1286	0	1212	0	0
6	1	93	0	36	16	0
6	2	31	0	12	1	0
6	3	62	0	24	2	0
6	4	62	0	24	8	0
6	5	62	0	24	7	0
6	6	62	0	24	4	0
All	All	57401	0	56854	816	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 816 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:764:PHE:CE1	3:C:213:LYS:HD3	1.97	0.99
2:3:764:PHE:CZ	3:C:213:LYS:CD	2.46	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:764:PHE:CZ	3:C:213:LYS:HD3	1.99	0.96
2:1:859:ARG:NH2	6:1:1003:AGS:O3A	1.98	0.95
2:6:437:LYS:HB3	2:6:437:LYS:HZ2	1.29	0.94

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	
2	1	715/906 (79%)	650 (91%)	61 (8%)	4 (1%)	25	65
2	2	715/906 (79%)	644 (90%)	69 (10%)	2 (0%)	41	76
2	3	715/906 (79%)	640 (90%)	71 (10%)	4 (1%)	25	65
2	4	715/906 (79%)	635 (89%)	75 (10%)	5 (1%)	22	62
2	5	714/906 (79%)	648 (91%)	63 (9%)	3 (0%)	34	72
2	6	714/906 (79%)	639 (90%)	71 (10%)	4 (1%)	25	65
3	A	189/287 (66%)	184 (97%)	5 (3%)	0	100	100
3	B	207/287 (72%)	200 (97%)	7 (3%)	0	100	100
3	C	207/287 (72%)	199 (96%)	8 (4%)	0	100	100
3	D	207/287 (72%)	201 (97%)	6 (3%)	0	100	100
3	E	208/287 (72%)	200 (96%)	8 (4%)	0	100	100
3	F	207/287 (72%)	196 (95%)	11 (5%)	0	100	100
3	G	189/287 (66%)	183 (97%)	6 (3%)	0	100	100
5	a	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	b	153/993 (15%)	143 (94%)	10 (6%)	0	100	100
5	c	153/993 (15%)	141 (92%)	12 (8%)	0	100	100
5	d	153/993 (15%)	143 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	e	153/993 (15%)	143 (94%)	10 (6%)	0	100 100
5	f	153/993 (15%)	143 (94%)	10 (6%)	0	100 100
5	g	153/993 (15%)	142 (93%)	11 (7%)	0	100 100
All	All	6773/14396 (47%)	6217 (92%)	534 (8%)	22 (0%)	44 76

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5	465	VAL
2	6	465	VAL
2	1	606	ASN
2	4	465	VAL
2	1	465	VAL

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
2	1	641/804 (80%)	637 (99%)	4 (1%)	86 92
2	2	641/804 (80%)	637 (99%)	4 (1%)	86 92
2	3	641/804 (80%)	640 (100%)	1 (0%)	93 96
2	4	641/804 (80%)	637 (99%)	4 (1%)	86 92
2	5	640/804 (80%)	636 (99%)	4 (1%)	86 92
2	6	640/804 (80%)	635 (99%)	5 (1%)	81 89
3	A	176/268 (66%)	176 (100%)	0	100 100
3	B	193/268 (72%)	193 (100%)	0	100 100
3	C	193/268 (72%)	193 (100%)	0	100 100
3	D	193/268 (72%)	193 (100%)	0	100 100
3	E	194/268 (72%)	194 (100%)	0	100 100
3	F	193/268 (72%)	190 (98%)	3 (2%)	62 79
3	G	176/268 (66%)	176 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	a	143/906 (16%)	143 (100%)	0	100 100
5	b	143/906 (16%)	143 (100%)	0	100 100
5	c	143/906 (16%)	141 (99%)	2 (1%)	67 80
5	d	143/906 (16%)	143 (100%)	0	100 100
5	e	143/906 (16%)	142 (99%)	1 (1%)	84 90
5	f	143/906 (16%)	143 (100%)	0	100 100
5	g	143/906 (16%)	143 (100%)	0	100 100
All	All	6163/13042 (47%)	6135 (100%)	28 (0%)	89 93

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5	322	THR
5	e	769	ASP
2	6	437	LYS
3	F	211	GLU
2	5	834	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
5	d	786	ASN
5	f	724	ASN
5	b	724	ASN
5	a	776	ASN
5	e	724	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)

12 ligands are modelled in this entry.

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	$\#\|Z\|>2$
6	AGS	4	1001	-	26,33,33	0.91	0	26,52,52	1.29	2 (7%)
6	AGS	1	1001	-	26,33,33	0.91	0	26,52,52	1.30	2 (7%)
6	AGS	1	1002	-	26,33,33	0.91	0	26,52,52	1.30	2 (7%)
6	AGS	5	1001	-	26,33,33	0.84	0	26,52,52	1.35	2 (7%)
6	AGS	6	1002	-	26,33,33	0.75	1 (3%)	26,52,52	1.19	3 (11%)
6	AGS	4	1002	-	26,33,33	0.81	0	26,52,52	1.06	3 (11%)
6	AGS	2	1001	-	26,33,33	0.81	0	26,52,52	1.07	3 (11%)
6	AGS	3	1002	-	26,33,33	0.81	0	26,52,52	1.07	3 (11%)
6	AGS	1	1003	-	26,33,33	1.89	4 (15%)	26,52,52	1.57	4 (15%)
6	AGS	6	1001	-	26,33,33	0.79	0	26,52,52	1.43	2 (7%)
6	AGS	5	1002	-	26,33,33	0.80	1 (3%)	26,52,52	0.93	2 (7%)
6	AGS	3	1001	-	26,33,33	0.91	0	26,52,52	1.30	2 (7%)

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
6	AGS	4	1001	-	-	2/17/38/38	0/3/3/3
6	AGS	1	1001	-	-	2/17/38/38	0/3/3/3
6	AGS	1	1002	-	-	2/17/38/38	0/3/3/3
6	AGS	5	1001	-	-	3/17/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AGS	6	1002	-	-	7/17/38/38	0/3/3/3
6	AGS	4	1002	-	-	3/17/38/38	0/3/3/3
6	AGS	2	1001	-	-	3/17/38/38	0/3/3/3
6	AGS	3	1002	-	-	3/17/38/38	0/3/3/3
6	AGS	1	1003	-	-	5/17/38/38	0/3/3/3
6	AGS	6	1001	-	-	3/17/38/38	0/3/3/3
6	AGS	5	1002	-	-	9/17/38/38	0/3/3/3
6	AGS	3	1001	-	-	2/17/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	1003	AGS	PG-S1G	7.96	2.08	1.90
6	1	1003	AGS	C5-C4	2.50	1.47	1.40
6	6	1002	AGS	PG-S1G	2.03	1.95	1.90
6	1	1003	AGS	PG-O2G	2.03	1.61	1.54
6	5	1002	AGS	PG-S1G	2.01	1.95	1.90

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	1001	AGS	PA-O3A-PB	-5.92	112.52	132.83
6	5	1001	AGS	PA-O3A-PB	-5.47	114.05	132.83
6	1	1001	AGS	PA-O3A-PB	-5.18	115.05	132.83
6	1	1002	AGS	PA-O3A-PB	-5.17	115.08	132.83
6	3	1001	AGS	PA-O3A-PB	-5.17	115.09	132.83

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	1003	AGS	O4'-C4'-C5'-O5'
6	6	1002	AGS	PB-O3B-PG-O2G
6	6	1002	AGS	C5'-O5'-PA-O1A
6	6	1002	AGS	C5'-O5'-PA-O2A
6	6	1002	AGS	C3'-C4'-C5'-O5'

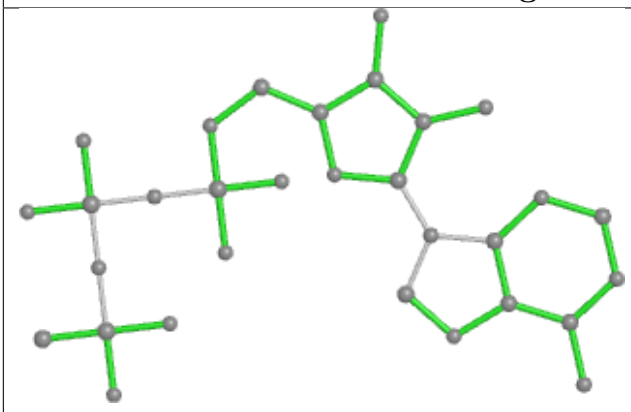
There are no ring outliers.

10 monomers are involved in 38 short contacts:

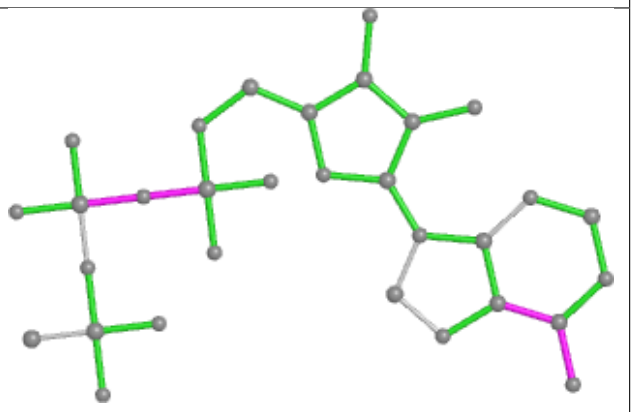
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	4	1001	AGS	2	0
6	1	1001	AGS	2	0
6	5	1001	AGS	5	0
6	6	1002	AGS	3	0
6	4	1002	AGS	6	0
6	2	1001	AGS	1	0
6	3	1002	AGS	2	0
6	1	1003	AGS	14	0
6	6	1001	AGS	1	0
6	5	1002	AGS	2	0

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.

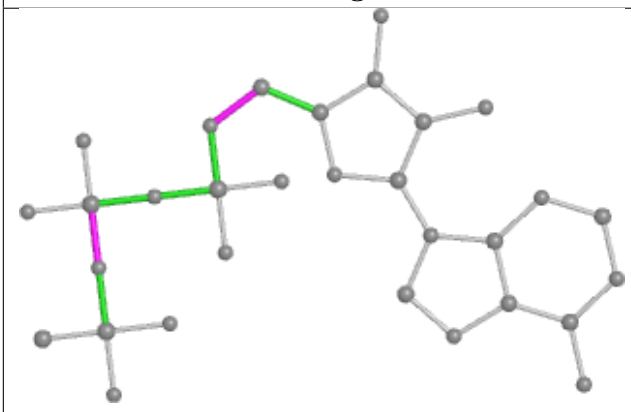
Ligand AGS 4 1001



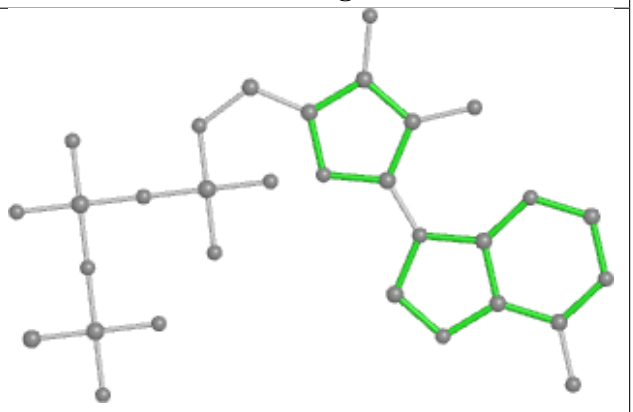
Bond lengths



Bond angles

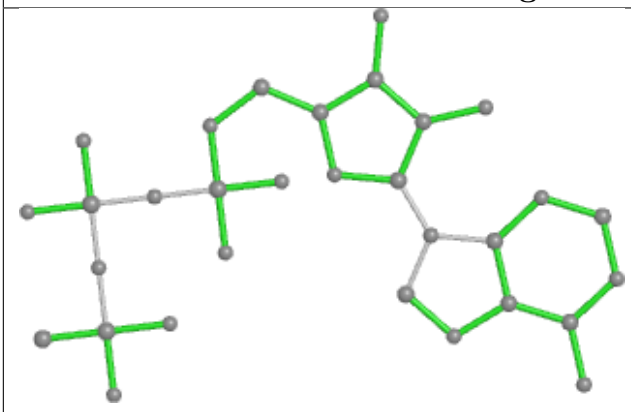


Torsions

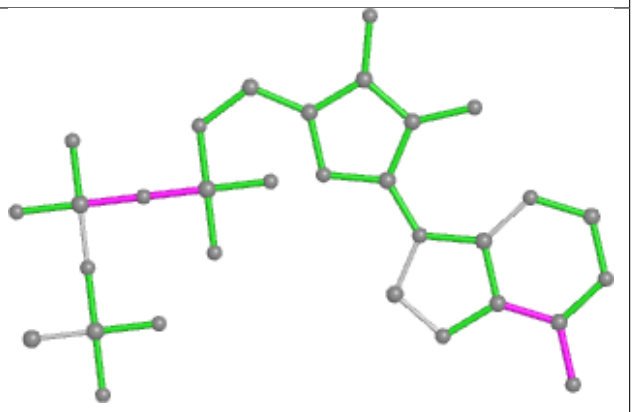


Rings

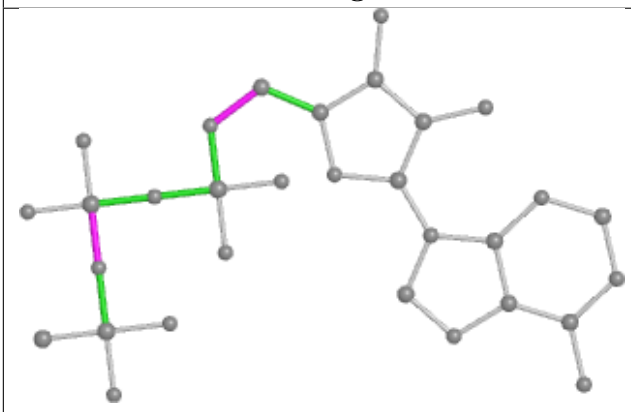
Ligand AGS 1 1001



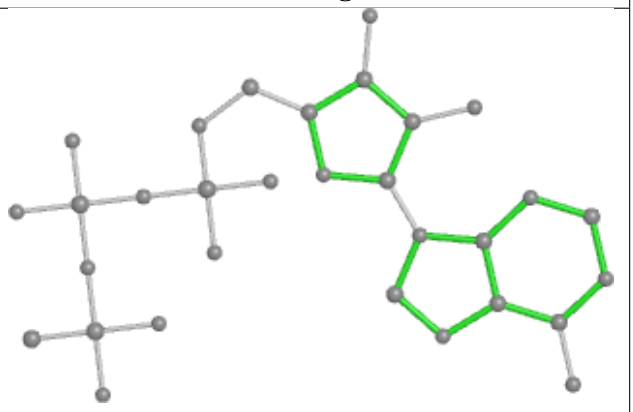
Bond lengths



Bond angles

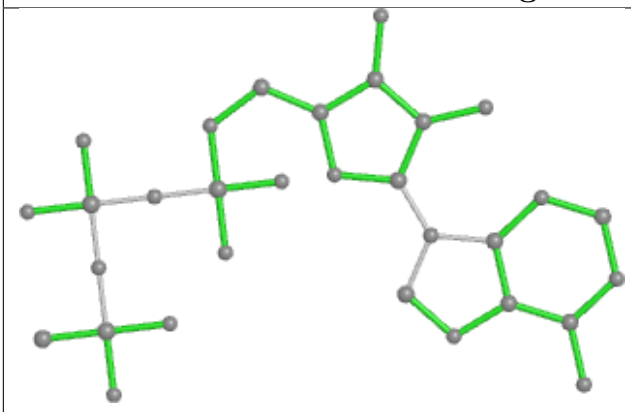


Torsions

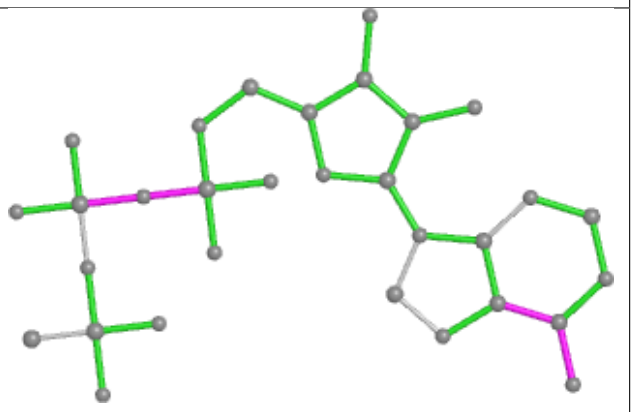


Rings

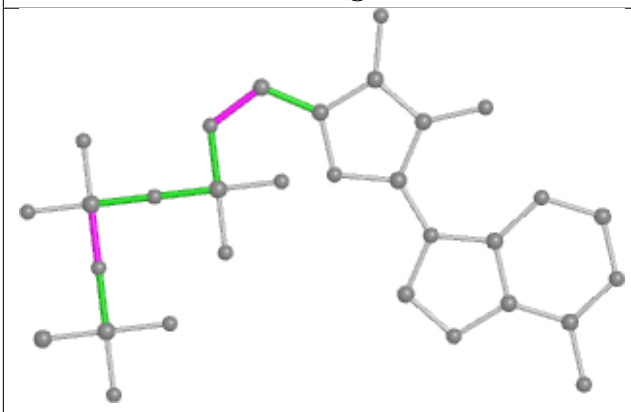
Ligand AGS 1 1002



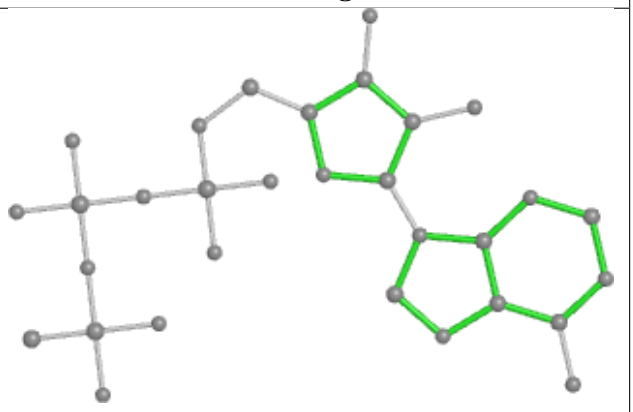
Bond lengths



Bond angles

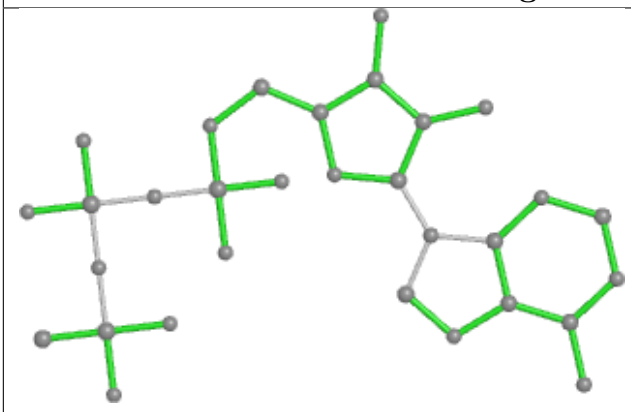


Torsions

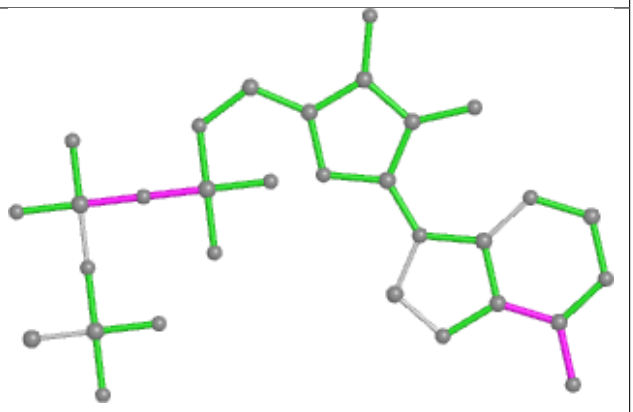


Rings

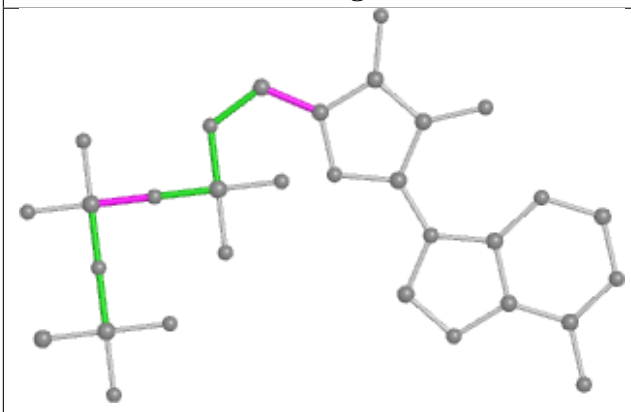
Ligand AGS 5 1001



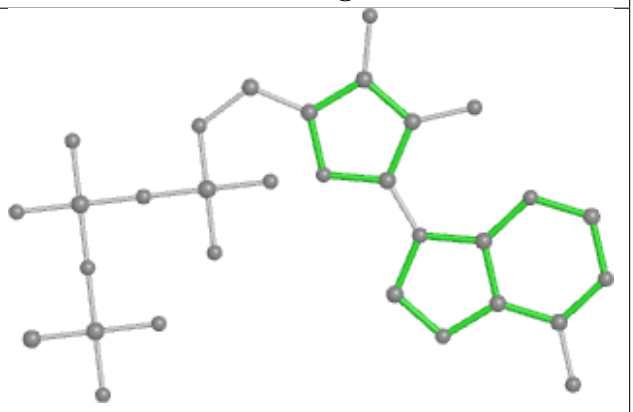
Bond lengths



Bond angles

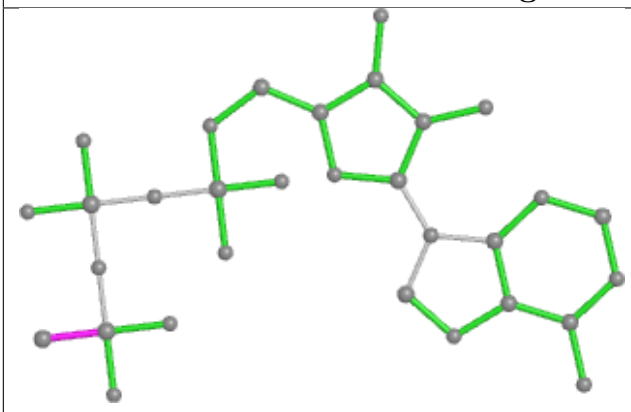


Torsions

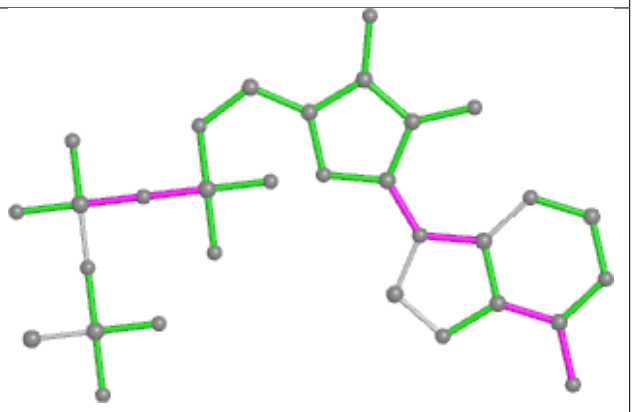


Rings

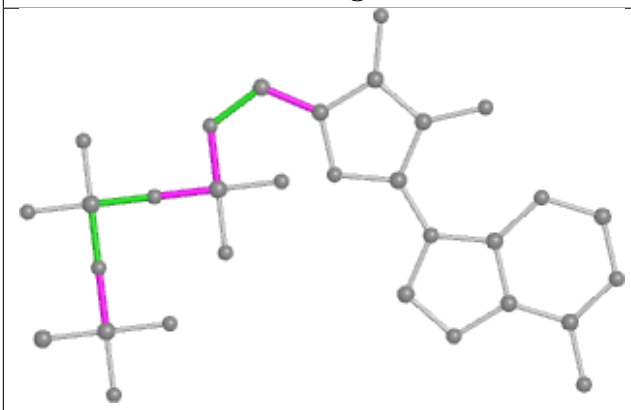
Ligand AGS 6 1002



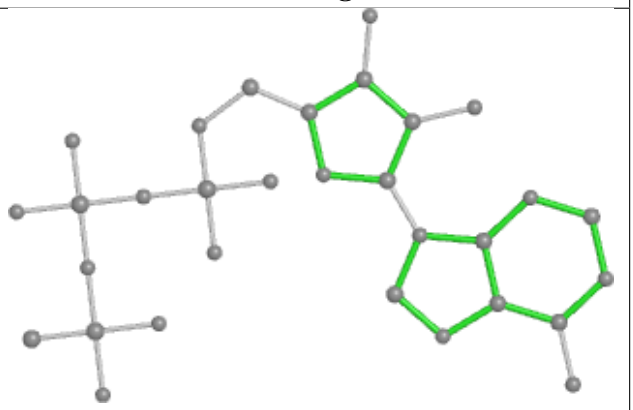
Bond lengths



Bond angles

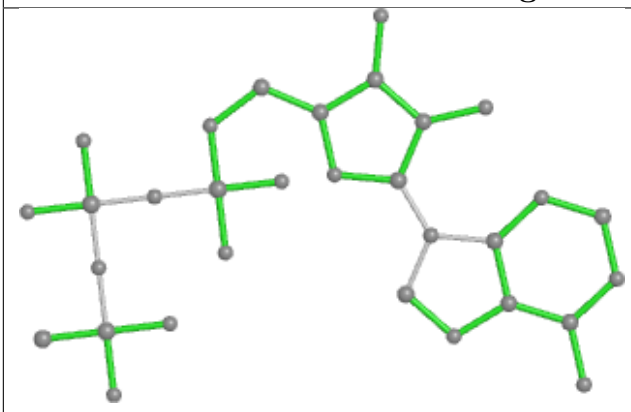


Torsions

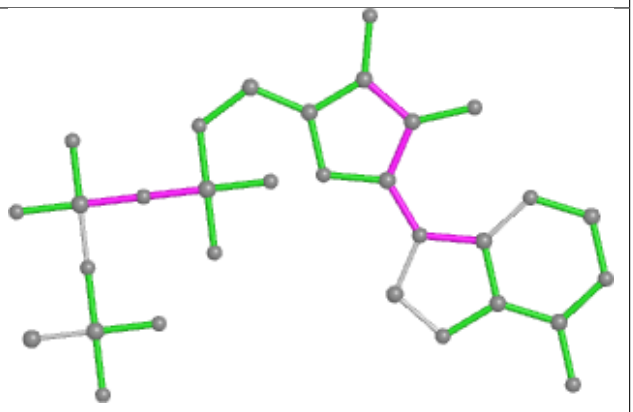


Rings

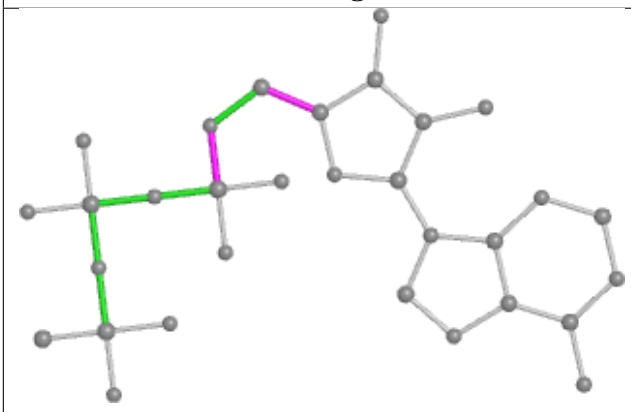
Ligand AGS 4 1002



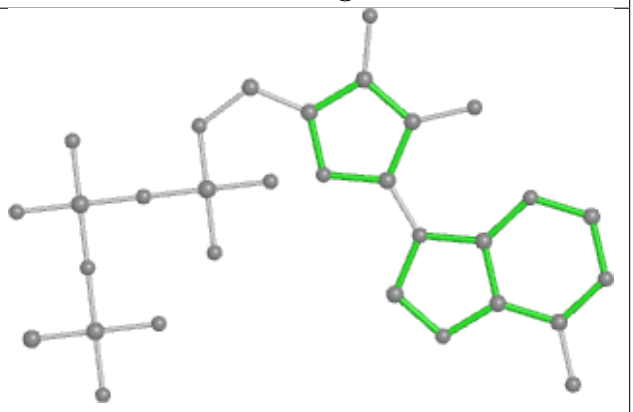
Bond lengths



Bond angles

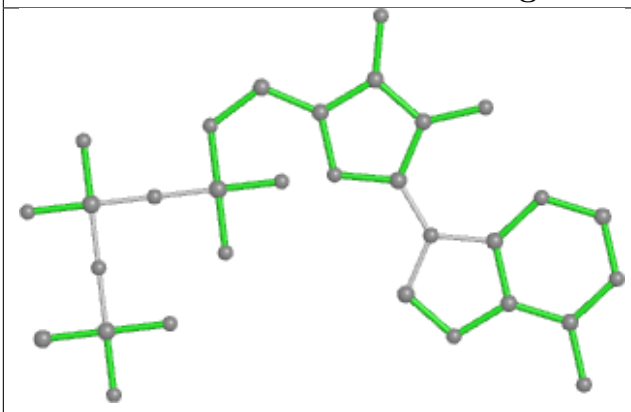


Torsions

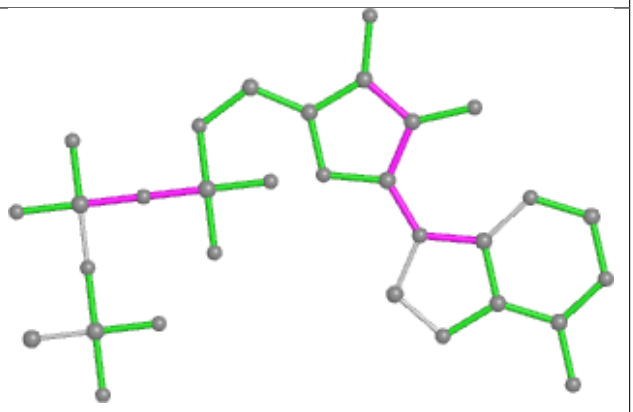


Rings

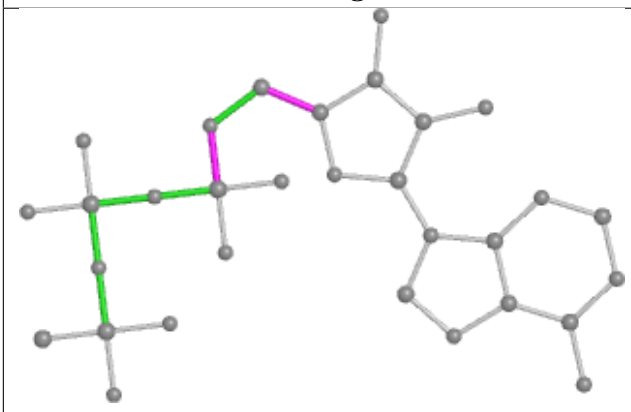
Ligand AGS 2 1001



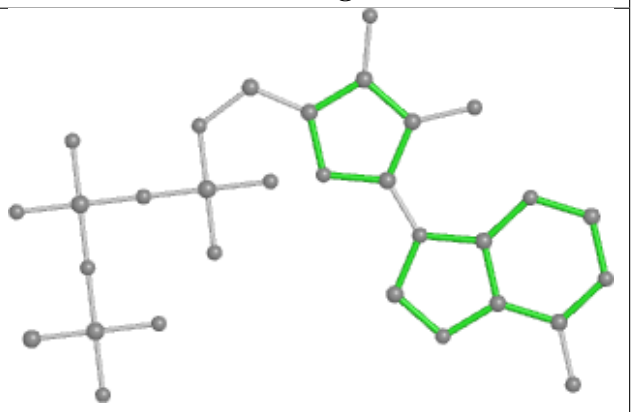
Bond lengths



Bond angles

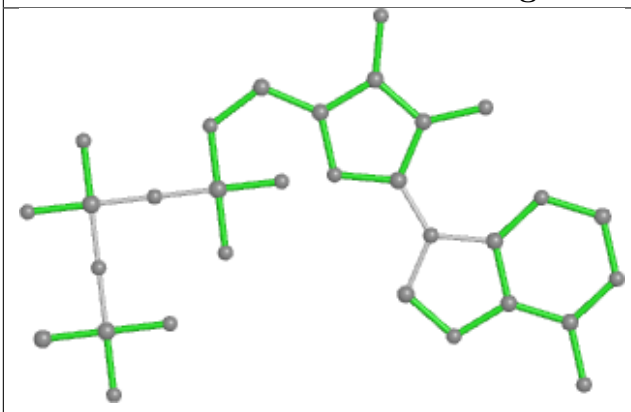


Torsions

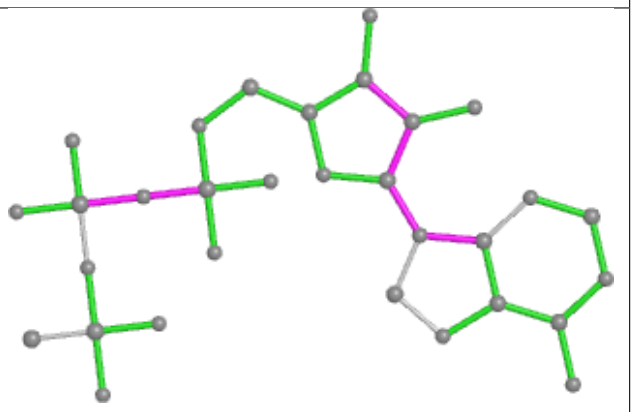


Rings

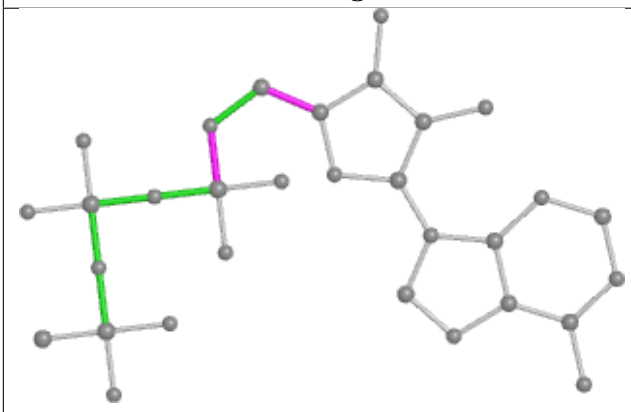
Ligand AGS 3 1002



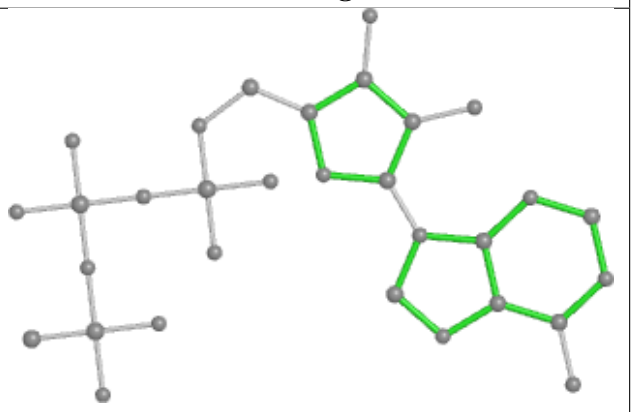
Bond lengths



Bond angles

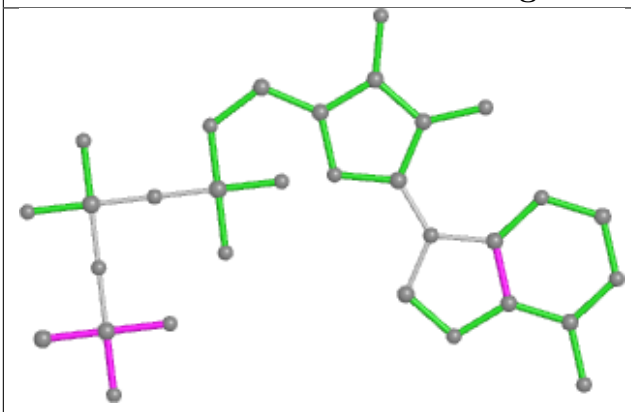


Torsions

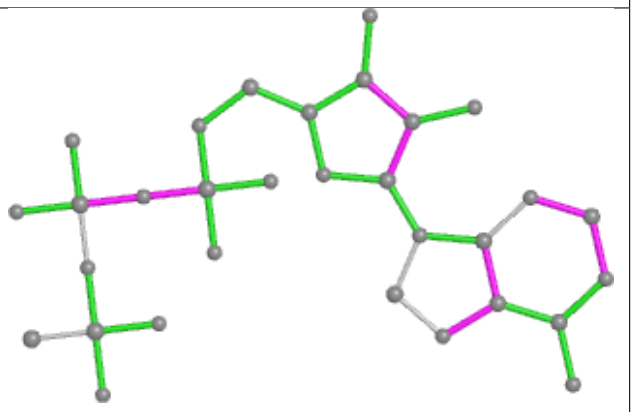


Rings

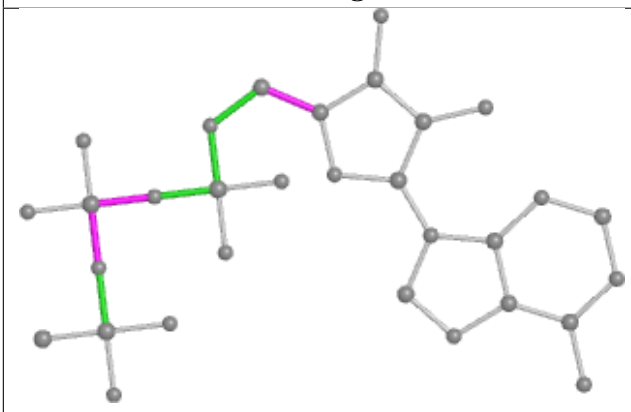
Ligand AGS 1 1003



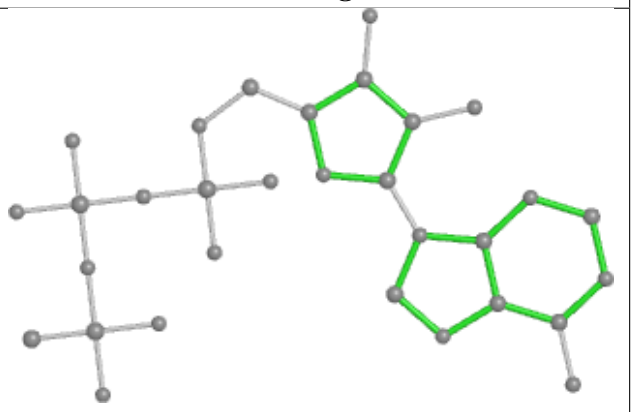
Bond lengths



Bond angles

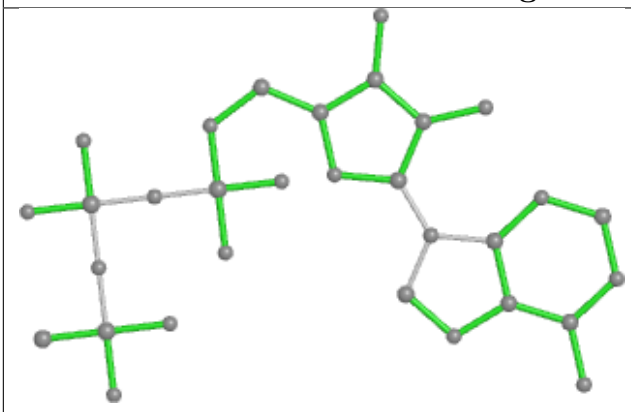


Torsions

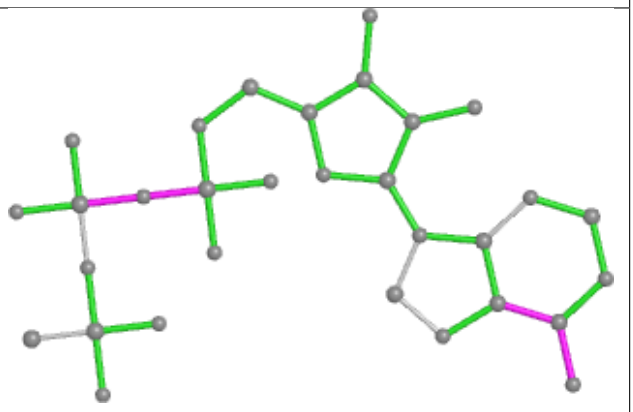


Rings

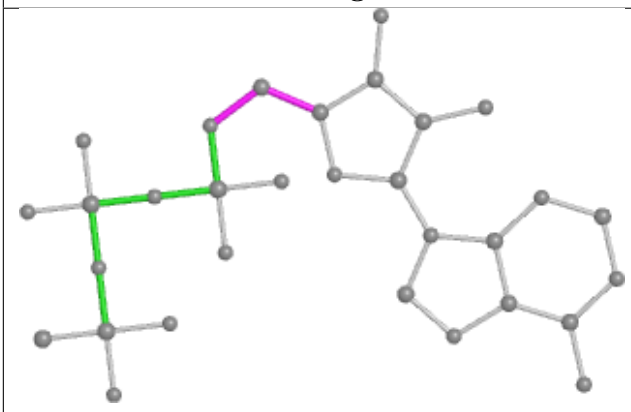
Ligand AGS 6 1001



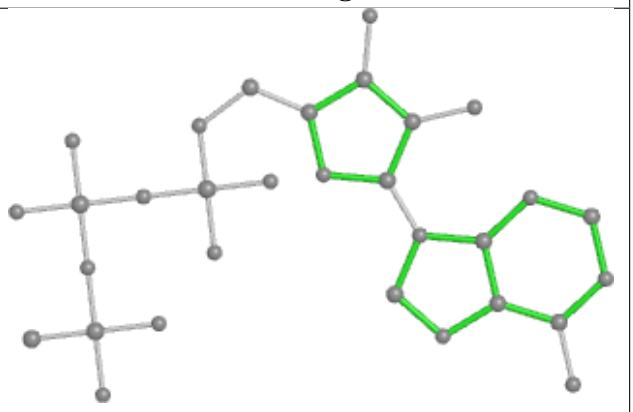
Bond lengths



Bond angles

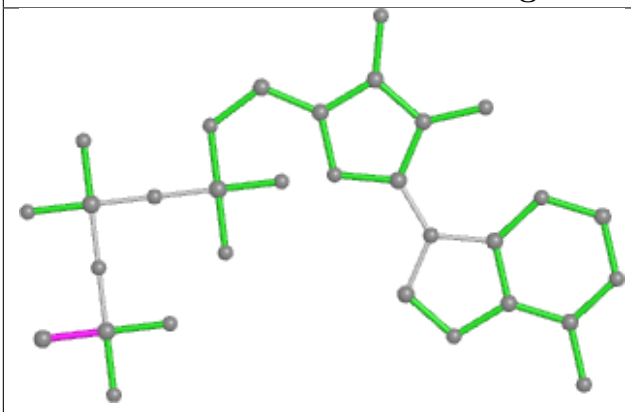


Torsions

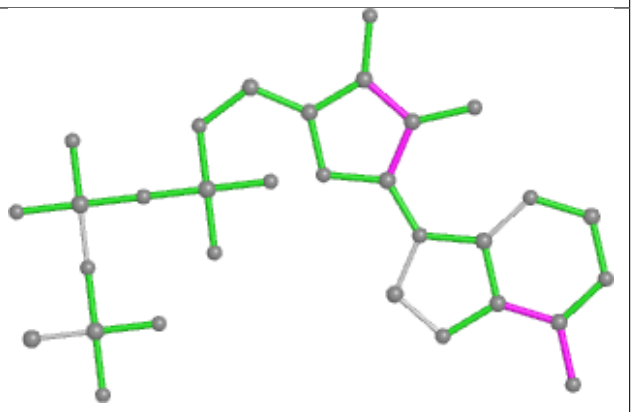


Rings

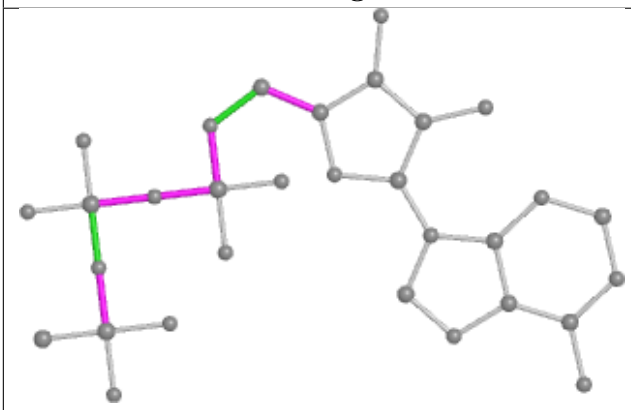
Ligand AGS 5 1002



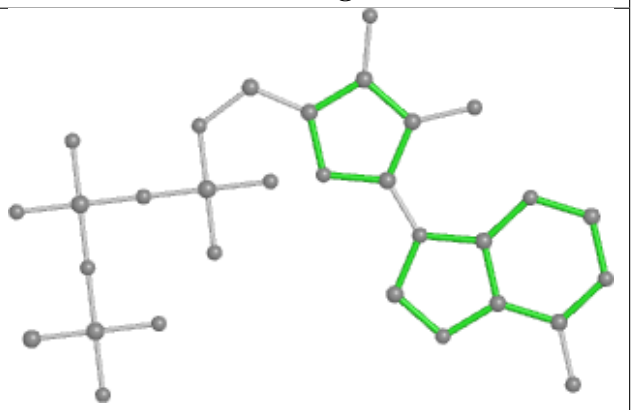
Bond lengths



Bond angles

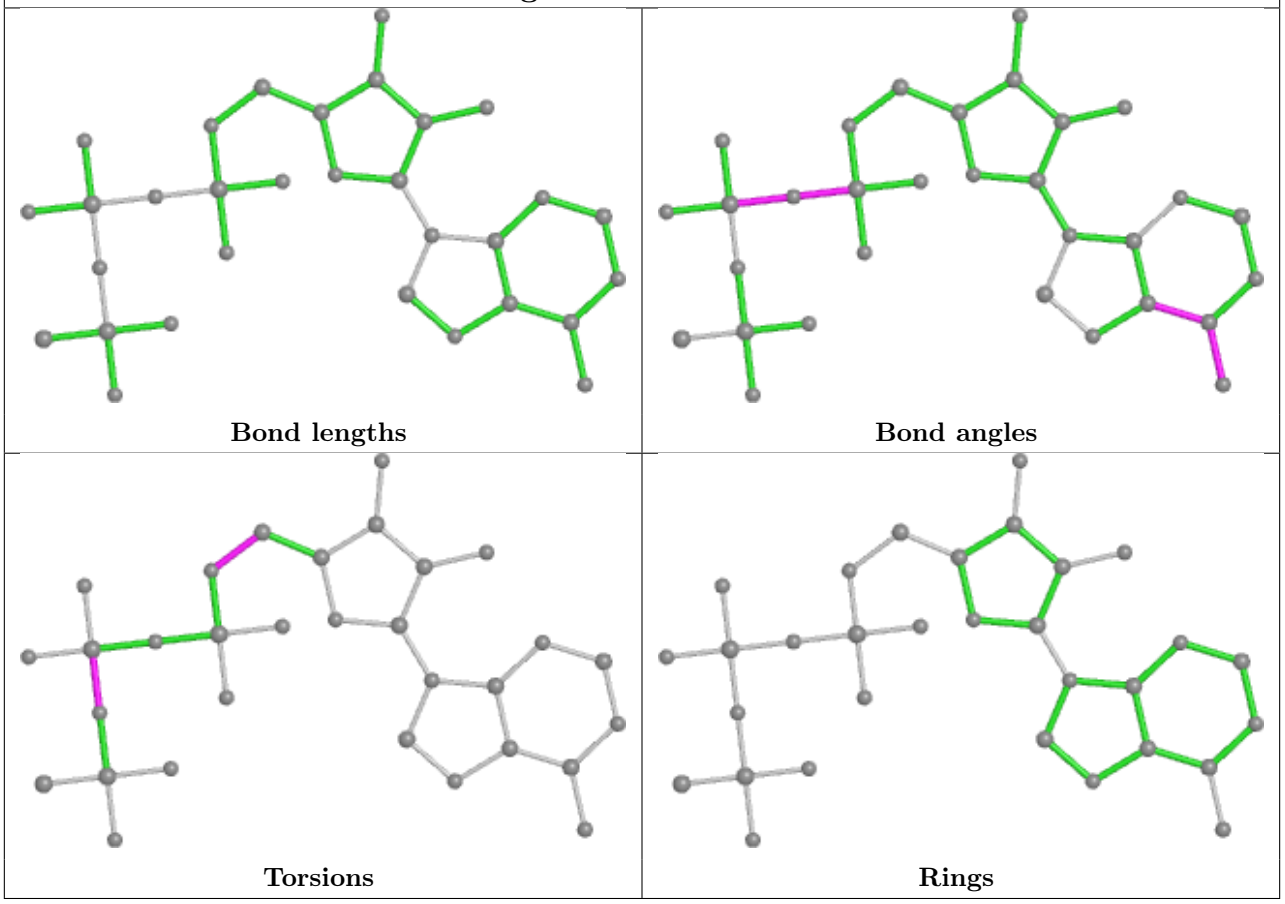


Torsions



Rings

Ligand AGS 3 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	h	1
1	i	1
1	l	1
1	j	1
1	k	1
1	m	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	28:UNK	C	988:UNK	N	44.65
1	i	29:UNK	C	988:UNK	N	43.96
1	l	33:UNK	C	986:UNK	N	33.84
1	j	32:UNK	C	981:UNK	N	24.35
1	k	33:UNK	C	980:UNK	N	19.33

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8952. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.