Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 01:31 am BST

PDB ID	:	7OFH
EMDB ID	:	EMD-12874
Title	:	CryoEM structure of the outer membrane secretin pore pIV from the f1 filamentous bacteriophage.
Authors	:	Conners, R.; Gold, V.A.M.
Deposited on	:	2021-05-05
Resolution	:	2.70 Å(reported)
Based on initial model	:	5W68

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

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

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

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

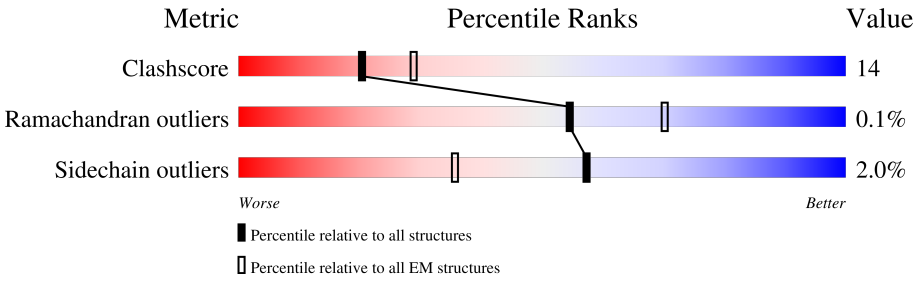
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	414	45% 10% 44%
1	B	414	44% 11% 44%
1	C	414	45% 11% 44%
1	D	414	45% 11% 44%
1	E	414	45% 10% 44%
1	F	414	45% 10% 44%
1	G	414	45% 10% 44%
1	H	414	46% 10% 44%

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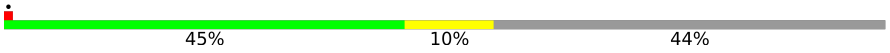
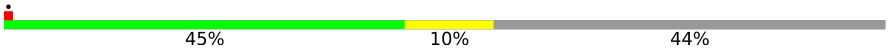
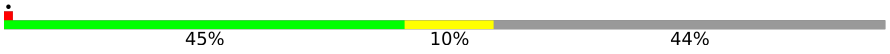
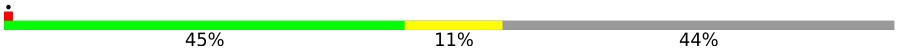
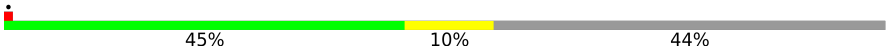
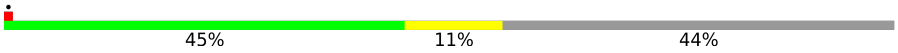
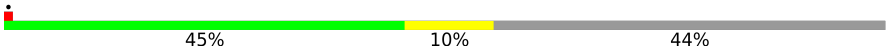
Mol	Chain	Length	Quality of chain
1	I	414	
1	J	414	
1	K	414	
1	L	414	
1	M	414	
1	N	414	
1	O	414	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27135 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 Virion export protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	B	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	C	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	D	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	E	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	F	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	G	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	H	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	I	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	J	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	K	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	L	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	M	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	N	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		
1	O	231	Total	C	N	O	S	0	0
			1742	1095	295	350	2		

There are 195 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	SER	variant	UNP P03666
A	49	ASN	ASP	variant	UNP P03666
A	66	ASN	ILE	variant	UNP P03666
A	308A	SER	-	insertion	UNP P03666
A	308B	ALA	-	insertion	UNP P03666
A	308C	HIS	-	insertion	UNP P03666
A	308D	HIS	-	insertion	UNP P03666
A	308E	HIS	-	insertion	UNP P03666
A	308F	HIS	-	insertion	UNP P03666
A	308G	HIS	-	insertion	UNP P03666
A	308H	HIS	-	insertion	UNP P03666
A	308I	HIS	-	insertion	UNP P03666
A	318	ILE	SER	engineered mutation	UNP P03666
B	9	PRO	SER	variant	UNP P03666
B	49	ASN	ASP	variant	UNP P03666
B	66	ASN	ILE	variant	UNP P03666
B	308A	SER	-	insertion	UNP P03666
B	308B	ALA	-	insertion	UNP P03666
B	308C	HIS	-	insertion	UNP P03666
B	308D	HIS	-	insertion	UNP P03666
B	308E	HIS	-	insertion	UNP P03666
B	308F	HIS	-	insertion	UNP P03666
B	308G	HIS	-	insertion	UNP P03666
B	308H	HIS	-	insertion	UNP P03666
B	308I	HIS	-	insertion	UNP P03666
B	318	ILE	SER	engineered mutation	UNP P03666
C	9	PRO	SER	variant	UNP P03666
C	49	ASN	ASP	variant	UNP P03666
C	66	ASN	ILE	variant	UNP P03666
C	308A	SER	-	insertion	UNP P03666
C	308B	ALA	-	insertion	UNP P03666
C	308C	HIS	-	insertion	UNP P03666
C	308D	HIS	-	insertion	UNP P03666
C	308E	HIS	-	insertion	UNP P03666
C	308F	HIS	-	insertion	UNP P03666
C	308G	HIS	-	insertion	UNP P03666
C	308H	HIS	-	insertion	UNP P03666
C	308I	HIS	-	insertion	UNP P03666
C	318	ILE	SER	engineered mutation	UNP P03666
D	9	PRO	SER	variant	UNP P03666
D	49	ASN	ASP	variant	UNP P03666
D	66	ASN	ILE	variant	UNP P03666
D	308A	SER	-	insertion	UNP P03666

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Chain	Residue	Modelled	Actual	Comment	Reference
D	308B	ALA	-	insertion	UNP P03666
D	308C	HIS	-	insertion	UNP P03666
D	308D	HIS	-	insertion	UNP P03666
D	308E	HIS	-	insertion	UNP P03666
D	308F	HIS	-	insertion	UNP P03666
D	308G	HIS	-	insertion	UNP P03666
D	308H	HIS	-	insertion	UNP P03666
D	308I	HIS	-	insertion	UNP P03666
D	318	ILE	SER	engineered mutation	UNP P03666
E	9	PRO	SER	variant	UNP P03666
E	49	ASN	ASP	variant	UNP P03666
E	66	ASN	ILE	variant	UNP P03666
E	308A	SER	-	insertion	UNP P03666
E	308B	ALA	-	insertion	UNP P03666
E	308C	HIS	-	insertion	UNP P03666
E	308D	HIS	-	insertion	UNP P03666
E	308E	HIS	-	insertion	UNP P03666
E	308F	HIS	-	insertion	UNP P03666
E	308G	HIS	-	insertion	UNP P03666
E	308H	HIS	-	insertion	UNP P03666
E	308I	HIS	-	insertion	UNP P03666
E	318	ILE	SER	engineered mutation	UNP P03666
F	9	PRO	SER	variant	UNP P03666
F	49	ASN	ASP	variant	UNP P03666
F	66	ASN	ILE	variant	UNP P03666
F	308A	SER	-	insertion	UNP P03666
F	308B	ALA	-	insertion	UNP P03666
F	308C	HIS	-	insertion	UNP P03666
F	308D	HIS	-	insertion	UNP P03666
F	308E	HIS	-	insertion	UNP P03666
F	308F	HIS	-	insertion	UNP P03666
F	308G	HIS	-	insertion	UNP P03666
F	308H	HIS	-	insertion	UNP P03666
F	308I	HIS	-	insertion	UNP P03666
F	318	ILE	SER	engineered mutation	UNP P03666
G	9	PRO	SER	variant	UNP P03666
G	49	ASN	ASP	variant	UNP P03666
G	66	ASN	ILE	variant	UNP P03666
G	308A	SER	-	insertion	UNP P03666
G	308B	ALA	-	insertion	UNP P03666
G	308C	HIS	-	insertion	UNP P03666
G	308D	HIS	-	insertion	UNP P03666

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Chain	Residue	Modelled	Actual	Comment	Reference
G	308E	HIS	-	insertion	UNP P03666
G	308F	HIS	-	insertion	UNP P03666
G	308G	HIS	-	insertion	UNP P03666
G	308H	HIS	-	insertion	UNP P03666
G	308I	HIS	-	insertion	UNP P03666
G	318	ILE	SER	engineered mutation	UNP P03666
H	9	PRO	SER	variant	UNP P03666
H	49	ASN	ASP	variant	UNP P03666
H	66	ASN	ILE	variant	UNP P03666
H	308A	SER	-	insertion	UNP P03666
H	308B	ALA	-	insertion	UNP P03666
H	308C	HIS	-	insertion	UNP P03666
H	308D	HIS	-	insertion	UNP P03666
H	308E	HIS	-	insertion	UNP P03666
H	308F	HIS	-	insertion	UNP P03666
H	308G	HIS	-	insertion	UNP P03666
H	308H	HIS	-	insertion	UNP P03666
H	308I	HIS	-	insertion	UNP P03666
H	318	ILE	SER	engineered mutation	UNP P03666
I	9	PRO	SER	variant	UNP P03666
I	49	ASN	ASP	variant	UNP P03666
I	66	ASN	ILE	variant	UNP P03666
I	308A	SER	-	insertion	UNP P03666
I	308B	ALA	-	insertion	UNP P03666
I	308C	HIS	-	insertion	UNP P03666
I	308D	HIS	-	insertion	UNP P03666
I	308E	HIS	-	insertion	UNP P03666
I	308F	HIS	-	insertion	UNP P03666
I	308G	HIS	-	insertion	UNP P03666
I	308H	HIS	-	insertion	UNP P03666
I	308I	HIS	-	insertion	UNP P03666
I	318	ILE	SER	engineered mutation	UNP P03666
J	9	PRO	SER	variant	UNP P03666
J	49	ASN	ASP	variant	UNP P03666
J	66	ASN	ILE	variant	UNP P03666
J	308A	SER	-	insertion	UNP P03666
J	308B	ALA	-	insertion	UNP P03666
J	308C	HIS	-	insertion	UNP P03666
J	308D	HIS	-	insertion	UNP P03666
J	308E	HIS	-	insertion	UNP P03666
J	308F	HIS	-	insertion	UNP P03666
J	308G	HIS	-	insertion	UNP P03666

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Chain	Residue	Modelled	Actual	Comment	Reference
J	308H	HIS	-	insertion	UNP P03666
J	308I	HIS	-	insertion	UNP P03666
J	318	ILE	SER	engineered mutation	UNP P03666
K	9	PRO	SER	variant	UNP P03666
K	49	ASN	ASP	variant	UNP P03666
K	66	ASN	ILE	variant	UNP P03666
K	308A	SER	-	insertion	UNP P03666
K	308B	ALA	-	insertion	UNP P03666
K	308C	HIS	-	insertion	UNP P03666
K	308D	HIS	-	insertion	UNP P03666
K	308E	HIS	-	insertion	UNP P03666
K	308F	HIS	-	insertion	UNP P03666
K	308G	HIS	-	insertion	UNP P03666
K	308H	HIS	-	insertion	UNP P03666
K	308I	HIS	-	insertion	UNP P03666
K	318	ILE	SER	engineered mutation	UNP P03666
L	9	PRO	SER	variant	UNP P03666
L	49	ASN	ASP	variant	UNP P03666
L	66	ASN	ILE	variant	UNP P03666
L	308A	SER	-	insertion	UNP P03666
L	308B	ALA	-	insertion	UNP P03666
L	308C	HIS	-	insertion	UNP P03666
L	308D	HIS	-	insertion	UNP P03666
L	308E	HIS	-	insertion	UNP P03666
L	308F	HIS	-	insertion	UNP P03666
L	308G	HIS	-	insertion	UNP P03666
L	308H	HIS	-	insertion	UNP P03666
L	308I	HIS	-	insertion	UNP P03666
L	318	ILE	SER	engineered mutation	UNP P03666
M	9	PRO	SER	variant	UNP P03666
M	49	ASN	ASP	variant	UNP P03666
M	66	ASN	ILE	variant	UNP P03666
M	308A	SER	-	insertion	UNP P03666
M	308B	ALA	-	insertion	UNP P03666
M	308C	HIS	-	insertion	UNP P03666
M	308D	HIS	-	insertion	UNP P03666
M	308E	HIS	-	insertion	UNP P03666
M	308F	HIS	-	insertion	UNP P03666
M	308G	HIS	-	insertion	UNP P03666
M	308H	HIS	-	insertion	UNP P03666
M	308I	HIS	-	insertion	UNP P03666
M	318	ILE	SER	engineered mutation	UNP P03666

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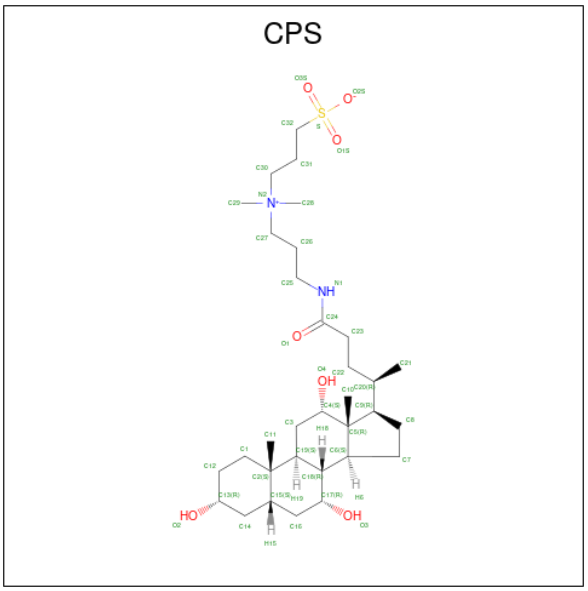
Chain	Residue	Modelled	Actual	Comment	Reference
N	9	PRO	SER	variant	UNP P03666
N	49	ASN	ASP	variant	UNP P03666
N	66	ASN	ILE	variant	UNP P03666
N	308A	SER	-	insertion	UNP P03666
N	308B	ALA	-	insertion	UNP P03666
N	308C	HIS	-	insertion	UNP P03666
N	308D	HIS	-	insertion	UNP P03666
N	308E	HIS	-	insertion	UNP P03666
N	308F	HIS	-	insertion	UNP P03666
N	308G	HIS	-	insertion	UNP P03666
N	308H	HIS	-	insertion	UNP P03666
N	308I	HIS	-	insertion	UNP P03666
N	318	ILE	SER	engineered mutation	UNP P03666
O	9	PRO	SER	variant	UNP P03666
O	49	ASN	ASP	variant	UNP P03666
O	66	ASN	ILE	variant	UNP P03666
O	308A	SER	-	insertion	UNP P03666
O	308B	ALA	-	insertion	UNP P03666
O	308C	HIS	-	insertion	UNP P03666
O	308D	HIS	-	insertion	UNP P03666
O	308E	HIS	-	insertion	UNP P03666
O	308F	HIS	-	insertion	UNP P03666
O	308G	HIS	-	insertion	UNP P03666
O	308H	HIS	-	insertion	UNP P03666
O	308I	HIS	-	insertion	UNP P03666
O	318	ILE	SER	engineered mutation	UNP P03666

- Molecule 2 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).



Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O S 42 32 2 7 1	0
2	A	1	Total C O 25 22 3	0
2	B	1	Total C N O S 42 32 2 7 1	0
2	B	1	Total C O 25 22 3	0
2	C	1	Total C N O S 42 32 2 7 1	0
2	C	1	Total C O 25 22 3	0
2	D	1	Total C N O S 42 32 2 7 1	0
2	D	1	Total C O 25 22 3	0
2	E	1	Total C N O S 42 32 2 7 1	0
2	E	1	Total C O 25 22 3	0
2	F	1	Total C N O S 42 32 2 7 1	0
2	F	1	Total C O 25 22 3	0
2	G	1	Total C N O S 42 32 2 7 1	0
2	G	1	Total C O 25 22 3	0

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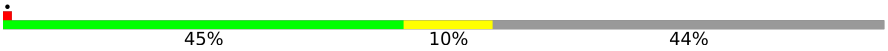
Mol	Chain	Residues	Atoms	AltConf
2	H	1	Total C N O S 42 32 2 7 1	0
2	H	1	Total C O 25 22 3	0
2	I	1	Total C N O S 42 32 2 7 1	0
2	I	1	Total C O 25 22 3	0
2	J	1	Total C N O S 42 32 2 7 1	0
2	J	1	Total C O 25 22 3	0
2	K	1	Total C N O S 42 32 2 7 1	0
2	K	1	Total C O 25 22 3	0
2	L	1	Total C N O S 42 32 2 7 1	0
2	L	1	Total C O 25 22 3	0
2	M	1	Total C N O S 42 32 2 7 1	0
2	M	1	Total C O 25 22 3	0
2	N	1	Total C N O S 42 32 2 7 1	0
2	N	1	Total C O 25 22 3	0
2	O	1	Total C O 25 22 3	0
2	O	1	Total C N O S 42 32 2 7 1	0

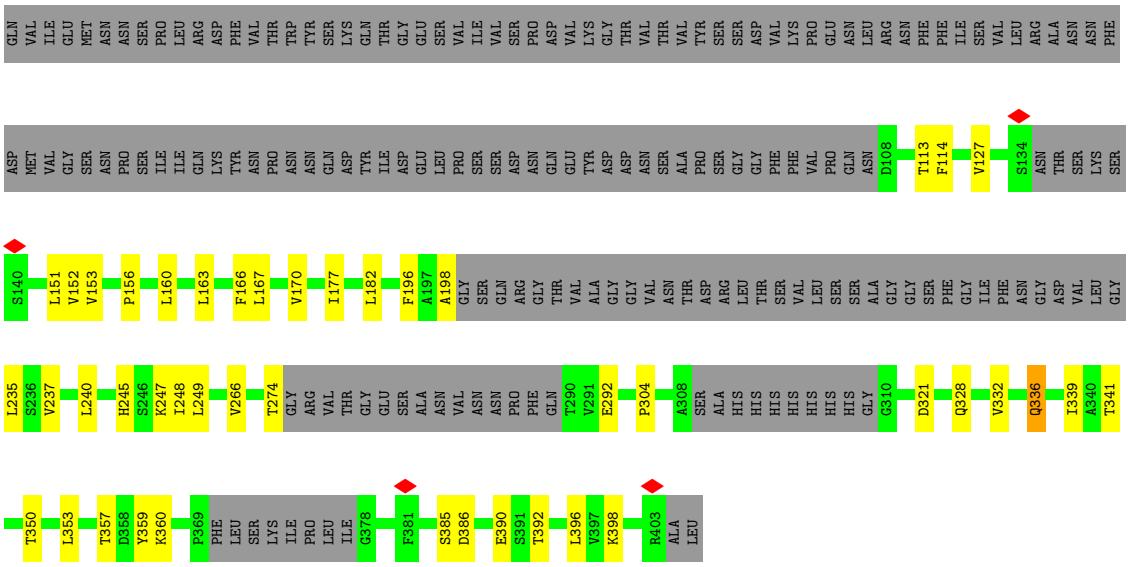
3 Residue-property plots (i)

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: Virion export protein

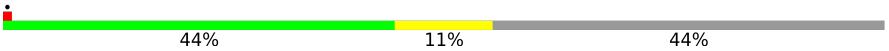
Chain A:

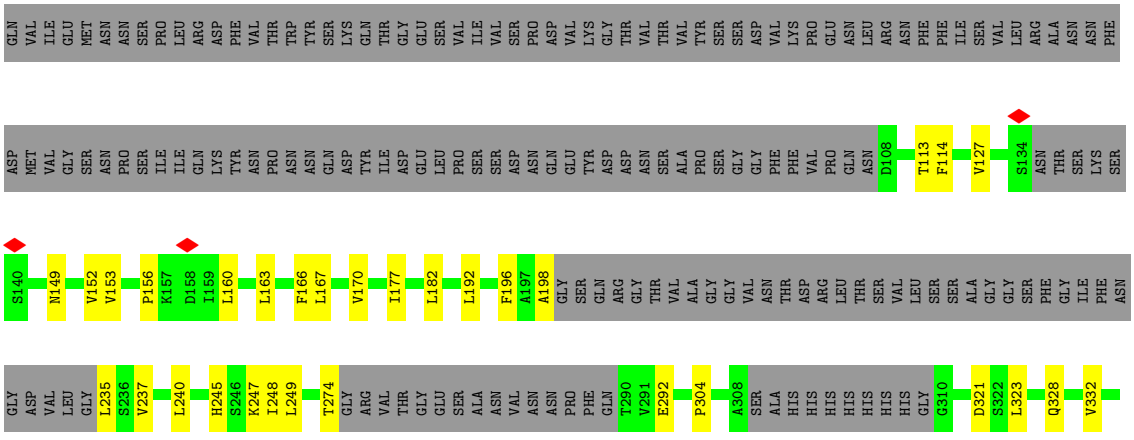


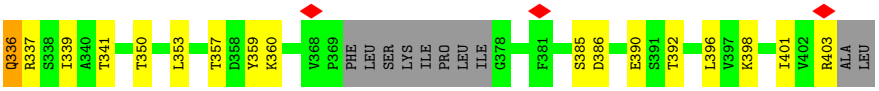


• Molecule 1: Virion export protein

Chain B:

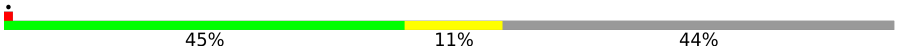


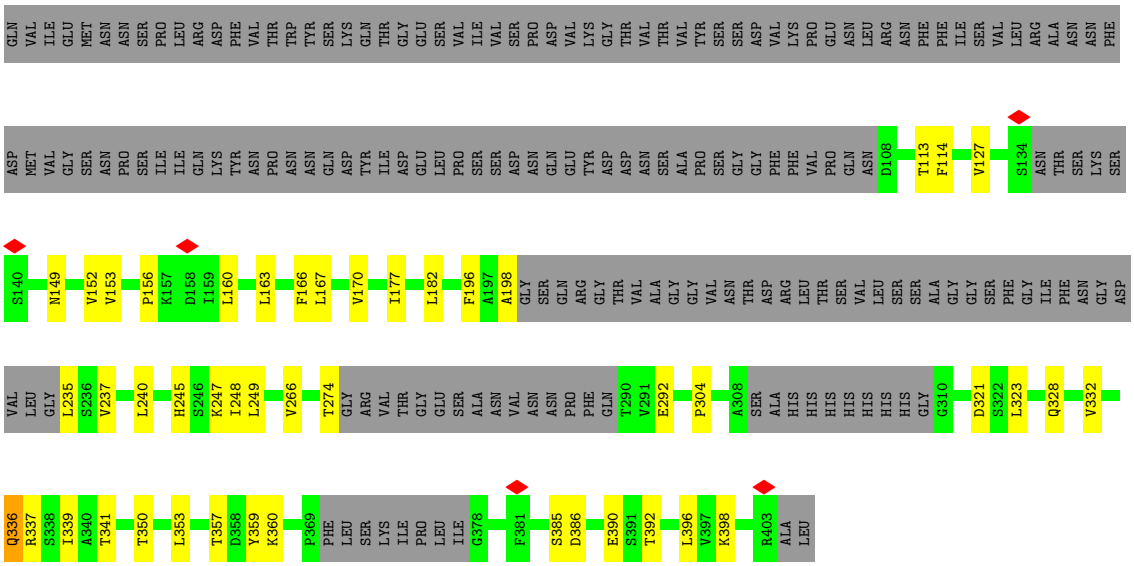




• Molecule 1: Virion export protein

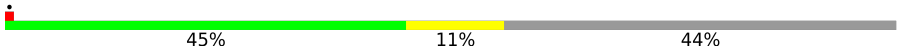
Chain C:

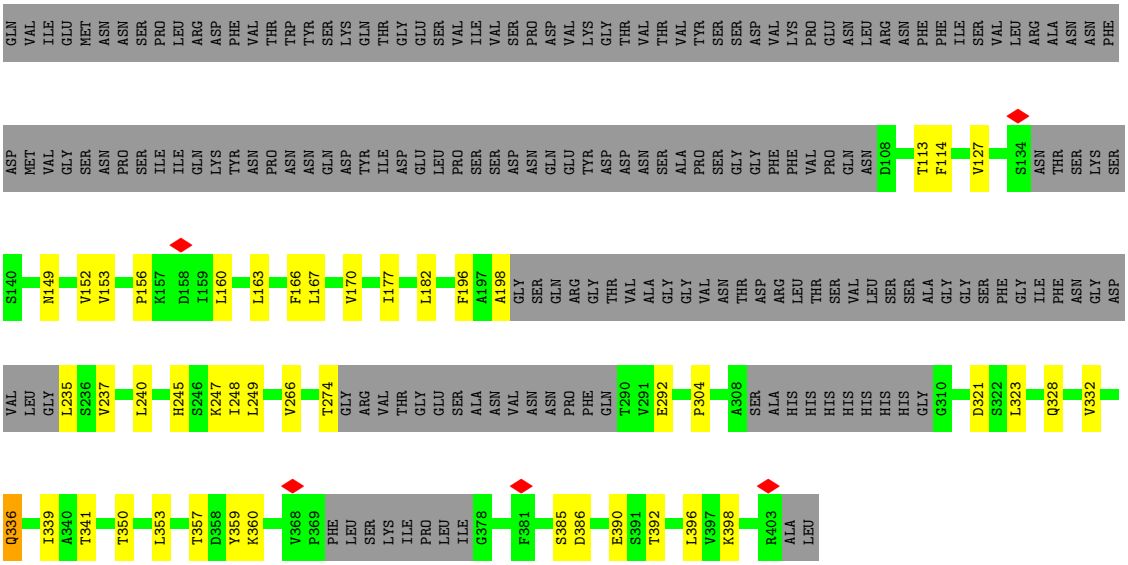




• Molecule 1: Virion export protein

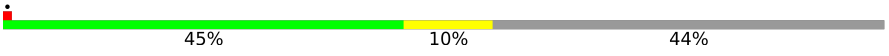
Chain D:

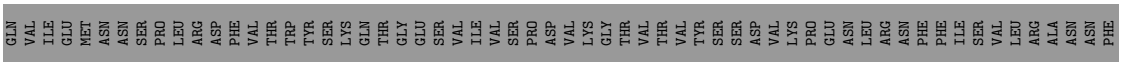


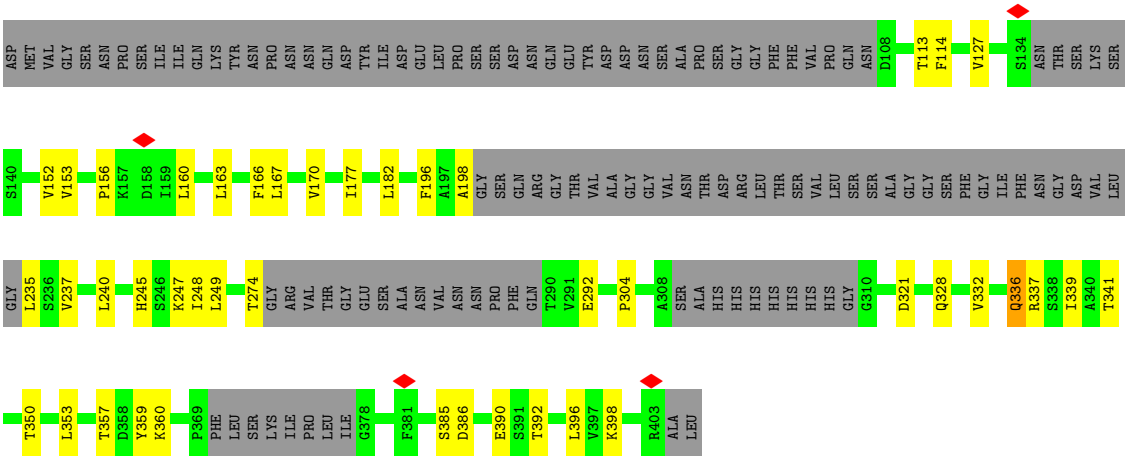


• Molecule 1: Virion export protein

Chain E:

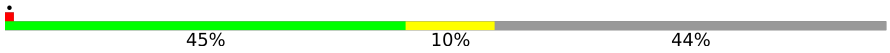


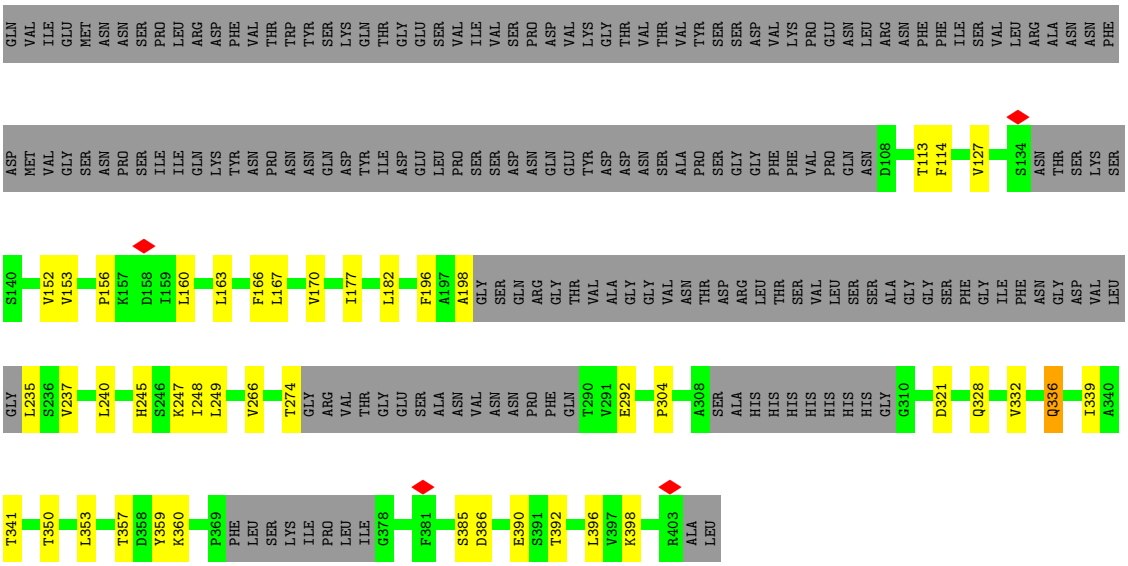




• Molecule 1: Virion export protein

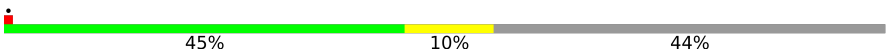
Chain F:

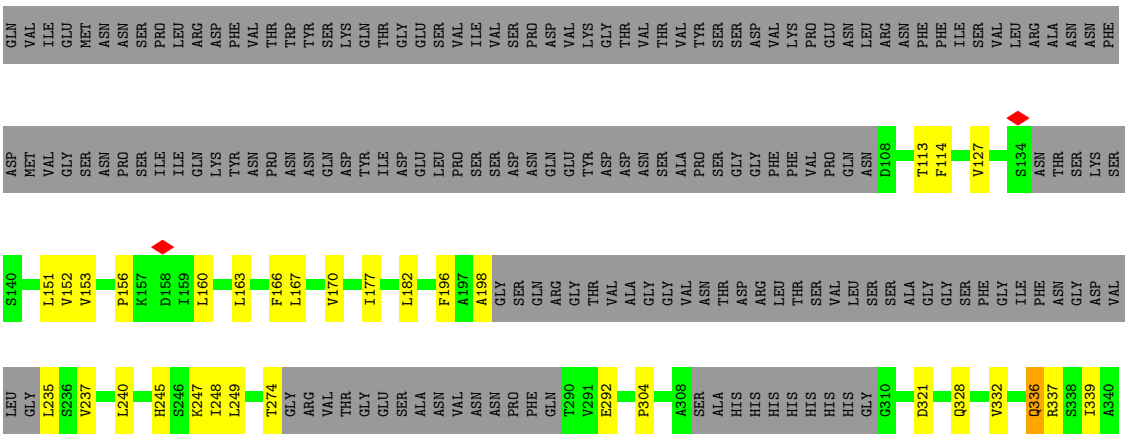


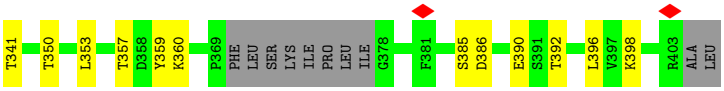


• Molecule 1: Virion export protein

Chain G:

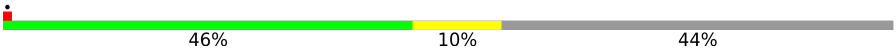


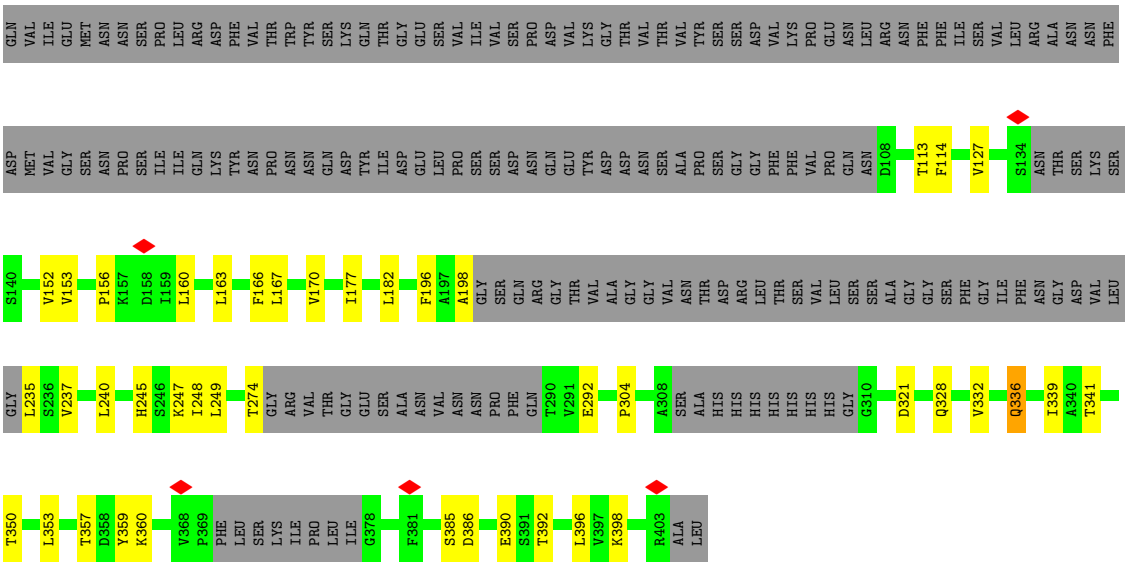




• Molecule 1: Virion export protein

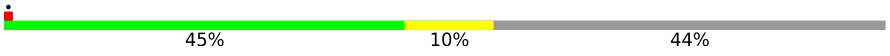
Chain H:

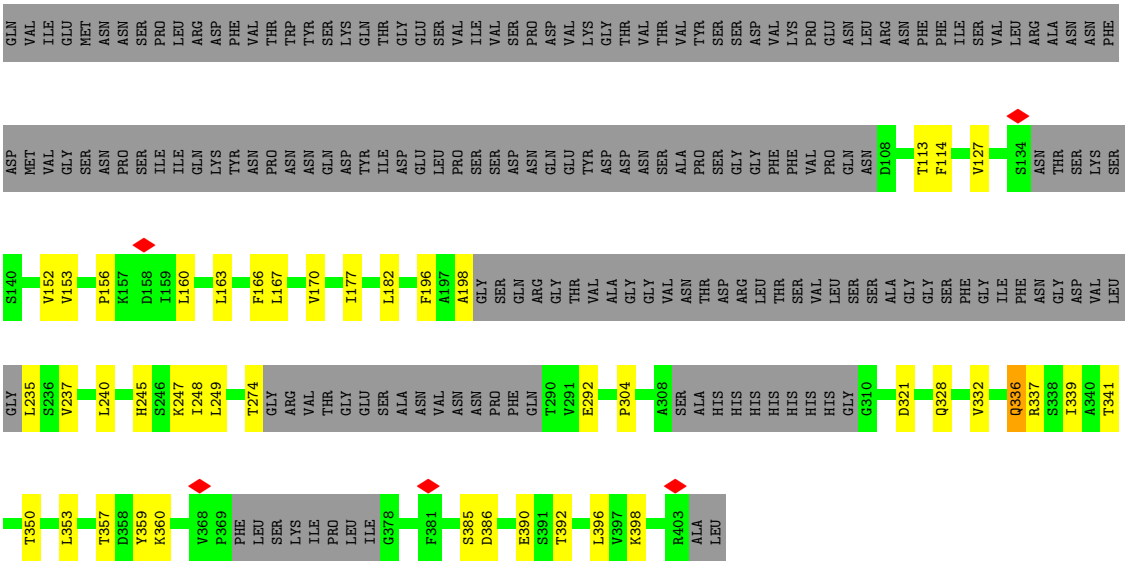




• Molecule 1: Virion export protein

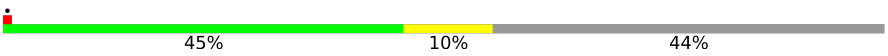
Chain I:

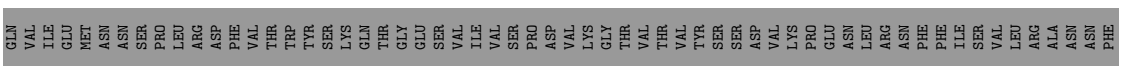


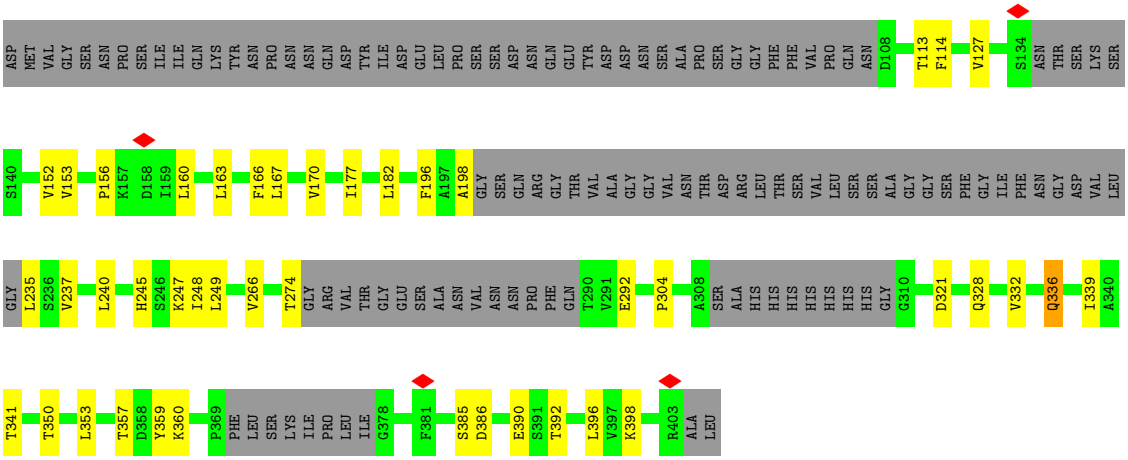


• Molecule 1: Virion export protein

Chain J:

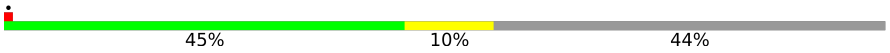


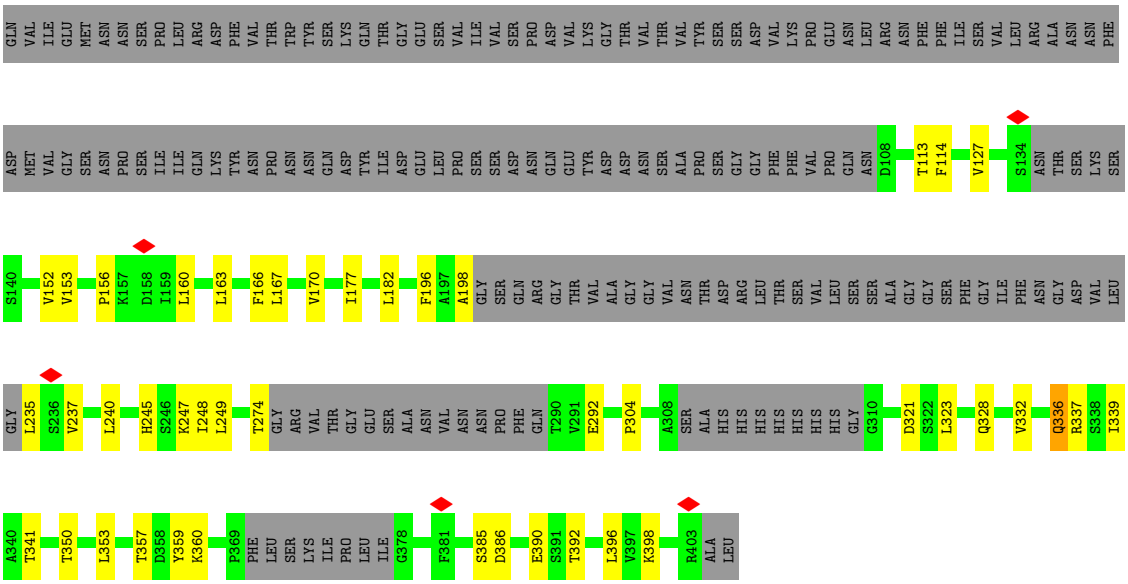




• Molecule 1: Virion export protein

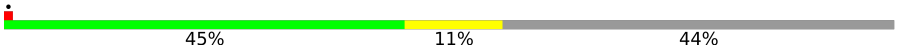
Chain K:

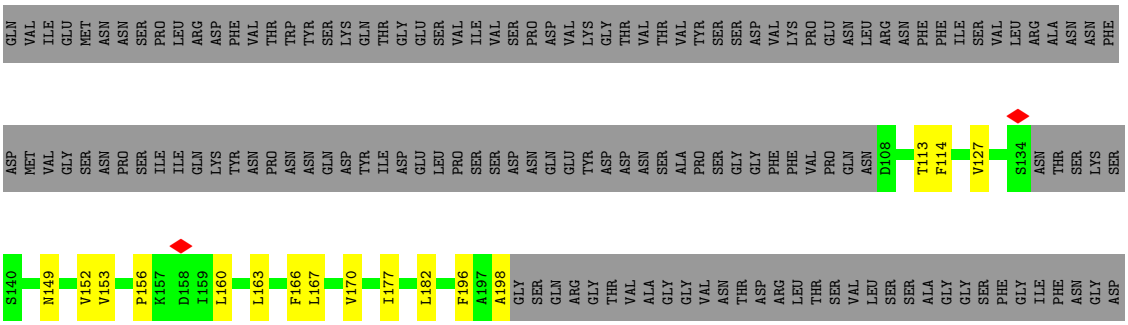


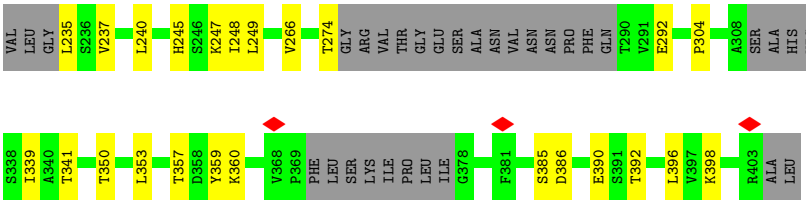


• Molecule 1: Virion export protein

Chain L:

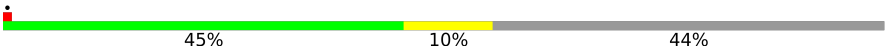


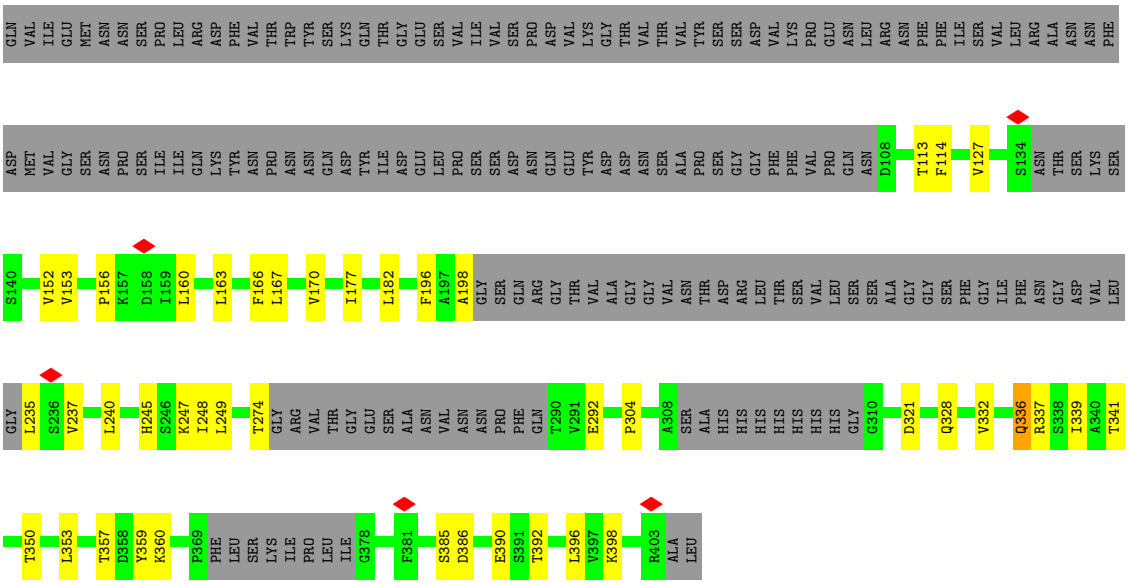




• Molecule 1: Virion export protein

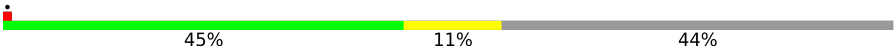
Chain M:

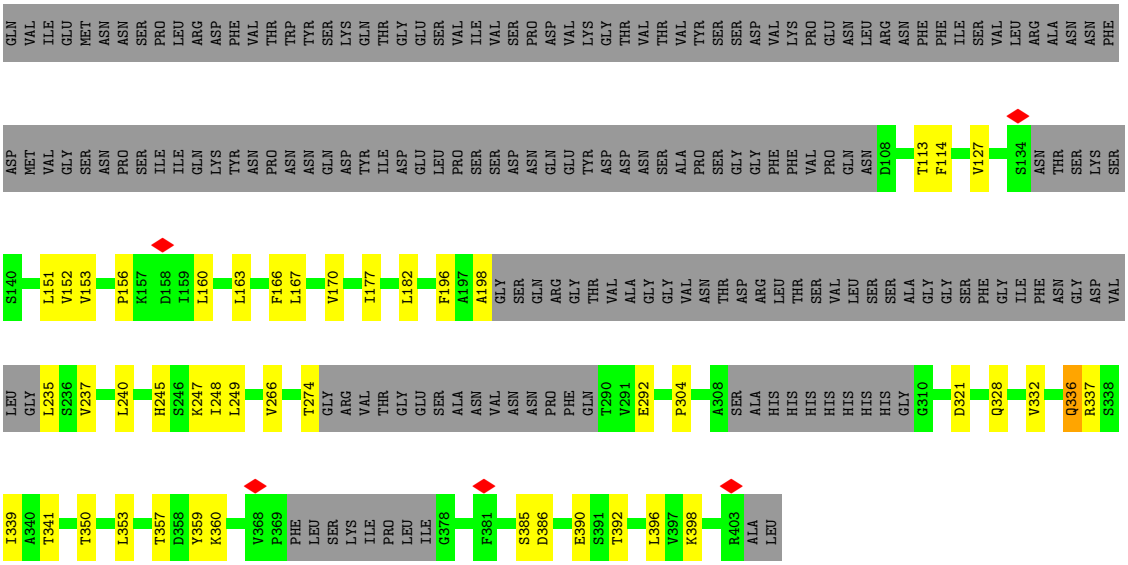




• Molecule 1: Virion export protein

Chain N:

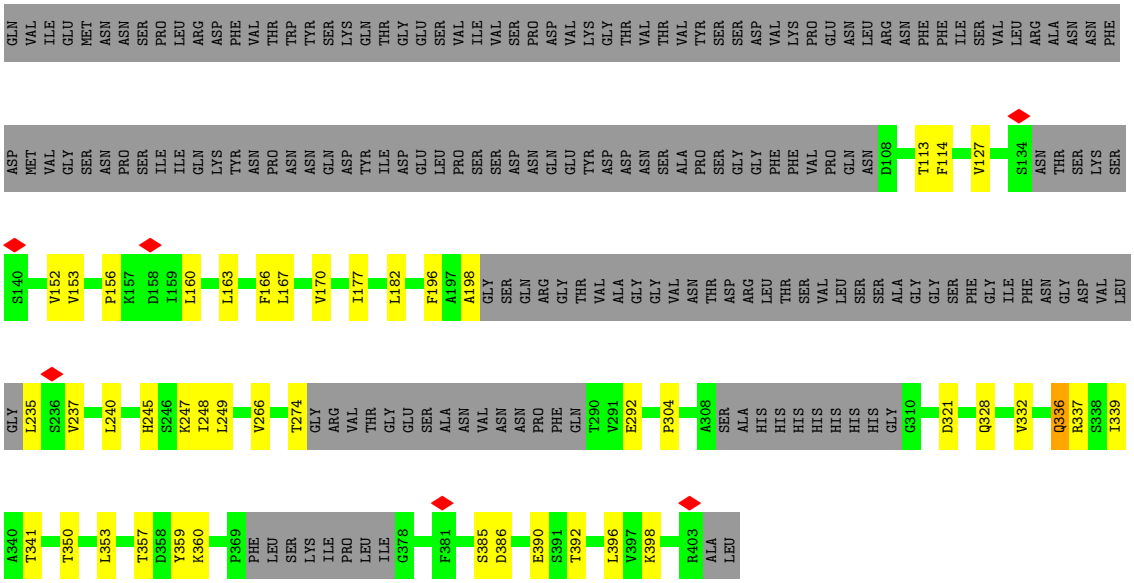




• Molecule 1: Virion export protein

Chain O:


45%
10%
44%


GLN VAL ILE GLU MET ASN ASN SER PRO LEU ARG ASP PHE VAL THR TRP TYR SER LYS GLN THR GLY GLU SER VAL ILE VAL SER PRO ASP VAL LYS GLY THR VAL THR VAL TYR SER SER ASP VAL LYS PRO GLU ASN LEU ARG ASN PHE PHE ILE SER VAL LEU ARG ALA ASN ASN PHE
ASP MET VAL GLY SER ASN PRO SER ILE ILE GLN LYS TYR ASN PRO ASN ASN GLN ASP TYR ILE ASP GLU LEU PRO SER SER ASP ASN GLN GLU TYR ASP ASP ASN SER ALA PRO SER GLY GLY PHE PHE VAL PRO GLN ASN D108 T113 F114 V127 S134 ASN THR SER LYS SER
S140 V152 V153 P156 K157 D158 I159 L160 L163 F166 L167 V170 I177 L182 F196 A197 A198 GLY SER GLN ARG GLY THR VAL ALA GLY GLY VAL ASN THR ASP ARG LEU THR SER VAL LEU SER SER ALA GLY GLY SER PHE GLY ILE PHE ASN GLY ASP VAL LEU
GLY L235 S236 V237 L240 H245 S246 K247 I248 L249 V266 T274 GLY ARG VAL THR GLY GLU SER ALA ASN VAL ASN ASN PRO PHE GLN T290 V291 E292 P304 A308 SER ALA HIS HIS HIS HIS HIS HIS HIS GLY G310 D321 Q328 V332 Q336 R337 S338 I339
A340 T341 T350 L353 T357 D358 Y359 K360 P369 PHE LEU SER LYS ILE PRO LEU ILE G378 F381 S385 D386 E390 S391 T392 L396 V397 K398 R403 ALA LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	111679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.059	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0226	Depositor
Map size (Å)	240.128, 240.128, 240.128	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CPS

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	0.47	0/1755	0.72	0/2377
1	B	0.47	0/1755	0.72	0/2377
1	C	0.48	0/1755	0.72	0/2377
1	D	0.48	0/1755	0.73	0/2377
1	E	0.48	0/1755	0.73	0/2377
1	F	0.48	0/1755	0.73	0/2377
1	G	0.48	0/1755	0.73	0/2377
1	H	0.47	0/1755	0.72	0/2377
1	I	0.47	0/1755	0.72	0/2377
1	J	0.48	0/1755	0.73	0/2377
1	K	0.48	0/1755	0.73	0/2377
1	L	0.48	0/1755	0.73	0/2377
1	M	0.48	0/1755	0.73	0/2377
1	N	0.48	0/1755	0.73	0/2377
1	O	0.48	0/1755	0.72	0/2377
All	All	0.48	0/26325	0.72	0/35655

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1742	0	1792	56	0
1	B	1742	0	1792	59	0
1	C	1742	0	1792	58	0
1	D	1742	0	1792	56	0
1	E	1742	0	1792	56	0
1	F	1742	0	1792	55	0
1	G	1742	0	1792	56	0
1	H	1742	0	1792	54	0
1	I	1742	0	1792	55	0
1	J	1742	0	1792	54	0
1	K	1742	0	1792	56	0
1	L	1742	0	1792	55	0
1	M	1742	0	1792	53	0
1	N	1742	0	1792	56	0
1	O	1742	0	1792	57	0
2	A	67	0	93	1	0
2	B	67	0	93	3	0
2	C	67	0	93	2	0
2	D	67	0	93	1	0
2	E	67	0	93	3	0
2	F	67	0	93	3	0
2	G	67	0	93	3	0
2	H	67	0	93	1	0
2	I	67	0	93	2	0
2	J	67	0	93	1	0
2	K	67	0	93	1	0
2	L	67	0	93	1	0
2	M	67	0	93	2	0
2	N	67	0	93	1	0
2	O	67	0	93	2	0
All	All	27135	0	28275	752	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (752) 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:F:341:THR:CG2	1:F:353:LEU:HD11	1.89	1.03
1:C:341:THR:CG2	1:C:353:LEU:HD11	1.89	1.03
1:O:341:THR:CG2	1:O:353:LEU:HD11	1.89	1.03
1:B:341:THR:CG2	1:B:353:LEU:HD11	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:THR:CG2	1:H:353:LEU:HD11	1.89	1.03
1:I:341:THR:CG2	1:I:353:LEU:HD11	1.89	1.03
1:N:341:THR:CG2	1:N:353:LEU:HD11	1.89	1.03
1:G:341:THR:CG2	1:G:353:LEU:HD11	1.89	1.02
1:L:341:THR:CG2	1:L:353:LEU:HD11	1.89	1.02
1:A:341:THR:CG2	1:A:353:LEU:HD11	1.89	1.02
1:E:341:THR:CG2	1:E:353:LEU:HD11	1.89	1.02
1:D:341:THR:CG2	1:D:353:LEU:HD11	1.89	1.02
1:J:341:THR:CG2	1:J:353:LEU:HD11	1.89	1.02
1:K:341:THR:CG2	1:K:353:LEU:HD11	1.89	1.02
1:M:341:THR:CG2	1:M:353:LEU:HD11	1.89	1.01
1:H:113:THR:HG22	1:H:152:VAL:HG22	1.50	0.94
1:G:113:THR:HG22	1:G:152:VAL:HG22	1.50	0.94
1:F:113:THR:HG22	1:F:152:VAL:HG22	1.49	0.93
1:A:113:THR:HG22	1:A:152:VAL:HG22	1.51	0.93
1:B:113:THR:HG22	1:B:152:VAL:HG22	1.51	0.93
1:C:113:THR:HG22	1:C:152:VAL:HG22	1.50	0.93
1:D:113:THR:HG22	1:D:152:VAL:HG22	1.49	0.92
1:O:113:THR:HG22	1:O:152:VAL:HG22	1.51	0.92
1:I:113:THR:HG22	1:I:152:VAL:HG22	1.50	0.92
1:E:113:THR:HG22	1:E:152:VAL:HG22	1.50	0.92
1:N:113:THR:HG22	1:N:152:VAL:HG22	1.50	0.91
1:K:113:THR:HG22	1:K:152:VAL:HG22	1.49	0.91
1:J:113:THR:HG22	1:J:152:VAL:HG22	1.50	0.91
1:K:359:TYR:HE1	1:K:390:GLU:HG3	1.37	0.90
1:M:113:THR:HG22	1:M:152:VAL:HG22	1.50	0.90
1:L:359:TYR:HE1	1:L:390:GLU:HG3	1.37	0.90
1:E:359:TYR:HE1	1:E:390:GLU:HG3	1.37	0.90
1:D:359:TYR:HE1	1:D:390:GLU:HG3	1.37	0.90
1:J:359:TYR:HE1	1:J:390:GLU:HG3	1.37	0.90
1:I:359:TYR:HE1	1:I:390:GLU:HG3	1.37	0.89
1:L:113:THR:HG22	1:L:152:VAL:HG22	1.50	0.89
1:M:359:TYR:HE1	1:M:390:GLU:HG3	1.37	0.89
1:G:359:TYR:HE1	1:G:390:GLU:HG3	1.37	0.89
1:C:359:TYR:HE1	1:C:390:GLU:HG3	1.37	0.89
1:F:359:TYR:HE1	1:F:390:GLU:HG3	1.37	0.89
1:H:359:TYR:HE1	1:H:390:GLU:HG3	1.37	0.89
1:B:359:TYR:HE1	1:B:390:GLU:HG3	1.36	0.89
1:N:359:TYR:HE1	1:N:390:GLU:HG3	1.37	0.88
1:O:359:TYR:HE1	1:O:390:GLU:HG3	1.37	0.88
1:A:359:TYR:HE1	1:A:390:GLU:HG3	1.37	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:321:ASP:OD1	1:L:336:GLN:HA	1.77	0.85
1:I:321:ASP:OD1	1:I:336:GLN:HA	1.77	0.85
1:M:321:ASP:OD1	1:M:336:GLN:HA	1.77	0.85
1:A:321:ASP:OD1	1:A:336:GLN:HA	1.77	0.85
1:C:321:ASP:OD1	1:C:336:GLN:HA	1.77	0.85
1:O:321:ASP:OD1	1:O:336:GLN:HA	1.77	0.85
1:D:321:ASP:OD1	1:D:336:GLN:HA	1.77	0.85
1:J:321:ASP:OD1	1:J:336:GLN:HA	1.77	0.85
1:E:321:ASP:OD1	1:E:336:GLN:HA	1.77	0.84
1:B:321:ASP:OD1	1:B:336:GLN:HA	1.77	0.84
1:F:321:ASP:OD1	1:F:336:GLN:HA	1.77	0.84
1:H:321:ASP:OD1	1:H:336:GLN:HA	1.77	0.84
1:G:321:ASP:OD1	1:G:336:GLN:HA	1.77	0.84
1:N:321:ASP:OD1	1:N:336:GLN:HA	1.77	0.83
1:K:321:ASP:OD1	1:K:336:GLN:HA	1.77	0.83
1:L:163:LEU:HD21	1:L:167:LEU:HD11	1.61	0.83
1:I:163:LEU:HD21	1:I:167:LEU:HD11	1.62	0.82
1:H:163:LEU:HD21	1:H:167:LEU:HD11	1.62	0.81
1:B:163:LEU:HD21	1:B:167:LEU:HD11	1.61	0.81
1:J:163:LEU:HD21	1:J:167:LEU:HD11	1.62	0.81
1:M:163:LEU:HD21	1:M:167:LEU:HD11	1.61	0.81
1:K:163:LEU:HD21	1:K:167:LEU:HD11	1.61	0.81
1:D:163:LEU:HD21	1:D:167:LEU:HD11	1.62	0.80
1:N:163:LEU:HD21	1:N:167:LEU:HD11	1.61	0.80
1:F:163:LEU:HD21	1:F:167:LEU:HD11	1.61	0.80
1:E:163:LEU:HD21	1:E:167:LEU:HD11	1.61	0.80
1:G:163:LEU:HD21	1:G:167:LEU:HD11	1.61	0.80
1:O:163:LEU:HD21	1:O:167:LEU:HD11	1.61	0.79
1:A:163:LEU:HD21	1:A:167:LEU:HD11	1.62	0.79
1:C:163:LEU:HD21	1:C:167:LEU:HD11	1.62	0.78
1:O:359:TYR:CE1	1:O:390:GLU:HG3	2.23	0.74
1:B:359:TYR:CE1	1:B:390:GLU:HG3	2.23	0.73
1:J:359:TYR:CE1	1:J:390:GLU:HG3	2.23	0.73
1:N:350:THR:HG22	1:N:398:LYS:HB2	1.71	0.73
1:H:359:TYR:CE1	1:H:390:GLU:HG3	2.23	0.73
1:D:359:TYR:CE1	1:D:390:GLU:HG3	2.23	0.73
1:F:359:TYR:CE1	1:F:390:GLU:HG3	2.23	0.73
1:K:341:THR:HG21	1:K:353:LEU:HD11	1.71	0.73
1:L:359:TYR:CE1	1:L:390:GLU:HG3	2.23	0.73
1:M:341:THR:HG22	1:M:353:LEU:HD11	1.71	0.73
1:A:350:THR:HG22	1:A:398:LYS:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:THR:HG22	1:H:353:LEU:HD11	1.71	0.72
1:B:341:THR:CG2	1:B:353:LEU:CD1	2.68	0.72
1:L:341:THR:HG21	1:L:353:LEU:CD1	2.19	0.72
1:I:341:THR:HG22	1:I:353:LEU:HD11	1.72	0.72
1:O:350:THR:HG22	1:O:398:LYS:HB2	1.71	0.72
1:F:341:THR:HG21	1:F:353:LEU:CD1	2.19	0.72
1:J:341:THR:HG21	1:J:353:LEU:HD11	1.72	0.72
1:B:341:THR:HG21	1:B:353:LEU:HD11	1.72	0.72
1:F:341:THR:CG2	1:F:353:LEU:CD1	2.67	0.72
1:G:341:THR:HG21	1:G:353:LEU:CD1	2.19	0.72
1:J:341:THR:HG21	1:J:353:LEU:CD1	2.19	0.72
1:J:341:THR:HG22	1:J:353:LEU:HD11	1.72	0.72
1:C:341:THR:HG21	1:C:353:LEU:CD1	2.20	0.72
1:L:341:THR:HG22	1:L:353:LEU:HD11	1.72	0.72
1:N:341:THR:HG21	1:N:353:LEU:CD1	2.20	0.72
1:B:163:LEU:HD21	1:B:167:LEU:CD1	2.19	0.72
1:K:341:THR:HG21	1:K:353:LEU:CD1	2.19	0.72
1:K:341:THR:HG22	1:K:353:LEU:HD11	1.72	0.72
1:B:350:THR:HG22	1:B:398:LYS:HB2	1.71	0.72
1:C:341:THR:HG21	1:C:353:LEU:HD11	1.72	0.72
1:D:341:THR:CG2	1:D:353:LEU:CD1	2.68	0.72
1:D:341:THR:HG21	1:D:353:LEU:CD1	2.20	0.72
1:E:341:THR:HG21	1:E:353:LEU:CD1	2.19	0.72
1:C:350:THR:HG22	1:C:398:LYS:HB2	1.71	0.72
1:I:341:THR:CG2	1:I:353:LEU:CD1	2.68	0.72
1:G:341:THR:HG22	1:G:353:LEU:HD11	1.72	0.72
1:L:341:THR:HG21	1:L:353:LEU:HD11	1.72	0.72
1:N:341:THR:HG22	1:N:353:LEU:HD11	1.72	0.72
1:A:341:THR:HG21	1:A:353:LEU:HD11	1.72	0.71
1:I:341:THR:HG21	1:I:353:LEU:CD1	2.19	0.71
1:O:341:THR:HG21	1:O:353:LEU:HD11	1.71	0.71
1:D:341:THR:HG21	1:D:353:LEU:HD11	1.71	0.71
1:F:341:THR:HG22	1:F:353:LEU:HD11	1.71	0.71
1:M:163:LEU:HD21	1:M:167:LEU:CD1	2.19	0.71
1:I:341:THR:HG21	1:I:353:LEU:HD11	1.72	0.71
1:O:341:THR:HG21	1:O:353:LEU:CD1	2.19	0.71
1:B:341:THR:HG21	1:B:353:LEU:CD1	2.19	0.71
1:E:245:HIS:NE2	1:E:247:LYS:HE3	2.06	0.71
1:H:350:THR:HG22	1:H:398:LYS:HB2	1.71	0.71
1:D:245:HIS:NE2	1:D:247:LYS:HE3	2.06	0.71
1:L:163:LEU:HD21	1:L:167:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:341:THR:CG2	1:N:353:LEU:CD1	2.68	0.71
1:N:359:TYR:CE1	1:N:390:GLU:HG3	2.23	0.71
1:F:245:HIS:NE2	1:F:247:LYS:HE3	2.06	0.71
1:O:341:THR:HG22	1:O:353:LEU:HD11	1.72	0.71
1:C:245:HIS:NE2	1:C:247:LYS:HE3	2.06	0.71
1:H:245:HIS:NE2	1:H:247:LYS:HE3	2.06	0.71
1:J:163:LEU:HD21	1:J:167:LEU:CD1	2.21	0.71
1:M:341:THR:HG21	1:M:353:LEU:CD1	2.19	0.71
1:D:153:VAL:HG23	1:D:160:LEU:HD21	1.73	0.71
1:H:341:THR:CG2	1:H:353:LEU:CD1	2.68	0.71
1:A:341:THR:CG2	1:A:353:LEU:CD1	2.68	0.71
1:E:350:THR:HG22	1:E:398:LYS:HB2	1.71	0.71
1:L:341:THR:CG2	1:L:353:LEU:CD1	2.68	0.71
1:A:341:THR:HG21	1:A:353:LEU:CD1	2.20	0.71
1:E:341:THR:HG21	1:E:353:LEU:HD11	1.71	0.71
1:F:350:THR:HG22	1:F:398:LYS:HB2	1.71	0.71
1:G:245:HIS:NE2	1:G:247:LYS:HE3	2.06	0.71
1:H:341:THR:HG21	1:H:353:LEU:CD1	2.19	0.71
1:L:350:THR:HG22	1:L:398:LYS:HB2	1.72	0.71
1:A:245:HIS:NE2	1:A:247:LYS:HE3	2.06	0.70
1:C:153:VAL:HG23	1:C:160:LEU:HD21	1.73	0.70
1:C:163:LEU:HD21	1:C:167:LEU:CD1	2.21	0.70
1:G:350:THR:HG22	1:G:398:LYS:HB2	1.71	0.70
1:J:350:THR:HG22	1:J:398:LYS:HB2	1.71	0.70
1:M:350:THR:HG22	1:M:398:LYS:HB2	1.73	0.70
1:N:163:LEU:HD21	1:N:167:LEU:CD1	2.20	0.70
1:A:359:TYR:CE1	1:A:390:GLU:HG3	2.23	0.70
1:B:245:HIS:NE2	1:B:247:LYS:HE3	2.06	0.70
1:I:163:LEU:HD21	1:I:167:LEU:CD1	2.21	0.70
1:I:245:HIS:NE2	1:I:247:LYS:HE3	2.06	0.70
1:A:153:VAL:HG23	1:A:160:LEU:HD21	1.73	0.70
1:A:341:THR:HG22	1:A:353:LEU:HD11	1.71	0.70
1:I:350:THR:HG22	1:I:398:LYS:HB2	1.71	0.70
1:L:245:HIS:NE2	1:L:247:LYS:HE3	2.06	0.70
1:C:341:THR:CG2	1:C:353:LEU:CD1	2.68	0.70
1:D:163:LEU:HD21	1:D:167:LEU:CD1	2.21	0.70
1:J:341:THR:CG2	1:J:353:LEU:CD1	2.68	0.70
1:I:359:TYR:CE1	1:I:390:GLU:HG3	2.23	0.70
1:O:153:VAL:HG23	1:O:160:LEU:HD21	1.73	0.70
1:O:163:LEU:HD21	1:O:167:LEU:CD1	2.20	0.70
1:A:163:LEU:HD21	1:A:167:LEU:CD1	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:TYR:CE1	1:G:390:GLU:HG3	2.23	0.70
1:K:341:THR:CG2	1:K:353:LEU:CD1	2.68	0.70
1:B:153:VAL:HG23	1:B:160:LEU:HD21	1.74	0.70
1:E:341:THR:HG22	1:E:353:LEU:HD11	1.72	0.70
1:G:163:LEU:HD21	1:G:167:LEU:CD1	2.21	0.70
1:M:245:HIS:NE2	1:M:247:LYS:HE3	2.06	0.70
1:D:350:THR:HG22	1:D:398:LYS:HB2	1.71	0.70
1:C:359:TYR:CE1	1:C:390:GLU:HG3	2.23	0.70
1:J:245:HIS:NE2	1:J:247:LYS:HE3	2.06	0.70
1:O:245:HIS:NE2	1:O:247:LYS:HE3	2.06	0.70
1:K:359:TYR:CE1	1:K:390:GLU:HG3	2.23	0.70
1:L:153:VAL:HG23	1:L:160:LEU:HD21	1.74	0.70
1:M:359:TYR:CE1	1:M:390:GLU:HG3	2.23	0.70
1:N:245:HIS:NE2	1:N:247:LYS:HE3	2.06	0.70
1:K:245:HIS:NE2	1:K:247:LYS:HE3	2.06	0.69
1:M:153:VAL:HG23	1:M:160:LEU:HD21	1.74	0.69
1:B:341:THR:HG22	1:B:353:LEU:HD11	1.72	0.69
1:E:359:TYR:CE1	1:E:390:GLU:HG3	2.23	0.69
1:F:153:VAL:HG23	1:F:160:LEU:HD21	1.74	0.69
1:D:341:THR:HG22	1:D:353:LEU:HD11	1.72	0.69
1:F:163:LEU:HD21	1:F:167:LEU:CD1	2.21	0.69
1:G:153:VAL:HG23	1:G:160:LEU:HD21	1.73	0.69
1:C:341:THR:HG22	1:C:353:LEU:HD11	1.72	0.69
1:E:153:VAL:HG23	1:E:160:LEU:HD21	1.74	0.69
1:H:163:LEU:HD21	1:H:167:LEU:CD1	2.22	0.69
1:K:163:LEU:HD21	1:K:167:LEU:CD1	2.21	0.69
1:E:163:LEU:HD21	1:E:167:LEU:CD1	2.21	0.69
1:K:350:THR:HG22	1:K:398:LYS:HB2	1.72	0.69
1:G:341:THR:CG2	1:G:353:LEU:CD1	2.68	0.69
1:K:153:VAL:HG23	1:K:160:LEU:HD21	1.75	0.69
1:N:153:VAL:HG23	1:N:160:LEU:HD21	1.75	0.69
1:M:341:THR:CG2	1:M:353:LEU:CD1	2.68	0.69
1:J:153:VAL:HG23	1:J:160:LEU:HD21	1.74	0.68
1:I:153:VAL:HG23	1:I:160:LEU:HD21	1.75	0.68
1:O:341:THR:CG2	1:O:353:LEU:CD1	2.68	0.68
1:L:274:THR:HG21	1:L:292:GLU:OE1	1.94	0.68
1:C:274:THR:HG21	1:C:292:GLU:OE1	1.94	0.68
1:M:274:THR:HG21	1:M:292:GLU:OE1	1.94	0.68
1:B:274:THR:HG21	1:B:292:GLU:OE1	1.94	0.68
1:D:274:THR:HG21	1:D:292:GLU:OE1	1.94	0.68
1:H:153:VAL:HG23	1:H:160:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:THR:HG21	1:E:292:GLU:OE1	1.94	0.67
1:H:341:THR:HG21	1:H:353:LEU:HD11	1.72	0.67
1:N:274:THR:HG21	1:N:292:GLU:OE1	1.94	0.67
1:K:274:THR:HG21	1:K:292:GLU:OE1	1.94	0.67
1:F:274:THR:HG21	1:F:292:GLU:OE1	1.94	0.67
1:H:274:THR:HG21	1:H:292:GLU:OE1	1.94	0.67
1:G:274:THR:HG21	1:G:292:GLU:OE1	1.94	0.67
1:I:274:THR:HG21	1:I:292:GLU:OE1	1.94	0.67
1:J:274:THR:HG21	1:J:292:GLU:OE1	1.94	0.67
1:E:341:THR:CG2	1:E:353:LEU:CD1	2.68	0.66
1:G:170:VAL:HG22	1:H:113:THR:HG21	1.77	0.66
1:G:341:THR:HG21	1:G:353:LEU:HD11	1.72	0.66
1:A:274:THR:HG21	1:A:292:GLU:OE1	1.94	0.66
1:H:274:THR:HG21	1:H:292:GLU:CD	2.16	0.66
1:O:274:THR:HG21	1:O:292:GLU:OE1	1.94	0.66
1:A:274:THR:HG21	1:A:292:GLU:CD	2.16	0.66
1:G:274:THR:HG21	1:G:292:GLU:CD	2.16	0.66
1:M:274:THR:HG21	1:M:292:GLU:CD	2.16	0.66
1:O:274:THR:HG21	1:O:292:GLU:CD	2.16	0.66
1:I:274:THR:HG21	1:I:292:GLU:CD	2.16	0.66
1:N:360:LYS:HG3	1:O:248:ILE:CD1	2.25	0.66
1:E:127:VAL:HG11	1:E:170:VAL:HG11	1.77	0.66
1:E:170:VAL:HG22	1:F:113:THR:HG21	1.78	0.66
1:N:274:THR:HG21	1:N:292:GLU:CD	2.16	0.66
1:D:274:THR:HG21	1:D:292:GLU:CD	2.16	0.65
1:F:170:VAL:HG22	1:G:113:THR:HG21	1.77	0.65
1:J:127:VAL:HG11	1:J:170:VAL:HG11	1.78	0.65
1:J:274:THR:HG21	1:J:292:GLU:CD	2.16	0.65
1:L:274:THR:HG21	1:L:292:GLU:CD	2.15	0.65
1:E:274:THR:HG21	1:E:292:GLU:CD	2.16	0.65
1:K:274:THR:HG21	1:K:292:GLU:CD	2.16	0.65
1:B:274:THR:HG21	1:B:292:GLU:CD	2.16	0.65
1:F:274:THR:HG21	1:F:292:GLU:CD	2.16	0.65
1:J:170:VAL:HG22	1:K:113:THR:HG21	1.78	0.65
1:I:170:VAL:HG22	1:J:113:THR:HG21	1.79	0.65
1:C:274:THR:HG21	1:C:292:GLU:CD	2.16	0.65
1:M:163:LEU:CD2	1:M:167:LEU:CD1	2.75	0.65
1:B:360:LYS:HG3	1:C:248:ILE:CD1	2.27	0.65
1:E:360:LYS:HG3	1:F:248:ILE:CD1	2.26	0.65
1:K:170:VAL:HG22	1:L:113:THR:HG21	1.79	0.65
1:H:170:VAL:HG22	1:I:113:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:VAL:HG11	1:I:170:VAL:HG11	1.79	0.64
1:J:360:LYS:HG3	1:K:248:ILE:CD1	2.27	0.64
1:H:360:LYS:HG3	1:I:248:ILE:CD1	2.28	0.64
1:N:163:LEU:CD2	1:N:167:LEU:CD1	2.76	0.64
1:B:163:LEU:CD2	1:B:167:LEU:CD1	2.75	0.64
1:A:360:LYS:HG3	1:B:248:ILE:CD1	2.28	0.64
1:G:360:LYS:HG3	1:H:248:ILE:CD1	2.28	0.64
1:L:127:VAL:HG11	1:L:170:VAL:HG11	1.80	0.64
1:D:360:LYS:HG3	1:E:248:ILE:CD1	2.28	0.64
1:C:360:LYS:HG3	1:D:248:ILE:CD1	2.28	0.64
1:F:360:LYS:HG3	1:G:248:ILE:CD1	2.28	0.64
1:L:163:LEU:CD2	1:L:167:LEU:CD1	2.76	0.64
1:A:113:THR:HG21	1:O:170:VAL:HG22	1.79	0.63
1:F:163:LEU:CD2	1:F:167:LEU:CD1	2.77	0.63
1:M:360:LYS:HG3	1:N:248:ILE:CD1	2.27	0.63
1:O:163:LEU:CD2	1:O:167:LEU:CD1	2.76	0.63
1:A:248:ILE:CD1	1:O:360:LYS:HG3	2.28	0.63
1:G:163:LEU:CD2	1:G:167:LEU:CD1	2.77	0.63
1:M:163:LEU:HD23	1:M:167:LEU:HD12	1.81	0.63
1:K:360:LYS:HG3	1:L:248:ILE:CD1	2.28	0.63
1:I:360:LYS:HG3	1:J:248:ILE:CD1	2.28	0.63
1:L:360:LYS:HG3	1:M:248:ILE:CD1	2.27	0.63
1:I:163:LEU:CD2	1:I:167:LEU:CD1	2.76	0.63
1:M:170:VAL:HG22	1:N:113:THR:HG21	1.79	0.63
1:N:170:VAL:HG22	1:O:113:THR:HG21	1.78	0.63
1:J:163:LEU:CD2	1:J:167:LEU:CD1	2.76	0.63
1:H:163:LEU:CD2	1:H:167:LEU:CD1	2.77	0.62
1:B:163:LEU:HD23	1:B:167:LEU:HD12	1.80	0.62
1:C:163:LEU:CD2	1:C:167:LEU:CD1	2.77	0.62
1:C:170:VAL:HG22	1:D:113:THR:HG21	1.80	0.62
1:J:163:LEU:HD23	1:J:167:LEU:HD12	1.82	0.62
1:A:163:LEU:CD2	1:A:167:LEU:CD1	2.76	0.62
1:E:163:LEU:CD2	1:E:167:LEU:CD1	2.77	0.62
1:K:163:LEU:CD2	1:K:167:LEU:CD1	2.77	0.62
1:B:127:VAL:HG11	1:B:170:VAL:HG11	1.81	0.62
1:D:170:VAL:HG22	1:E:113:THR:HG21	1.79	0.62
1:K:127:VAL:HG11	1:K:170:VAL:HG11	1.82	0.62
1:D:163:LEU:CD2	1:D:167:LEU:CD1	2.76	0.62
1:G:127:VAL:HG11	1:G:170:VAL:HG11	1.80	0.62
1:N:360:LYS:HG3	1:O:248:ILE:HD13	1.81	0.62
1:I:163:LEU:HD23	1:I:167:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:163:LEU:HD23	1:N:167:LEU:HD12	1.82	0.62
1:B:170:VAL:HG22	1:C:113:THR:HG21	1.80	0.62
1:F:127:VAL:HG11	1:F:170:VAL:HG11	1.81	0.62
1:B:163:LEU:CD2	1:B:167:LEU:HD12	2.30	0.62
1:M:163:LEU:CD2	1:M:167:LEU:HD12	2.30	0.61
1:L:360:LYS:HG3	1:M:248:ILE:HD13	1.82	0.61
1:A:170:VAL:HG22	1:B:113:THR:HG21	1.81	0.61
1:L:170:VAL:HG22	1:M:113:THR:HG21	1.80	0.61
1:M:127:VAL:HG11	1:M:170:VAL:HG11	1.82	0.61
1:M:360:LYS:HG3	1:N:248:ILE:HD13	1.82	0.61
1:L:163:LEU:HD23	1:L:167:LEU:HD12	1.82	0.61
1:O:163:LEU:HD23	1:O:167:LEU:HD12	1.82	0.61
1:A:163:LEU:HD23	1:A:167:LEU:HD12	1.82	0.60
1:D:163:LEU:HD23	1:D:167:LEU:HD12	1.82	0.60
1:K:360:LYS:HG3	1:L:248:ILE:HD13	1.82	0.60
1:C:163:LEU:HD23	1:C:167:LEU:HD12	1.83	0.60
1:K:163:LEU:HD23	1:K:167:LEU:HD12	1.83	0.60
1:J:360:LYS:HG3	1:K:248:ILE:HD13	1.83	0.60
1:A:163:LEU:CD2	1:A:167:LEU:HD12	2.32	0.60
1:F:163:LEU:HD23	1:F:167:LEU:HD12	1.83	0.60
1:N:163:LEU:CD2	1:N:167:LEU:HD12	2.32	0.60
1:O:163:LEU:CD2	1:O:167:LEU:HD12	2.32	0.60
1:A:360:LYS:HG3	1:B:248:ILE:HD13	1.83	0.60
1:G:163:LEU:HD23	1:G:167:LEU:HD12	1.83	0.60
1:I:163:LEU:CD2	1:I:167:LEU:HD12	2.32	0.60
1:J:163:LEU:CD2	1:J:167:LEU:HD12	2.32	0.60
1:D:127:VAL:HG11	1:D:170:VAL:HG11	1.83	0.59
1:H:163:LEU:HD23	1:H:167:LEU:HD12	1.83	0.59
1:E:163:LEU:HD23	1:E:167:LEU:HD12	1.84	0.59
1:E:360:LYS:HG3	1:F:248:ILE:HD13	1.83	0.59
1:D:163:LEU:CD2	1:D:167:LEU:HD12	2.32	0.59
1:C:163:LEU:CD2	1:C:167:LEU:HD12	2.33	0.59
1:B:360:LYS:HG3	1:C:248:ILE:HD13	1.84	0.58
1:F:360:LYS:HG3	1:G:248:ILE:HD13	1.83	0.58
1:A:248:ILE:HD13	1:O:360:LYS:HG3	1.84	0.58
1:H:360:LYS:HG3	1:I:248:ILE:HD13	1.84	0.58
1:H:127:VAL:HG11	1:H:170:VAL:HG11	1.84	0.58
1:I:360:LYS:HG3	1:J:248:ILE:HD13	1.84	0.58
1:A:127:VAL:HG11	1:A:170:VAL:HG11	1.86	0.58
1:K:163:LEU:CD2	1:K:167:LEU:HD12	2.34	0.58
1:L:163:LEU:CD2	1:L:167:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LYS:HG3	1:E:248:ILE:HD13	1.85	0.58
1:F:341:THR:HG21	1:F:353:LEU:HD11	1.72	0.58
1:G:360:LYS:HG3	1:H:248:ILE:HD13	1.84	0.57
1:N:127:VAL:HG11	1:N:170:VAL:HG11	1.85	0.57
1:C:360:LYS:HG3	1:D:248:ILE:HD13	1.85	0.57
1:F:163:LEU:CD2	1:F:167:LEU:HD12	2.34	0.57
1:G:163:LEU:CD2	1:G:167:LEU:HD12	2.34	0.57
1:O:127:VAL:HG11	1:O:170:VAL:HG11	1.87	0.57
1:H:163:LEU:CD2	1:H:167:LEU:HD12	2.35	0.56
1:C:153:VAL:CG2	1:C:160:LEU:CD2	2.84	0.56
1:D:153:VAL:CG2	1:D:160:LEU:CD2	2.83	0.56
1:E:163:LEU:CD2	1:E:167:LEU:HD12	2.35	0.56
1:E:385:SER:O	1:E:386:ASP:OD1	2.24	0.56
1:A:153:VAL:CG2	1:A:160:LEU:CD2	2.84	0.56
1:O:153:VAL:CG2	1:O:160:LEU:CD2	2.84	0.56
1:B:153:VAL:CG2	1:B:160:LEU:CD2	2.84	0.56
1:F:385:SER:O	1:F:386:ASP:OD1	2.24	0.56
1:H:385:SER:O	1:H:386:ASP:OD1	2.24	0.56
1:I:385:SER:O	1:I:386:ASP:OD1	2.24	0.56
1:M:385:SER:O	1:M:386:ASP:OD1	2.24	0.56
1:L:385:SER:O	1:L:386:ASP:OD1	2.24	0.56
1:A:385:SER:O	1:A:386:ASP:OD1	2.24	0.56
1:G:385:SER:O	1:G:386:ASP:OD1	2.24	0.56
1:J:359:TYR:HE1	1:J:390:GLU:CG	2.16	0.56
1:G:153:VAL:CG2	1:G:160:LEU:CD2	2.84	0.56
1:J:153:VAL:HG23	1:J:160:LEU:CD2	2.36	0.56
1:O:385:SER:O	1:O:386:ASP:OD1	2.24	0.56
1:B:385:SER:O	1:B:386:ASP:OD1	2.24	0.56
1:J:385:SER:O	1:J:386:ASP:OD1	2.24	0.56
1:K:385:SER:O	1:K:386:ASP:OD1	2.24	0.56
1:N:385:SER:O	1:N:386:ASP:OD1	2.24	0.56
1:D:385:SER:O	1:D:386:ASP:OD1	2.24	0.55
1:J:153:VAL:CG2	1:J:160:LEU:CD2	2.84	0.55
1:C:385:SER:O	1:C:386:ASP:OD1	2.24	0.55
1:I:153:VAL:HG23	1:I:160:LEU:CD2	2.36	0.55
1:N:153:VAL:CG2	1:N:160:LEU:CD2	2.84	0.55
1:E:153:VAL:CG2	1:E:160:LEU:CD2	2.84	0.55
1:H:153:VAL:HG23	1:H:160:LEU:CD2	2.36	0.55
1:H:153:VAL:CG2	1:H:160:LEU:CD2	2.84	0.55
1:I:153:VAL:CG2	1:I:160:LEU:CD2	2.84	0.55
1:K:153:VAL:HG23	1:K:160:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:VAL:HG13	1:F:152:VAL:HG21	1.88	0.55
1:J:127:VAL:HG13	1:K:152:VAL:HG21	1.89	0.55
1:C:127:VAL:HG11	1:C:170:VAL:HG11	1.88	0.55
1:C:153:VAL:HG23	1:C:160:LEU:CD2	2.36	0.55
1:K:153:VAL:CG2	1:K:160:LEU:CD2	2.84	0.55
1:O:153:VAL:HG23	1:O:160:LEU:CD2	2.36	0.55
1:A:152:VAL:HG21	1:O:127:VAL:HG13	1.88	0.55
1:A:357:THR:HG22	1:A:392:THR:OG1	2.07	0.55
1:M:153:VAL:CG2	1:M:160:LEU:CD2	2.84	0.55
1:D:127:VAL:HG13	1:E:152:VAL:HG21	1.89	0.55
1:G:153:VAL:HG23	1:G:160:LEU:CD2	2.36	0.55
1:L:153:VAL:CG2	1:L:160:LEU:CD2	2.84	0.55
1:E:153:VAL:HG23	1:E:160:LEU:CD2	2.36	0.55
1:F:153:VAL:HG23	1:F:160:LEU:CD2	2.36	0.55
1:H:359:TYR:HE1	1:H:390:GLU:CG	2.16	0.55
1:A:359:TYR:HE1	1:A:390:GLU:CG	2.16	0.54
1:C:357:THR:HG22	1:C:392:THR:OG1	2.08	0.54
1:L:153:VAL:HG23	1:L:160:LEU:CD2	2.36	0.54
1:D:153:VAL:HG23	1:D:160:LEU:CD2	2.36	0.54
1:F:153:VAL:CG2	1:F:160:LEU:CD2	2.84	0.54
1:B:127:VAL:HG13	1:C:152:VAL:HG21	1.89	0.54
1:D:357:THR:HG22	1:D:392:THR:OG1	2.07	0.54
1:F:127:VAL:HG13	1:G:152:VAL:HG21	1.89	0.54
1:D:237:VAL:O	1:D:237:VAL:HG23	2.07	0.54
1:N:127:VAL:HG13	1:O:152:VAL:HG21	1.90	0.54
1:B:153:VAL:HG23	1:B:160:LEU:CD2	2.37	0.54
1:G:127:VAL:HG13	1:H:152:VAL:HG21	1.90	0.54
1:A:153:VAL:HG23	1:A:160:LEU:CD2	2.37	0.54
1:O:357:THR:HG22	1:O:392:THR:OG1	2.07	0.54
1:M:153:VAL:HG23	1:M:160:LEU:CD2	2.36	0.54
1:B:237:VAL:HG23	1:B:237:VAL:O	2.08	0.54
1:H:357:THR:HG22	1:H:392:THR:OG1	2.08	0.54
1:I:357:THR:HG22	1:I:392:THR:OG1	2.08	0.54
1:B:357:THR:HG22	1:B:392:THR:OG1	2.08	0.54
1:F:359:TYR:HE1	1:F:390:GLU:CG	2.16	0.53
1:L:357:THR:HG22	1:L:392:THR:OG1	2.08	0.53
1:M:127:VAL:HG13	1:N:152:VAL:HG21	1.90	0.53
1:G:357:THR:HG22	1:G:392:THR:OG1	2.08	0.53
1:L:127:VAL:HG13	1:M:152:VAL:HG21	1.90	0.53
1:M:237:VAL:HG23	1:M:237:VAL:O	2.08	0.53
1:M:357:THR:HG22	1:M:392:THR:OG1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:153:VAL:HG23	1:N:160:LEU:CD2	2.36	0.53
1:K:357:THR:HG22	1:K:392:THR:OG1	2.08	0.53
1:I:127:VAL:HG13	1:J:152:VAL:HG21	1.91	0.53
1:I:196:PHE:O	1:I:196:PHE:CD2	2.61	0.53
1:J:357:THR:HG22	1:J:392:THR:OG1	2.09	0.53
1:N:357:THR:HG22	1:N:392:THR:OG1	2.08	0.53
1:H:127:VAL:HG13	1:I:152:VAL:HG21	1.91	0.53
1:I:237:VAL:HG23	1:I:237:VAL:O	2.08	0.53
1:K:127:VAL:HG13	1:L:152:VAL:HG21	1.91	0.53
1:L:196:PHE:CD2	1:L:196:PHE:O	2.61	0.53
1:O:196:PHE:O	1:O:196:PHE:CD2	2.62	0.53
1:F:357:THR:HG22	1:F:392:THR:OG1	2.08	0.53
1:E:357:THR:HG22	1:E:392:THR:OG1	2.08	0.53
1:K:196:PHE:O	1:K:196:PHE:CD2	2.62	0.53
1:A:196:PHE:O	1:A:196:PHE:CD2	2.62	0.53
1:E:196:PHE:CD2	1:E:196:PHE:O	2.61	0.53
1:A:127:VAL:HG13	1:B:152:VAL:HG21	1.90	0.53
1:C:237:VAL:HG23	1:C:237:VAL:O	2.09	0.53
1:D:196:PHE:O	1:D:196:PHE:CD2	2.62	0.53
1:G:196:PHE:CD2	1:G:196:PHE:O	2.62	0.53
1:N:196:PHE:O	1:N:196:PHE:CD2	2.62	0.53
1:B:196:PHE:CD2	1:B:196:PHE:O	2.61	0.53
1:J:196:PHE:CD2	1:J:196:PHE:O	2.62	0.53
1:L:237:VAL:HG23	1:L:237:VAL:O	2.08	0.53
1:C:196:PHE:O	1:C:196:PHE:CD2	2.62	0.52
1:E:237:VAL:HG23	1:E:237:VAL:O	2.08	0.52
1:F:237:VAL:HG23	1:F:237:VAL:O	2.08	0.52
1:N:237:VAL:HG23	1:N:237:VAL:O	2.09	0.52
1:H:196:PHE:O	1:H:196:PHE:CD2	2.62	0.52
1:H:237:VAL:HG23	1:H:237:VAL:O	2.08	0.52
1:K:359:TYR:HE1	1:K:390:GLU:CG	2.16	0.52
1:M:196:PHE:O	1:M:196:PHE:CD2	2.61	0.52
1:A:237:VAL:HG23	1:A:237:VAL:O	2.09	0.52
1:D:153:VAL:CG2	1:D:160:LEU:HD21	2.38	0.52
1:D:359:TYR:HE1	1:D:390:GLU:CG	2.16	0.52
1:F:196:PHE:O	1:F:196:PHE:CD2	2.62	0.52
1:O:359:TYR:HE1	1:O:390:GLU:CG	2.16	0.52
1:F:153:VAL:CG2	1:F:160:LEU:HD21	2.39	0.52
1:C:127:VAL:HG13	1:D:152:VAL:HG21	1.91	0.52
1:L:341:THR:HG21	1:L:353:LEU:HD12	1.92	0.52
1:M:359:TYR:HE1	1:M:390:GLU:CG	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:VAL:CG2	1:O:113:THR:HG21	2.40	0.52
1:N:359:TYR:HD2	1:O:249:LEU:HD23	1.75	0.52
1:C:153:VAL:CG2	1:C:160:LEU:HD21	2.39	0.52
1:G:237:VAL:HG23	1:G:237:VAL:O	2.09	0.52
1:K:359:TYR:HD2	1:L:249:LEU:HD23	1.75	0.52
1:A:153:VAL:CG2	1:A:160:LEU:HD21	2.38	0.52
1:E:153:VAL:CG2	1:E:160:LEU:HD21	2.39	0.52
1:J:237:VAL:HG23	1:J:237:VAL:O	2.09	0.52
1:G:153:VAL:CG2	1:G:160:LEU:HD21	2.39	0.51
1:K:237:VAL:O	1:K:237:VAL:HG23	2.09	0.51
1:K:341:THR:HG21	1:K:353:LEU:HD12	1.92	0.51
1:M:359:TYR:HD2	1:N:249:LEU:HD23	1.75	0.51
1:O:237:VAL:HG23	1:O:237:VAL:O	2.10	0.51
1:I:359:TYR:HD2	1:J:249:LEU:HD23	1.75	0.51
1:A:359:TYR:CE1	1:A:390:GLU:CG	2.93	0.51
1:C:359:TYR:HE1	1:C:390:GLU:CG	2.16	0.51
1:J:359:TYR:CE1	1:J:390:GLU:CG	2.93	0.51
1:M:341:THR:HG21	1:M:353:LEU:HD12	1.92	0.51
1:B:359:TYR:HE1	1:B:390:GLU:CG	2.16	0.51
1:N:153:VAL:CG2	1:N:160:LEU:HD21	2.40	0.51
1:A:196:PHE:O	1:A:196:PHE:CG	2.64	0.51
1:C:341:THR:HG21	1:C:353:LEU:HD12	1.92	0.51
1:F:170:VAL:CG2	1:G:113:THR:HG21	2.41	0.51
1:G:341:THR:HG21	1:G:353:LEU:HD12	1.91	0.51
1:H:341:THR:HG21	1:H:353:LEU:HD12	1.91	0.51
1:F:359:TYR:CE1	1:F:390:GLU:CG	2.94	0.51
1:I:341:THR:HG21	1:I:353:LEU:HD12	1.91	0.51
1:B:359:TYR:CE1	1:B:390:GLU:CG	2.94	0.51
1:A:113:THR:HG21	1:O:170:VAL:CG2	2.42	0.50
1:B:339:ILE:HG21	1:B:353:LEU:HG	1.93	0.50
1:J:153:VAL:CG2	1:J:160:LEU:HD21	2.40	0.50
1:A:339:ILE:HG21	1:A:353:LEU:HG	1.93	0.50
1:C:359:TYR:CE1	1:C:390:GLU:CG	2.93	0.50
1:E:359:TYR:HD2	1:F:249:LEU:HD23	1.76	0.50
1:F:339:ILE:HG21	1:F:353:LEU:HG	1.94	0.50
1:K:359:TYR:CE1	1:K:390:GLU:CG	2.93	0.50
1:D:341:THR:HG21	1:D:353:LEU:HD12	1.92	0.50
1:F:341:THR:HG21	1:F:353:LEU:HD12	1.92	0.50
1:B:359:TYR:HD2	1:C:249:LEU:HD23	1.75	0.50
1:I:339:ILE:HG21	1:I:353:LEU:HG	1.93	0.50
1:D:196:PHE:O	1:D:196:PHE:CG	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:359:TYR:HD2	1:M:249:LEU:HD23	1.76	0.50
1:A:341:THR:HG21	1:A:353:LEU:HD12	1.92	0.50
1:H:153:VAL:CG2	1:H:160:LEU:HD21	2.41	0.50
1:J:196:PHE:O	1:J:196:PHE:CG	2.64	0.50
1:M:196:PHE:O	1:M:196:PHE:CG	2.62	0.50
1:N:341:THR:HG21	1:N:353:LEU:HD12	1.93	0.50
1:O:341:THR:HG21	1:O:353:LEU:HD12	1.92	0.50
1:C:339:ILE:HG21	1:C:353:LEU:HG	1.94	0.50
1:G:359:TYR:CE1	1:G:390:GLU:CG	2.94	0.50
1:O:153:VAL:CG2	1:O:160:LEU:HD21	2.39	0.50
1:E:170:VAL:CG2	1:F:113:THR:HG21	2.42	0.50
1:K:153:VAL:CG2	1:K:160:LEU:HD21	2.41	0.50
1:O:339:ILE:HG21	1:O:353:LEU:HG	1.94	0.50
1:F:359:TYR:HD2	1:G:249:LEU:HD23	1.75	0.50
1:H:359:TYR:HD2	1:I:249:LEU:HD23	1.77	0.50
1:G:170:VAL:CG2	1:H:113:THR:HG21	2.42	0.49
1:N:359:TYR:HE1	1:N:390:GLU:CG	2.16	0.49
1:A:359:TYR:HD2	1:B:249:LEU:HD23	1.77	0.49
1:E:341:THR:HG21	1:E:353:LEU:HD12	1.92	0.49
1:J:359:TYR:HD2	1:K:249:LEU:HD23	1.77	0.49
1:L:359:TYR:HE1	1:L:390:GLU:CG	2.16	0.49
1:M:153:VAL:CG2	1:M:160:LEU:HD21	2.40	0.49
1:E:359:TYR:HE1	1:E:390:GLU:CG	2.16	0.49
1:G:339:ILE:HG21	1:G:353:LEU:HG	1.95	0.49
1:I:196:PHE:O	1:I:196:PHE:CG	2.63	0.49
1:O:196:PHE:O	1:O:196:PHE:CG	2.64	0.49
1:O:359:TYR:CE1	1:O:390:GLU:CG	2.93	0.49
1:E:196:PHE:O	1:E:196:PHE:CG	2.63	0.49
1:L:153:VAL:CG2	1:L:160:LEU:HD21	2.40	0.49
1:B:153:VAL:CG2	1:B:160:LEU:HD21	2.39	0.49
1:C:359:TYR:HD2	1:D:249:LEU:HD23	1.78	0.49
1:D:177:ILE:HD13	1:D:304:PRO:HB2	1.95	0.49
1:B:196:PHE:O	1:B:196:PHE:CG	2.63	0.49
1:E:339:ILE:HG21	1:E:353:LEU:HG	1.95	0.49
1:L:359:TYR:CE1	1:L:390:GLU:CG	2.93	0.49
1:N:196:PHE:O	1:N:196:PHE:CG	2.64	0.49
1:B:170:VAL:CG2	1:C:113:THR:HG21	2.42	0.49
1:G:359:TYR:HD2	1:H:249:LEU:HD23	1.77	0.49
1:H:196:PHE:O	1:H:196:PHE:CG	2.65	0.49
1:H:170:VAL:CG2	1:I:113:THR:HG21	2.43	0.49
1:L:196:PHE:O	1:L:196:PHE:CG	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:VAL:CG2	1:E:113:THR:HG21	2.43	0.49
1:G:196:PHE:O	1:G:196:PHE:CG	2.64	0.49
1:I:153:VAL:CG2	1:I:160:LEU:HD21	2.41	0.49
1:I:359:TYR:HE1	1:I:390:GLU:CG	2.16	0.49
1:J:170:VAL:CG2	1:K:113:THR:HG21	2.43	0.49
1:C:196:PHE:O	1:C:196:PHE:CG	2.64	0.49
1:D:359:TYR:CE1	1:D:390:GLU:CG	2.94	0.49
1:O:177:ILE:HD13	1:O:304:PRO:HB2	1.95	0.49
1:A:249:LEU:HD23	1:O:359:TYR:HD2	1.77	0.48
1:D:339:ILE:HG21	1:D:353:LEU:HG	1.95	0.48
1:B:341:THR:HG21	1:B:353:LEU:HD12	1.92	0.48
1:G:177:ILE:HD13	1:G:304:PRO:HB2	1.96	0.48
1:J:341:THR:HG21	1:J:353:LEU:HD12	1.92	0.48
1:F:177:ILE:HD13	1:F:304:PRO:HB2	1.96	0.48
1:L:339:ILE:HG21	1:L:353:LEU:HG	1.95	0.48
1:A:170:VAL:CG2	1:B:113:THR:HG21	2.43	0.48
1:C:170:VAL:CG2	1:D:113:THR:HG21	2.43	0.48
1:B:177:ILE:HD13	1:B:304:PRO:HB2	1.96	0.48
1:E:177:ILE:HD13	1:E:304:PRO:HB2	1.95	0.48
1:H:339:ILE:HG21	1:H:353:LEU:HG	1.95	0.48
1:H:359:TYR:CE1	1:H:390:GLU:CG	2.94	0.48
1:J:339:ILE:HG21	1:J:353:LEU:HG	1.95	0.48
1:L:177:ILE:HD13	1:L:304:PRO:HB2	1.95	0.48
1:K:196:PHE:O	1:K:196:PHE:CG	2.64	0.48
1:M:170:VAL:CG2	1:N:113:THR:HG21	2.44	0.48
1:M:359:TYR:CE1	1:M:390:GLU:CG	2.94	0.48
1:C:177:ILE:HD13	1:C:304:PRO:HB2	1.96	0.48
1:D:359:TYR:HD2	1:E:249:LEU:HD23	1.78	0.48
1:F:196:PHE:O	1:F:196:PHE:CG	2.63	0.48
1:H:177:ILE:HD13	1:H:304:PRO:HB2	1.96	0.48
1:I:170:VAL:CG2	1:J:113:THR:HG21	2.43	0.48
1:K:339:ILE:HG21	1:K:353:LEU:HG	1.95	0.48
1:J:127:VAL:HG12	1:J:166:PHE:CE2	2.49	0.48
1:A:177:ILE:HD13	1:A:304:PRO:HB2	1.96	0.47
1:G:359:TYR:HE1	1:G:390:GLU:CG	2.16	0.47
1:K:170:VAL:CG2	1:L:113:THR:HG21	2.43	0.47
1:N:177:ILE:HD13	1:N:304:PRO:HB2	1.96	0.47
1:N:339:ILE:HG21	1:N:353:LEU:HG	1.96	0.47
1:J:177:ILE:HD13	1:J:304:PRO:HB2	1.96	0.47
1:A:152:VAL:HG21	1:O:127:VAL:CG1	2.45	0.47
1:I:177:ILE:HD13	1:I:304:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:ILE:HD13	1:K:304:PRO:HB2	1.97	0.47
1:M:177:ILE:HD13	1:M:304:PRO:HB2	1.96	0.47
1:M:339:ILE:HG21	1:M:353:LEU:HG	1.96	0.47
1:I:127:VAL:HG12	1:I:166:PHE:CE2	2.50	0.47
1:E:359:TYR:CE1	1:E:390:GLU:CG	2.94	0.47
1:H:153:VAL:CG2	1:H:160:LEU:HD22	2.45	0.46
1:N:396:LEU:N	1:N:396:LEU:HD12	2.31	0.46
1:L:170:VAL:CG2	1:M:113:THR:HG21	2.45	0.46
1:N:153:VAL:CG2	1:N:160:LEU:HD22	2.46	0.46
1:N:359:TYR:CE1	1:N:390:GLU:CG	2.94	0.46
1:C:337:ARG:HE	1:C:337:ARG:HB2	1.57	0.46
1:H:127:VAL:HG12	1:H:166:PHE:CE2	2.51	0.46
1:M:153:VAL:CG2	1:M:160:LEU:HD22	2.46	0.46
1:I:359:TYR:CE1	1:I:390:GLU:CG	2.94	0.46
1:G:153:VAL:CG2	1:G:160:LEU:HD22	2.46	0.46
1:O:153:VAL:CG2	1:O:160:LEU:HD22	2.46	0.46
1:J:153:VAL:CG2	1:J:160:LEU:HD22	2.46	0.46
1:K:127:VAL:HG12	1:K:166:PHE:CE2	2.51	0.46
1:C:127:VAL:CG1	1:D:152:VAL:HG21	2.46	0.46
1:K:153:VAL:CG2	1:K:160:LEU:HD22	2.45	0.46
1:L:153:VAL:CG2	1:L:160:LEU:HD22	2.46	0.46
1:N:127:VAL:CG1	1:O:152:VAL:HG21	2.46	0.46
1:I:396:LEU:N	1:I:396:LEU:HD12	2.31	0.45
1:J:396:LEU:HD12	1:J:396:LEU:N	2.31	0.45
1:E:153:VAL:CG2	1:E:160:LEU:HD22	2.46	0.45
1:F:396:LEU:N	1:F:396:LEU:HD12	2.31	0.45
1:G:396:LEU:HD12	1:G:396:LEU:N	2.30	0.45
1:M:127:VAL:HG12	1:M:166:PHE:CE2	2.52	0.45
1:D:127:VAL:CG1	1:E:152:VAL:HG21	2.47	0.45
1:L:127:VAL:HG12	1:L:166:PHE:CE2	2.51	0.45
1:E:127:VAL:HG12	1:E:166:PHE:CE2	2.51	0.45
1:F:153:VAL:CG2	1:F:160:LEU:HD22	2.46	0.45
1:G:127:VAL:HG12	1:G:166:PHE:CE2	2.51	0.45
1:O:114:PHE:HE1	1:O:153:VAL:HG22	1.82	0.45
1:A:127:VAL:HG12	1:A:166:PHE:CE2	2.52	0.45
2:I:501:CPS:H21B	2:I:501:CPS:C10	2.46	0.45
1:B:153:VAL:CG2	1:B:160:LEU:HD22	2.47	0.45
2:C:501:CPS:H21B	2:C:501:CPS:C10	2.47	0.45
1:E:396:LEU:HD12	1:E:396:LEU:N	2.32	0.45
1:F:127:VAL:HG12	1:F:166:PHE:CE2	2.51	0.45
1:N:114:PHE:HE1	1:N:153:VAL:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG12	1:B:166:PHE:CE2	2.52	0.45
1:C:396:LEU:N	1:C:396:LEU:HD12	2.32	0.45
1:I:153:VAL:CG2	1:I:160:LEU:HD22	2.46	0.45
1:L:198:ALA:HA	1:L:235:LEU:HD23	1.99	0.45
1:A:114:PHE:HE1	1:A:153:VAL:HG22	1.82	0.45
1:A:153:VAL:CG2	1:A:160:LEU:HD22	2.47	0.45
1:C:153:VAL:CG2	1:C:160:LEU:HD22	2.46	0.45
1:N:127:VAL:HG12	1:N:166:PHE:CE2	2.52	0.45
1:D:153:VAL:CG2	1:D:160:LEU:HD22	2.47	0.44
1:D:127:VAL:HG12	1:D:166:PHE:CE2	2.52	0.44
1:E:114:PHE:HE1	1:E:153:VAL:HG22	1.82	0.44
1:C:114:PHE:HE1	1:C:153:VAL:HG22	1.82	0.44
1:I:198:ALA:HA	1:I:235:LEU:HD23	2.00	0.44
1:A:127:VAL:CG1	1:B:152:VAL:HG21	2.48	0.44
1:B:114:PHE:HE1	1:B:153:VAL:HG22	1.83	0.44
1:B:337:ARG:HG2	1:C:266:VAL:HG22	1.99	0.44
1:B:127:VAL:CG1	1:C:152:VAL:HG21	2.48	0.44
1:B:396:LEU:HD12	1:B:396:LEU:N	2.33	0.44
1:D:114:PHE:HE1	1:D:153:VAL:HG22	1.83	0.44
1:E:198:ALA:HA	1:E:235:LEU:HD23	1.99	0.44
1:G:198:ALA:HA	1:G:235:LEU:HD23	2.00	0.44
1:H:114:PHE:HE1	1:H:153:VAL:HG22	1.82	0.44
1:K:114:PHE:HE1	1:K:153:VAL:HG22	1.81	0.44
1:N:198:ALA:HA	1:N:235:LEU:HD23	1.99	0.44
1:N:337:ARG:HG2	1:O:266:VAL:HG22	1.99	0.44
1:O:127:VAL:HG12	1:O:166:PHE:CE2	2.53	0.44
2:O:502:CPS:H21B	2:O:502:CPS:C10	2.48	0.44
1:A:182:LEU:HB3	1:A:396:LEU:HB2	2.00	0.44
1:J:198:ALA:HA	1:J:235:LEU:HD23	2.00	0.44
1:M:182:LEU:HB3	1:M:396:LEU:HB2	2.00	0.44
2:M:501:CPS:H21B	2:M:501:CPS:C10	2.48	0.44
1:H:396:LEU:N	1:H:396:LEU:HD12	2.32	0.44
1:L:396:LEU:HD12	1:L:396:LEU:N	2.32	0.44
1:C:127:VAL:HG12	1:C:166:PHE:CE2	2.52	0.44
1:G:114:PHE:HE1	1:G:153:VAL:HG22	1.83	0.44
1:K:182:LEU:HB3	1:K:396:LEU:HB2	2.00	0.44
2:B:501:CPS:H21B	2:B:501:CPS:C10	2.48	0.44
1:H:182:LEU:HB3	1:H:396:LEU:HB2	2.00	0.44
1:K:396:LEU:N	1:K:396:LEU:HD12	2.33	0.43
1:O:182:LEU:HB3	1:O:396:LEU:HB2	2.00	0.43
1:I:337:ARG:HE	1:I:337:ARG:HB2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:PHE:HE1	1:J:153:VAL:HG22	1.82	0.43
1:K:198:ALA:HA	1:K:235:LEU:HD23	2.00	0.43
1:A:198:ALA:HA	1:A:235:LEU:HD23	2.00	0.43
1:B:337:ARG:HE	1:B:337:ARG:HB2	1.57	0.43
1:C:198:ALA:HA	1:C:235:LEU:HD23	1.99	0.43
1:D:396:LEU:N	1:D:396:LEU:HD12	2.32	0.43
1:G:337:ARG:HE	1:G:337:ARG:HB2	1.57	0.43
1:L:337:ARG:HE	1:L:337:ARG:HB2	1.57	0.43
1:M:114:PHE:HE1	1:M:153:VAL:HG22	1.82	0.43
1:H:328:GLN:O	1:H:328:GLN:CG	2.67	0.43
1:I:182:LEU:HB3	1:I:396:LEU:HB2	2.00	0.43
1:F:114:PHE:HE1	1:F:153:VAL:HG22	1.82	0.43
1:B:182:LEU:HB3	1:B:396:LEU:HB2	2.01	0.43
2:G:501:CPS:H21B	2:G:501:CPS:C10	2.48	0.43
1:L:114:PHE:HE1	1:L:153:VAL:HG22	1.82	0.43
2:C:501:CPS:H21B	2:C:501:CPS:H10B	2.01	0.43
2:I:501:CPS:H21B	2:I:501:CPS:H10B	2.00	0.43
1:D:182:LEU:HB3	1:D:396:LEU:HB2	2.01	0.43
2:F:501:CPS:H21B	2:F:501:CPS:C10	2.48	0.43
1:H:198:ALA:HA	1:H:235:LEU:HD23	2.00	0.43
1:J:182:LEU:HB3	1:J:396:LEU:HB2	2.01	0.43
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.91	0.43
1:E:182:LEU:HB3	1:E:396:LEU:HB2	2.01	0.43
1:M:198:ALA:HA	1:M:235:LEU:HD23	2.00	0.43
1:M:337:ARG:HG2	1:N:266:VAL:HG22	2.00	0.43
1:L:182:LEU:HB3	1:L:396:LEU:HB2	2.01	0.42
1:D:198:ALA:HA	1:D:235:LEU:HD23	1.99	0.42
1:G:328:GLN:CG	1:G:328:GLN:O	2.67	0.42
1:I:328:GLN:O	1:I:328:GLN:CG	2.68	0.42
1:J:328:GLN:O	1:J:328:GLN:CG	2.67	0.42
1:D:328:GLN:O	1:D:328:GLN:CG	2.67	0.42
2:L:501:CPS:H21B	2:L:501:CPS:C10	2.50	0.42
1:M:328:GLN:O	1:M:328:GLN:CG	2.67	0.42
1:H:127:VAL:CG1	1:I:152:VAL:HG21	2.49	0.42
1:N:328:GLN:O	1:N:328:GLN:CG	2.67	0.42
1:O:198:ALA:HA	1:O:235:LEU:HD23	2.00	0.42
1:C:182:LEU:HB3	1:C:396:LEU:HB2	2.02	0.42
1:C:328:GLN:O	1:C:328:GLN:CG	2.67	0.42
1:F:198:ALA:HA	1:F:235:LEU:HD23	2.00	0.42
1:F:182:LEU:HB3	1:F:396:LEU:HB2	2.01	0.42
1:G:151:LEU:HD23	1:G:151:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:396:LEU:N	1:M:396:LEU:HD12	2.34	0.42
1:N:182:LEU:HB3	1:N:396:LEU:HB2	2.02	0.42
1:B:198:ALA:HA	1:B:235:LEU:HD23	2.00	0.42
1:E:337:ARG:HE	1:E:337:ARG:HB2	1.57	0.42
2:M:501:CPS:H21B	2:M:501:CPS:H10B	2.02	0.42
2:N:501:CPS:H21B	2:N:501:CPS:C10	2.49	0.42
2:O:502:CPS:H21B	2:O:502:CPS:H10B	2.02	0.42
1:A:328:GLN:O	1:A:328:GLN:CG	2.67	0.42
1:E:328:GLN:O	1:E:328:GLN:CG	2.67	0.42
1:F:127:VAL:CG1	1:G:152:VAL:HG21	2.50	0.42
1:F:328:GLN:CG	1:F:328:GLN:O	2.67	0.42
1:G:182:LEU:HB3	1:G:396:LEU:HB2	2.01	0.42
1:M:127:VAL:CG1	1:N:152:VAL:HG21	2.49	0.42
1:B:328:GLN:O	1:B:328:GLN:CG	2.67	0.42
1:L:328:GLN:O	1:L:328:GLN:CG	2.67	0.42
1:O:396:LEU:HD12	1:O:396:LEU:N	2.35	0.42
2:B:501:CPS:H21B	2:B:501:CPS:H10B	2.02	0.42
1:I:114:PHE:HE1	1:I:153:VAL:HG22	1.83	0.42
1:K:328:GLN:CG	1:K:328:GLN:O	2.68	0.42
1:A:396:LEU:N	1:A:396:LEU:HD12	2.34	0.41
2:A:501:CPS:H21B	2:A:501:CPS:C10	2.50	0.41
1:C:323:LEU:HD23	1:C:323:LEU:HA	1.91	0.41
2:J:501:CPS:H21B	2:J:501:CPS:C10	2.50	0.41
2:K:501:CPS:H21B	2:K:501:CPS:C10	2.49	0.41
1:O:328:GLN:CG	1:O:328:GLN:O	2.67	0.41
1:E:127:VAL:CG1	1:F:152:VAL:HG21	2.50	0.41
2:E:501:CPS:H21B	2:E:501:CPS:C10	2.49	0.41
1:K:323:LEU:HD23	1:K:323:LEU:HA	1.91	0.41
1:C:337:ARG:HG2	1:D:266:VAL:HG22	2.02	0.41
1:O:337:ARG:HE	1:O:337:ARG:HB2	1.57	0.41
2:E:501:CPS:H23	2:E:501:CPS:H9	1.98	0.41
1:K:337:ARG:HG2	1:L:266:VAL:HG22	2.01	0.41
1:A:266:VAL:HG22	1:O:337:ARG:HG2	2.02	0.41
2:D:501:CPS:H21B	2:D:501:CPS:C10	2.50	0.41
2:F:501:CPS:H23	2:F:501:CPS:H9	1.98	0.41
1:G:127:VAL:CG1	1:H:152:VAL:HG21	2.51	0.41
1:D:323:LEU:HD23	1:D:323:LEU:HA	1.91	0.41
2:H:501:CPS:H21B	2:H:501:CPS:C10	2.50	0.41
1:I:337:ARG:HG2	1:J:266:VAL:HG22	2.02	0.41
1:K:127:VAL:CG1	1:L:152:VAL:HG21	2.50	0.41
1:N:151:LEU:HD23	1:N:151:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:VAL:CG1	1:K:152:VAL:HG21	2.51	0.40
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.93	0.40
1:B:401:ILE:HG22	1:B:403:ARG:HG3	2.04	0.40
1:E:337:ARG:HG2	1:F:266:VAL:HG22	2.03	0.40
2:G:501:CPS:H21B	2:G:501:CPS:H10B	2.02	0.40
1:B:192:LEU:HD23	1:B:192:LEU:O	2.22	0.40
2:B:501:CPS:H23	2:B:501:CPS:H9	1.97	0.40
2:E:501:CPS:H21B	2:E:501:CPS:H10B	2.03	0.40
2:F:501:CPS:H21B	2:F:501:CPS:H10B	2.03	0.40
2:G:501:CPS:H23	2:G:501:CPS:H9	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	B	219/414 (53%)	193 (88%)	25 (11%)	1 (0%)	29	54
1	C	219/414 (53%)	192 (88%)	26 (12%)	1 (0%)	29	54
1	D	219/414 (53%)	193 (88%)	25 (11%)	1 (0%)	29	54
1	E	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	F	219/414 (53%)	191 (87%)	28 (13%)	0	100	100
1	G	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	H	219/414 (53%)	191 (87%)	28 (13%)	0	100	100
1	I	219/414 (53%)	191 (87%)	28 (13%)	0	100	100
1	J	219/414 (53%)	191 (87%)	28 (13%)	0	100	100
1	K	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	L	219/414 (53%)	192 (88%)	26 (12%)	1 (0%)	29	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	N	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
1	O	219/414 (53%)	192 (88%)	27 (12%)	0	100	100
All	All	3285/6210 (53%)	2878 (88%)	403 (12%)	4 (0%)	54	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	C	149	ASN
1	D	149	ASN
1	L	149	ASN

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	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	B	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	C	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	D	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	E	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	F	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	G	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	H	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	I	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	J	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	K	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	L	205/365 (56%)	201 (98%)	4 (2%)	55	81
1	M	205/365 (56%)	201 (98%)	4 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	205/365 (56%)	201 (98%)	4 (2%)	55 81
1	O	205/365 (56%)	201 (98%)	4 (2%)	55 81
All	All	3075/5475 (56%)	3015 (98%)	60 (2%)	57 81

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	PRO
1	A	240	LEU
1	A	332	VAL
1	A	336	GLN
1	B	156	PRO
1	B	240	LEU
1	B	332	VAL
1	B	336	GLN
1	C	156	PRO
1	C	240	LEU
1	C	332	VAL
1	C	336	GLN
1	D	156	PRO
1	D	240	LEU
1	D	332	VAL
1	D	336	GLN
1	E	156	PRO
1	E	240	LEU
1	E	332	VAL
1	E	336	GLN
1	F	156	PRO
1	F	240	LEU
1	F	332	VAL
1	F	336	GLN
1	G	156	PRO
1	G	240	LEU
1	G	332	VAL
1	G	336	GLN
1	H	156	PRO
1	H	240	LEU
1	H	332	VAL
1	H	336	GLN
1	I	156	PRO
1	I	240	LEU

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Mol	Chain	Res	Type
1	I	332	VAL
1	I	336	GLN
1	J	156	PRO
1	J	240	LEU
1	J	332	VAL
1	J	336	GLN
1	K	156	PRO
1	K	240	LEU
1	K	332	VAL
1	K	336	GLN
1	L	156	PRO
1	L	240	LEU
1	L	332	VAL
1	L	336	GLN
1	M	156	PRO
1	M	240	LEU
1	M	332	VAL
1	M	336	GLN
1	N	156	PRO
1	N	240	LEU
1	N	332	VAL
1	N	336	GLN
1	O	156	PRO
1	O	240	LEU
1	O	332	VAL
1	O	336	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	B	361	ASN
1	C	361	ASN
1	D	361	ASN
1	E	361	ASN
1	F	361	ASN
1	G	361	ASN
1	H	361	ASN
1	I	361	ASN
1	J	361	ASN
1	K	361	ASN
1	L	361	ASN

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Mol	Chain	Res	Type
1	M	361	ASN
1	N	361	ASN
1	O	361	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)

30 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	$\#\|Z\| > 2$
2	CPS	L	501	-	45,45,45	0.68	0	69,70,70	1.19	6 (8%)
2	CPS	N	501	-	45,45,45	0.68	0	69,70,70	1.21	6 (8%)
2	CPS	G	502	-	28,28,45	0.68	0	46,46,70	0.97	1 (2%)
2	CPS	E	501	-	45,45,45	0.69	0	69,70,70	1.18	6 (8%)
2	CPS	N	502	-	28,28,45	0.68	0	46,46,70	0.99	1 (2%)
2	CPS	D	502	-	28,28,45	0.68	0	46,46,70	0.98	1 (2%)
2	CPS	A	502	-	28,28,45	0.68	0	46,46,70	0.98	1 (2%)
2	CPS	C	501	-	45,45,45	0.69	0	69,70,70	1.20	5 (7%)
2	CPS	E	502	-	28,28,45	0.68	0	46,46,70	1.00	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CPS	H	502	-	28,28,45	0.67	0	46,46,70	0.97	1 (2%)
2	CPS	J	501	-	45,45,45	0.68	0	69,70,70	1.19	6 (8%)
2	CPS	O	501	-	28,28,45	0.68	0	46,46,70	0.97	1 (2%)
2	CPS	K	502	-	28,28,45	0.68	0	46,46,70	0.97	1 (2%)
2	CPS	A	501	-	45,45,45	0.69	0	69,70,70	1.19	5 (7%)
2	CPS	L	502	-	28,28,45	0.68	0	46,46,70	0.98	1 (2%)
2	CPS	B	502	-	28,28,45	0.67	0	46,46,70	0.99	1 (2%)
2	CPS	I	502	-	28,28,45	0.68	0	46,46,70	0.97	1 (2%)
2	CPS	G	501	-	45,45,45	0.68	0	69,70,70	1.21	6 (8%)
2	CPS	H	501	-	45,45,45	0.67	0	69,70,70	1.18	6 (8%)
2	CPS	D	501	-	45,45,45	0.68	0	69,70,70	1.18	5 (7%)
2	CPS	M	501	-	45,45,45	0.68	0	69,70,70	1.20	5 (7%)
2	CPS	J	502	-	28,28,45	0.67	0	46,46,70	0.97	1 (2%)
2	CPS	C	502	-	28,28,45	0.67	0	46,46,70	0.97	1 (2%)
2	CPS	O	502	-	45,45,45	0.69	0	69,70,70	1.20	6 (8%)
2	CPS	B	501	-	45,45,45	0.69	0	69,70,70	1.21	5 (7%)
2	CPS	F	502	-	28,28,45	0.67	0	46,46,70	0.99	1 (2%)
2	CPS	M	502	-	28,28,45	0.68	0	46,46,70	0.98	1 (2%)
2	CPS	I	501	-	45,45,45	0.68	0	69,70,70	1.18	6 (8%)
2	CPS	K	501	-	45,45,45	0.68	0	69,70,70	1.19	6 (8%)
2	CPS	F	501	-	45,45,45	0.69	0	69,70,70	1.22	6 (8%)

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
2	CPS	L	501	-	-	16/25/90/90	0/4/4/4
2	CPS	N	501	-	-	16/25/90/90	0/4/4/4
2	CPS	G	502	-	-	0/4/69/90	0/4/4/4
2	CPS	E	501	-	-	16/25/90/90	0/4/4/4
2	CPS	N	502	-	-	0/4/69/90	0/4/4/4
2	CPS	D	502	-	-	0/4/69/90	0/4/4/4
2	CPS	A	502	-	-	0/4/69/90	0/4/4/4
2	CPS	C	501	-	-	16/25/90/90	0/4/4/4
2	CPS	E	502	-	-	0/4/69/90	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPS	H	502	-	-	0/4/69/90	0/4/4/4
2	CPS	J	501	-	-	16/25/90/90	0/4/4/4
2	CPS	O	501	-	-	0/4/69/90	0/4/4/4
2	CPS	K	502	-	-	0/4/69/90	0/4/4/4
2	CPS	A	501	-	-	16/25/90/90	0/4/4/4
2	CPS	L	502	-	-	0/4/69/90	0/4/4/4
2	CPS	B	502	-	-	0/4/69/90	0/4/4/4
2	CPS	I	502	-	-	0/4/69/90	0/4/4/4
2	CPS	G	501	-	-	16/25/90/90	0/4/4/4
2	CPS	H	501	-	-	16/25/90/90	0/4/4/4
2	CPS	D	501	-	-	16/25/90/90	0/4/4/4
2	CPS	M	501	-	-	16/25/90/90	0/4/4/4
2	CPS	J	502	-	-	0/4/69/90	0/4/4/4
2	CPS	C	502	-	-	0/4/69/90	0/4/4/4
2	CPS	O	502	-	-	16/25/90/90	0/4/4/4
2	CPS	B	501	-	-	16/25/90/90	0/4/4/4
2	CPS	F	502	-	-	0/4/69/90	0/4/4/4
2	CPS	M	502	-	-	0/4/69/90	0/4/4/4
2	CPS	I	501	-	-	16/25/90/90	0/4/4/4
2	CPS	K	501	-	-	16/25/90/90	0/4/4/4
2	CPS	F	501	-	-	16/25/90/90	0/4/4/4

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	501	CPS	C5-C9-C20	4.20	124.50	119.50
2	L	501	CPS	C5-C9-C20	4.19	124.49	119.50
2	B	501	CPS	C5-C9-C20	4.16	124.47	119.50
2	A	501	CPS	C5-C9-C20	4.15	124.45	119.50
2	F	501	CPS	C5-C9-C20	4.15	124.45	119.50
2	J	501	CPS	C5-C9-C20	4.13	124.42	119.50
2	G	501	CPS	C5-C9-C20	4.12	124.41	119.50
2	K	501	CPS	C5-C9-C20	4.10	124.39	119.50
2	C	501	CPS	C5-C9-C20	4.09	124.38	119.50
2	D	501	CPS	C5-C9-C20	4.09	124.37	119.50
2	M	501	CPS	C5-C9-C20	4.08	124.37	119.50
2	E	501	CPS	C5-C9-C20	4.07	124.35	119.50
2	O	502	CPS	C5-C9-C20	4.06	124.34	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	501	CPS	C5-C9-C20	4.01	124.28	119.50
2	F	501	CPS	C25-N1-C24	3.99	130.24	122.84
2	G	501	CPS	C25-N1-C24	3.96	130.19	122.84
2	M	501	CPS	C25-N1-C24	3.94	130.15	122.84
2	O	502	CPS	C25-N1-C24	3.90	130.08	122.84
2	C	501	CPS	C25-N1-C24	3.87	130.03	122.84
2	B	501	CPS	C25-N1-C24	3.86	130.00	122.84
2	I	501	CPS	C5-C9-C20	3.86	124.10	119.50
2	J	501	CPS	C25-N1-C24	3.84	129.96	122.84
2	N	501	CPS	C25-N1-C24	3.82	129.94	122.84
2	I	501	CPS	C25-N1-C24	3.81	129.91	122.84
2	A	501	CPS	C25-N1-C24	3.80	129.90	122.84
2	K	501	CPS	C25-N1-C24	3.78	129.86	122.84
2	L	501	CPS	C25-N1-C24	3.76	129.82	122.84
2	H	501	CPS	C25-N1-C24	3.76	129.81	122.84
2	E	501	CPS	C25-N1-C24	3.70	129.72	122.84
2	D	501	CPS	C25-N1-C24	3.69	129.69	122.84
2	G	501	CPS	C2-C19-C18	2.85	114.87	111.82
2	K	501	CPS	C2-C19-C18	2.84	114.86	111.82
2	F	501	CPS	C2-C19-C18	2.83	114.86	111.82
2	M	501	CPS	C2-C19-C18	2.83	114.86	111.82
2	C	501	CPS	C2-C19-C18	2.82	114.85	111.82
2	I	501	CPS	C2-C19-C18	2.81	114.84	111.82
2	B	501	CPS	C2-C19-C18	2.77	114.80	111.82
2	E	501	CPS	C2-C19-C18	2.75	114.77	111.82
2	H	501	CPS	C2-C19-C18	2.73	114.75	111.82
2	L	501	CPS	C2-C19-C18	2.70	114.72	111.82
2	D	501	CPS	C2-C19-C18	2.69	114.71	111.82
2	N	501	CPS	C2-C19-C18	2.68	114.70	111.82
2	J	501	CPS	C2-C19-C18	2.67	114.69	111.82
2	A	501	CPS	C2-C19-C18	2.67	114.69	111.82
2	O	502	CPS	C2-C19-C18	2.66	114.68	111.82
2	M	501	CPS	C14-C15-C2	2.37	115.17	112.66
2	O	502	CPS	C14-C15-C2	2.34	115.14	112.66
2	D	501	CPS	C14-C15-C2	2.33	115.14	112.66
2	L	501	CPS	C14-C15-C2	2.33	115.13	112.66
2	N	501	CPS	C14-C15-C2	2.32	115.12	112.66
2	J	501	CPS	C14-C15-C2	2.31	115.11	112.66
2	A	501	CPS	C14-C15-C2	2.31	115.11	112.66
2	F	501	CPS	C14-C15-C2	2.31	115.11	112.66
2	G	501	CPS	C14-C15-C2	2.29	115.09	112.66
2	E	501	CPS	C14-C15-C2	2.28	115.08	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	501	CPS	C14-C15-C2	2.27	115.07	112.66
2	B	501	CPS	C14-C15-C2	2.27	115.07	112.66
2	C	501	CPS	C14-C15-C2	2.26	115.06	112.66
2	H	501	CPS	C14-C15-C2	2.25	115.05	112.66
2	I	501	CPS	C14-C15-C2	2.24	115.03	112.66
2	I	501	CPS	C15-C14-C13	2.13	115.89	112.76
2	B	501	CPS	C15-C14-C13	2.13	115.89	112.76
2	M	502	CPS	C12-C1-C2	2.12	116.42	112.78
2	E	501	CPS	C15-C14-C13	2.12	115.88	112.76
2	G	501	CPS	C15-C14-C13	2.12	115.88	112.76
2	H	501	CPS	C15-C14-C13	2.12	115.87	112.76
2	C	501	CPS	C15-C14-C13	2.11	115.86	112.76
2	D	501	CPS	C15-C14-C13	2.10	115.84	112.76
2	N	501	CPS	C15-C14-C13	2.10	115.84	112.76
2	B	502	CPS	C12-C1-C2	2.10	116.37	112.78
2	I	502	CPS	C12-C1-C2	2.09	116.37	112.78
2	H	502	CPS	C12-C1-C2	2.09	116.37	112.78
2	K	502	CPS	C12-C1-C2	2.09	116.37	112.78
2	E	502	CPS	C12-C1-C2	2.09	116.36	112.78
2	C	502	CPS	C12-C1-C2	2.09	116.36	112.78
2	F	502	CPS	C12-C1-C2	2.09	116.36	112.78
2	A	502	CPS	C12-C1-C2	2.08	116.36	112.78
2	J	502	CPS	C12-C1-C2	2.08	116.36	112.78
2	G	502	CPS	C12-C1-C2	2.08	116.35	112.78
2	F	501	CPS	C15-C14-C13	2.08	115.81	112.76
2	M	501	CPS	C15-C14-C13	2.08	115.81	112.76
2	D	502	CPS	C12-C1-C2	2.07	116.33	112.78
2	L	501	CPS	C15-C14-C13	2.07	115.80	112.76
2	K	501	CPS	C15-C14-C13	2.07	115.79	112.76
2	O	501	CPS	C12-C1-C2	2.06	116.32	112.78
2	J	501	CPS	C15-C14-C13	2.06	115.78	112.76
2	H	501	CPS	C5-C6-C18	2.05	117.36	114.74
2	O	502	CPS	C5-C6-C18	2.05	117.36	114.74
2	K	501	CPS	C5-C6-C18	2.05	117.35	114.74
2	I	501	CPS	C5-C6-C18	2.04	117.35	114.74
2	A	501	CPS	C15-C14-C13	2.04	115.76	112.76
2	O	502	CPS	C15-C14-C13	2.04	115.75	112.76
2	F	501	CPS	C5-C6-C18	2.04	117.34	114.74
2	G	501	CPS	C5-C6-C18	2.04	117.34	114.74
2	L	501	CPS	C5-C6-C18	2.03	117.34	114.74
2	N	502	CPS	C12-C1-C2	2.03	116.25	112.78
2	L	502	CPS	C12-C1-C2	2.03	116.25	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	501	CPS	C5-C6-C18	2.03	117.32	114.74
2	J	501	CPS	C5-C6-C18	2.00	117.30	114.74
2	E	501	CPS	C5-C6-C18	2.00	117.29	114.74

There are no chirality outliers.

All (240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CPS	C26-C27-N2-C28
2	A	501	CPS	C26-C27-N2-C30
2	A	501	CPS	C31-C30-N2-C27
2	A	501	CPS	C31-C30-N2-C29
2	A	501	CPS	C31-C32-S-O1S
2	B	501	CPS	C26-C27-N2-C28
2	B	501	CPS	C26-C27-N2-C30
2	B	501	CPS	C31-C30-N2-C27
2	B	501	CPS	C31-C30-N2-C29
2	B	501	CPS	C31-C32-S-O1S
2	C	501	CPS	C26-C27-N2-C28
2	C	501	CPS	C26-C27-N2-C29
2	C	501	CPS	C26-C27-N2-C30
2	C	501	CPS	C31-C30-N2-C27
2	C	501	CPS	C31-C30-N2-C29
2	C	501	CPS	C31-C32-S-O1S
2	D	501	CPS	C26-C27-N2-C28
2	D	501	CPS	C26-C27-N2-C29
2	D	501	CPS	C26-C27-N2-C30
2	D	501	CPS	C31-C30-N2-C27
2	D	501	CPS	C31-C30-N2-C29
2	D	501	CPS	C31-C32-S-O1S
2	E	501	CPS	C26-C27-N2-C28
2	E	501	CPS	C26-C27-N2-C29
2	E	501	CPS	C26-C27-N2-C30
2	E	501	CPS	C31-C30-N2-C27
2	E	501	CPS	C31-C30-N2-C29
2	E	501	CPS	C31-C32-S-O1S
2	F	501	CPS	C26-C27-N2-C28
2	F	501	CPS	C26-C27-N2-C29
2	F	501	CPS	C26-C27-N2-C30
2	F	501	CPS	C31-C30-N2-C27
2	F	501	CPS	C31-C30-N2-C29
2	F	501	CPS	C31-C32-S-O1S

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Mol	Chain	Res	Type	Atoms
2	G	501	CPS	C26-C27-N2-C28
2	G	501	CPS	C26-C27-N2-C30
2	G	501	CPS	C31-C30-N2-C27
2	G	501	CPS	C31-C30-N2-C29
2	G	501	CPS	C31-C32-S-O1S
2	H	501	CPS	C26-C27-N2-C28
2	H	501	CPS	C26-C27-N2-C29
2	H	501	CPS	C26-C27-N2-C30
2	H	501	CPS	C31-C30-N2-C27
2	H	501	CPS	C31-C30-N2-C29
2	H	501	CPS	C31-C32-S-O1S
2	I	501	CPS	C26-C27-N2-C28
2	I	501	CPS	C26-C27-N2-C29
2	I	501	CPS	C26-C27-N2-C30
2	I	501	CPS	C31-C30-N2-C27
2	I	501	CPS	C31-C30-N2-C29
2	I	501	CPS	C31-C32-S-O1S
2	J	501	CPS	C26-C27-N2-C28
2	J	501	CPS	C26-C27-N2-C29
2	J	501	CPS	C26-C27-N2-C30
2	J	501	CPS	C31-C30-N2-C27
2	J	501	CPS	C31-C30-N2-C29
2	J	501	CPS	C31-C32-S-O1S
2	K	501	CPS	C26-C27-N2-C28
2	K	501	CPS	C26-C27-N2-C29
2	K	501	CPS	C26-C27-N2-C30
2	K	501	CPS	C31-C30-N2-C27
2	K	501	CPS	C31-C30-N2-C29
2	K	501	CPS	C31-C32-S-O1S
2	L	501	CPS	C26-C27-N2-C28
2	L	501	CPS	C26-C27-N2-C30
2	L	501	CPS	C31-C30-N2-C27
2	L	501	CPS	C31-C30-N2-C29
2	L	501	CPS	C31-C32-S-O1S
2	M	501	CPS	C26-C27-N2-C28
2	M	501	CPS	C26-C27-N2-C30
2	M	501	CPS	C31-C30-N2-C27
2	M	501	CPS	C31-C30-N2-C29
2	M	501	CPS	C31-C32-S-O1S
2	N	501	CPS	C26-C27-N2-C28
2	N	501	CPS	C26-C27-N2-C30
2	N	501	CPS	C31-C30-N2-C27

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Mol	Chain	Res	Type	Atoms
2	N	501	CPS	C31-C30-N2-C29
2	N	501	CPS	C31-C32-S-O1S
2	O	502	CPS	C26-C27-N2-C28
2	O	502	CPS	C26-C27-N2-C30
2	O	502	CPS	C31-C30-N2-C27
2	O	502	CPS	C31-C30-N2-C29
2	O	502	CPS	C31-C32-S-O1S
2	A	501	CPS	C23-C24-N1-C25
2	B	501	CPS	C23-C24-N1-C25
2	C	501	CPS	C23-C24-N1-C25
2	D	501	CPS	C23-C24-N1-C25
2	E	501	CPS	C23-C24-N1-C25
2	F	501	CPS	C23-C24-N1-C25
2	G	501	CPS	C23-C24-N1-C25
2	H	501	CPS	C23-C24-N1-C25
2	I	501	CPS	C23-C24-N1-C25
2	J	501	CPS	C23-C24-N1-C25
2	K	501	CPS	C23-C24-N1-C25
2	L	501	CPS	C23-C24-N1-C25
2	M	501	CPS	C23-C24-N1-C25
2	N	501	CPS	C23-C24-N1-C25
2	O	502	CPS	C23-C24-N1-C25
2	A	501	CPS	C26-C27-N2-C29
2	A	501	CPS	C31-C30-N2-C28
2	B	501	CPS	C26-C27-N2-C29
2	B	501	CPS	C31-C30-N2-C28
2	C	501	CPS	C31-C30-N2-C28
2	D	501	CPS	C31-C30-N2-C28
2	E	501	CPS	C31-C30-N2-C28
2	F	501	CPS	C31-C30-N2-C28
2	G	501	CPS	C26-C27-N2-C29
2	G	501	CPS	C31-C30-N2-C28
2	H	501	CPS	C31-C30-N2-C28
2	I	501	CPS	C31-C30-N2-C28
2	J	501	CPS	C31-C30-N2-C28
2	K	501	CPS	C31-C30-N2-C28
2	L	501	CPS	C26-C27-N2-C29
2	L	501	CPS	C31-C30-N2-C28
2	M	501	CPS	C26-C27-N2-C29
2	M	501	CPS	C31-C30-N2-C28
2	N	501	CPS	C26-C27-N2-C29
2	N	501	CPS	C31-C30-N2-C28

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Mol	Chain	Res	Type	Atoms
2	O	502	CPS	C26-C27-N2-C29
2	O	502	CPS	C31-C30-N2-C28
2	A	501	CPS	O1-C24-N1-C25
2	B	501	CPS	O1-C24-N1-C25
2	C	501	CPS	O1-C24-N1-C25
2	D	501	CPS	O1-C24-N1-C25
2	E	501	CPS	O1-C24-N1-C25
2	F	501	CPS	O1-C24-N1-C25
2	G	501	CPS	O1-C24-N1-C25
2	H	501	CPS	O1-C24-N1-C25
2	I	501	CPS	O1-C24-N1-C25
2	J	501	CPS	O1-C24-N1-C25
2	K	501	CPS	O1-C24-N1-C25
2	L	501	CPS	O1-C24-N1-C25
2	M	501	CPS	O1-C24-N1-C25
2	N	501	CPS	O1-C24-N1-C25
2	O	502	CPS	O1-C24-N1-C25
2	A	501	CPS	C31-C32-S-O2S
2	B	501	CPS	C31-C32-S-O2S
2	C	501	CPS	C31-C32-S-O2S
2	D	501	CPS	C31-C32-S-O2S
2	E	501	CPS	C31-C32-S-O2S
2	F	501	CPS	C31-C32-S-O2S
2	G	501	CPS	C31-C32-S-O2S
2	H	501	CPS	C31-C32-S-O2S
2	I	501	CPS	C31-C32-S-O2S
2	J	501	CPS	C31-C32-S-O2S
2	K	501	CPS	C31-C32-S-O2S
2	L	501	CPS	C31-C32-S-O2S
2	M	501	CPS	C31-C32-S-O2S
2	N	501	CPS	C31-C32-S-O2S
2	O	502	CPS	C31-C32-S-O2S
2	A	501	CPS	C22-C20-C9-C5
2	F	501	CPS	C22-C20-C9-C5
2	H	501	CPS	C22-C20-C9-C5
2	J	501	CPS	C22-C20-C9-C5
2	L	501	CPS	C22-C20-C9-C5
2	N	501	CPS	C22-C20-C9-C5
2	B	501	CPS	C22-C20-C9-C5
2	C	501	CPS	C22-C20-C9-C5
2	D	501	CPS	C22-C20-C9-C5
2	E	501	CPS	C22-C20-C9-C5

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Mol	Chain	Res	Type	Atoms
2	G	501	CPS	C22-C20-C9-C5
2	I	501	CPS	C22-C20-C9-C5
2	K	501	CPS	C22-C20-C9-C5
2	M	501	CPS	C22-C20-C9-C5
2	O	502	CPS	C22-C20-C9-C5
2	A	501	CPS	C22-C20-C9-C8
2	F	501	CPS	C22-C20-C9-C8
2	G	501	CPS	C22-C20-C9-C8
2	J	501	CPS	C22-C20-C9-C8
2	L	501	CPS	C22-C20-C9-C8
2	M	501	CPS	C22-C20-C9-C8
2	N	501	CPS	C22-C20-C9-C8
2	A	501	CPS	C21-C20-C9-C8
2	B	501	CPS	C21-C20-C9-C8
2	D	501	CPS	C21-C20-C9-C8
2	E	501	CPS	C21-C20-C9-C8
2	F	501	CPS	C21-C20-C9-C8
2	G	501	CPS	C21-C20-C9-C8
2	H	501	CPS	C21-C20-C9-C8
2	J	501	CPS	C21-C20-C9-C8
2	K	501	CPS	C21-C20-C9-C8
2	L	501	CPS	C21-C20-C9-C8
2	M	501	CPS	C21-C20-C9-C8
2	N	501	CPS	C21-C20-C9-C8
2	B	501	CPS	C22-C20-C9-C8
2	C	501	CPS	C22-C20-C9-C8
2	D	501	CPS	C22-C20-C9-C8
2	E	501	CPS	C22-C20-C9-C8
2	H	501	CPS	C22-C20-C9-C8
2	I	501	CPS	C22-C20-C9-C8
2	K	501	CPS	C22-C20-C9-C8
2	O	502	CPS	C22-C20-C9-C8
2	C	501	CPS	C21-C20-C9-C8
2	I	501	CPS	C21-C20-C9-C8
2	O	502	CPS	C21-C20-C9-C8
2	A	501	CPS	C31-C32-S-O3S
2	B	501	CPS	C31-C32-S-O3S
2	C	501	CPS	C31-C32-S-O3S
2	D	501	CPS	C31-C32-S-O3S
2	E	501	CPS	C31-C32-S-O3S
2	F	501	CPS	C31-C32-S-O3S
2	G	501	CPS	C31-C32-S-O3S

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Mol	Chain	Res	Type	Atoms
2	H	501	CPS	C31-C32-S-O3S
2	I	501	CPS	C31-C32-S-O3S
2	J	501	CPS	C31-C32-S-O3S
2	K	501	CPS	C31-C32-S-O3S
2	L	501	CPS	C31-C32-S-O3S
2	M	501	CPS	C31-C32-S-O3S
2	N	501	CPS	C31-C32-S-O3S
2	O	502	CPS	C31-C32-S-O3S
2	A	501	CPS	C30-C31-C32-S
2	B	501	CPS	C30-C31-C32-S
2	C	501	CPS	C30-C31-C32-S
2	D	501	CPS	C30-C31-C32-S
2	E	501	CPS	C30-C31-C32-S
2	F	501	CPS	C30-C31-C32-S
2	G	501	CPS	C30-C31-C32-S
2	H	501	CPS	C30-C31-C32-S
2	I	501	CPS	C30-C31-C32-S
2	J	501	CPS	C30-C31-C32-S
2	K	501	CPS	C30-C31-C32-S
2	L	501	CPS	C30-C31-C32-S
2	M	501	CPS	C30-C31-C32-S
2	N	501	CPS	C30-C31-C32-S
2	O	502	CPS	C30-C31-C32-S
2	A	501	CPS	C21-C20-C22-C23
2	D	501	CPS	C21-C20-C22-C23
2	E	501	CPS	C21-C20-C22-C23
2	H	501	CPS	C21-C20-C22-C23
2	J	501	CPS	C21-C20-C22-C23
2	F	501	CPS	C21-C20-C22-C23
2	G	501	CPS	C21-C20-C22-C23
2	K	501	CPS	C21-C20-C22-C23
2	L	501	CPS	C21-C20-C22-C23
2	M	501	CPS	C21-C20-C22-C23
2	N	501	CPS	C21-C20-C22-C23
2	B	501	CPS	C21-C20-C22-C23
2	C	501	CPS	C21-C20-C22-C23
2	I	501	CPS	C21-C20-C22-C23
2	O	502	CPS	C21-C20-C22-C23

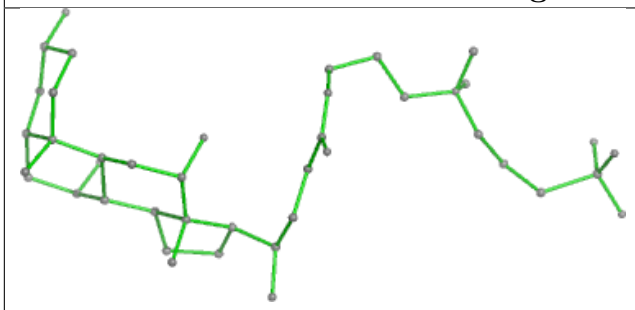
There are no ring outliers.

15 monomers are involved in 27 short contacts:

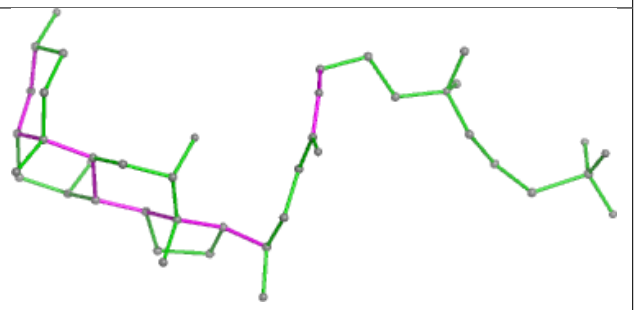
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	CPS	1	0
2	N	501	CPS	1	0
2	E	501	CPS	3	0
2	C	501	CPS	2	0
2	J	501	CPS	1	0
2	A	501	CPS	1	0
2	G	501	CPS	3	0
2	H	501	CPS	1	0
2	D	501	CPS	1	0
2	M	501	CPS	2	0
2	O	502	CPS	2	0
2	B	501	CPS	3	0
2	I	501	CPS	2	0
2	K	501	CPS	1	0
2	F	501	CPS	3	0

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.

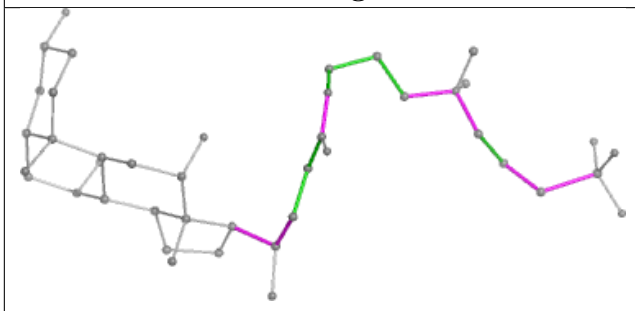
Ligand CPS L 501



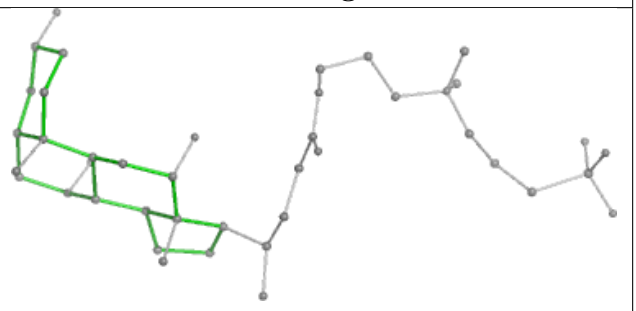
Bond lengths



Bond angles

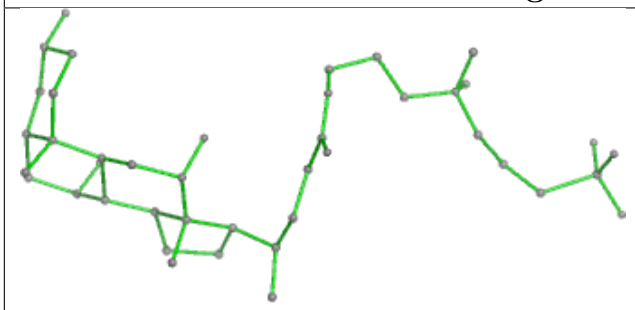


Torsions

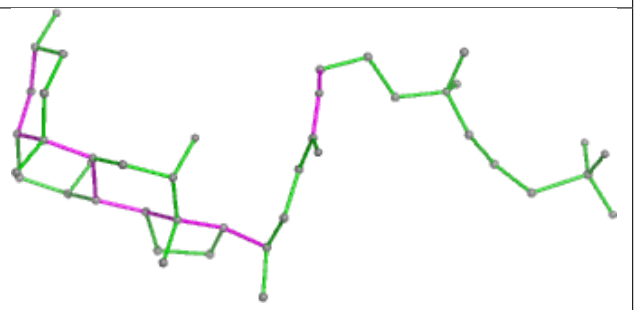


Rings

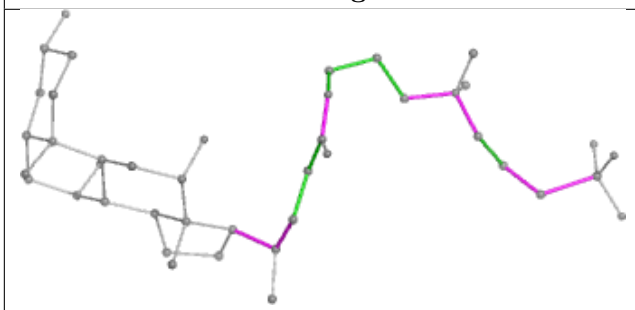
Ligand CPS N 501



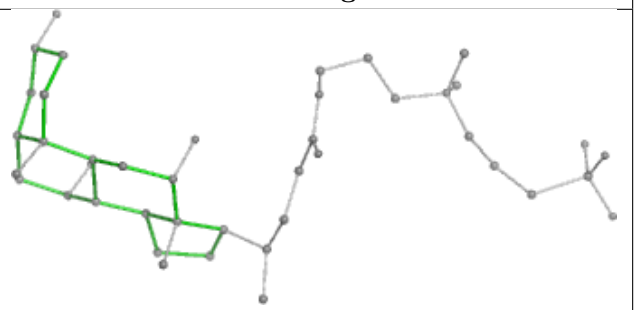
Bond lengths



Bond angles

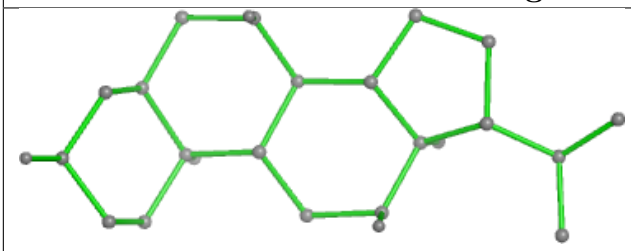


Torsions

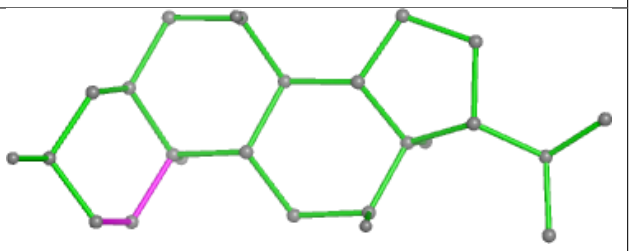


Rings

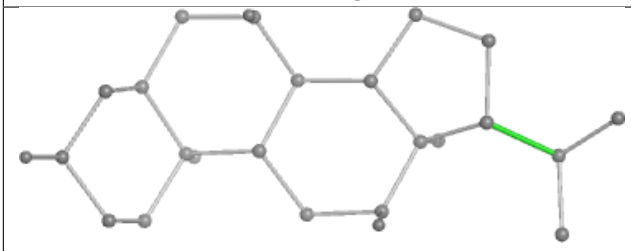
Ligand CPS G 502



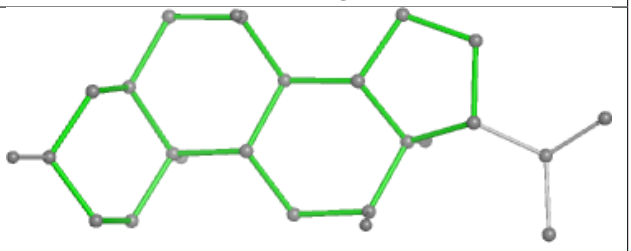
Bond lengths



Bond angles

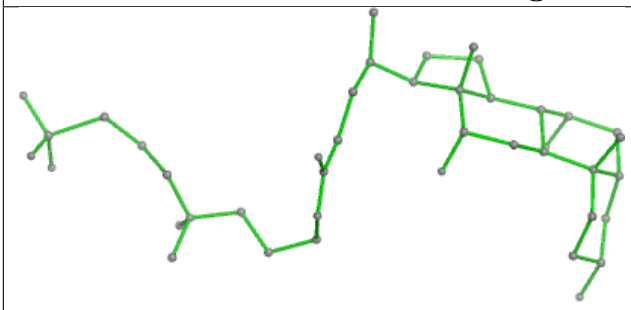


Torsions

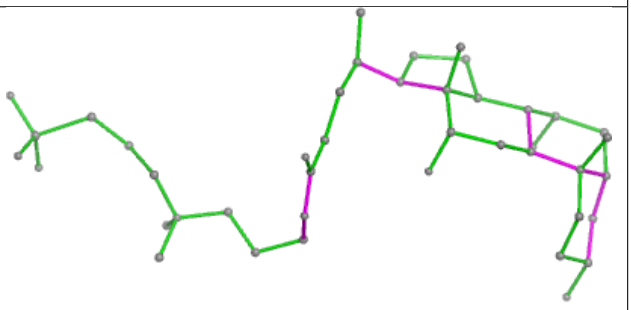


Rings

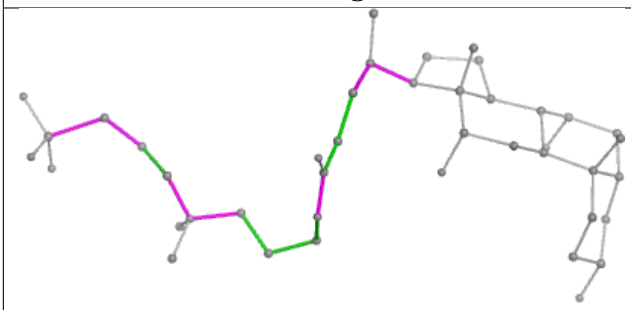
Ligand CPS E 501



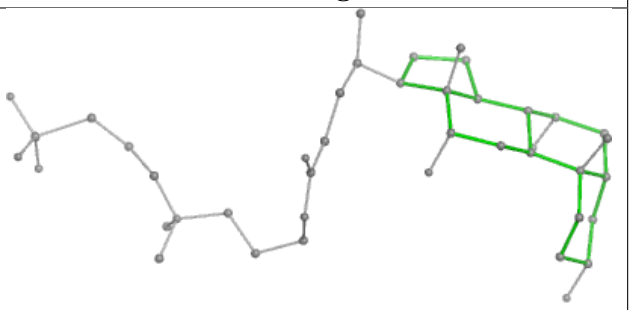
Bond lengths



Bond angles

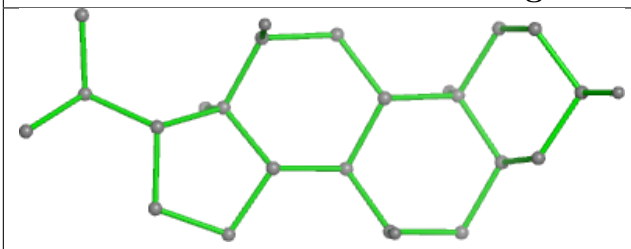


Torsions

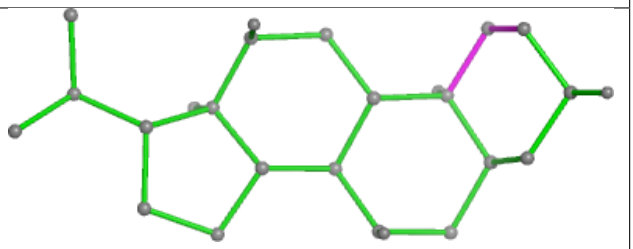


Rings

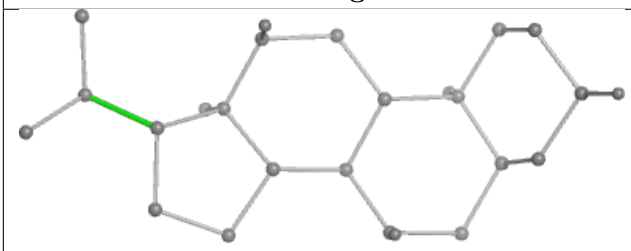
Ligand CPS N 502



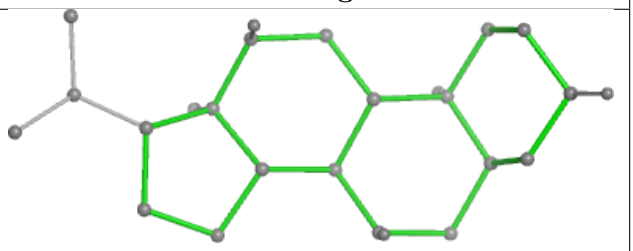
Bond lengths



Bond angles

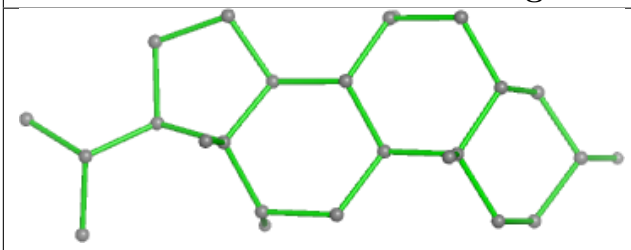


Torsions

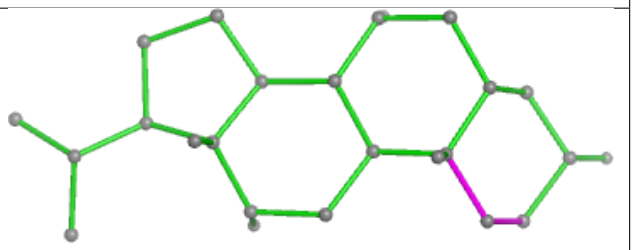


Rings

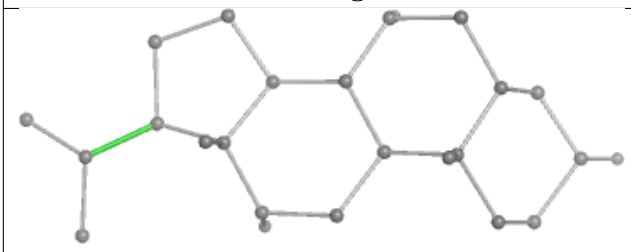
Ligand CPS D 502



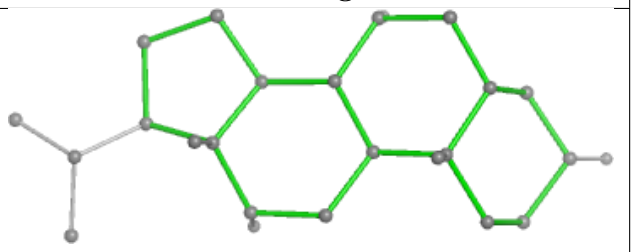
Bond lengths



Bond angles

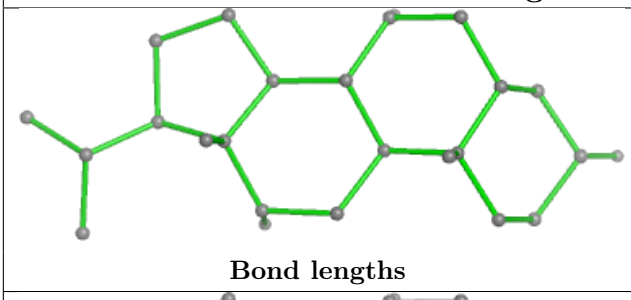


Torsions

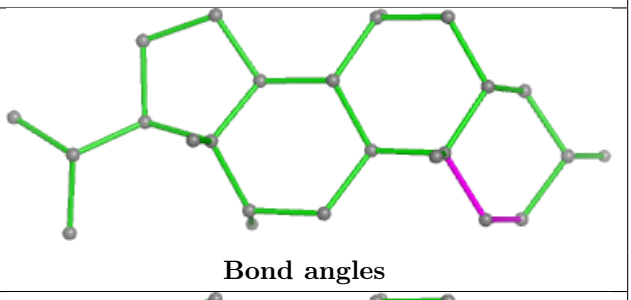


Rings

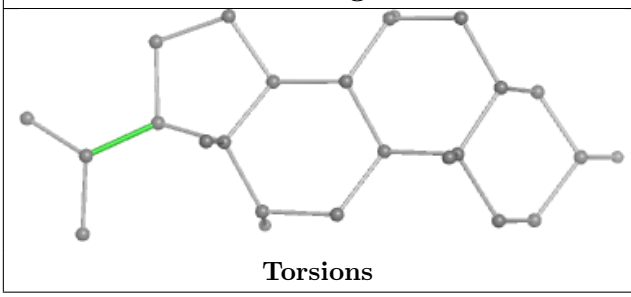
Ligand CPS A 502



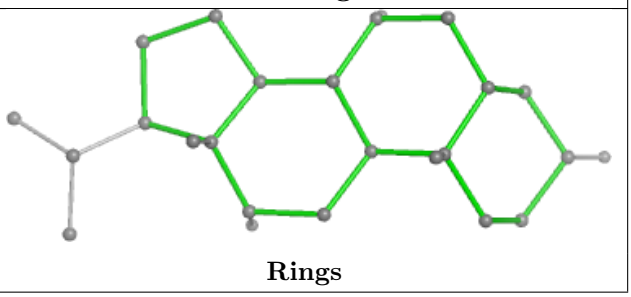
Bond lengths



Bond angles

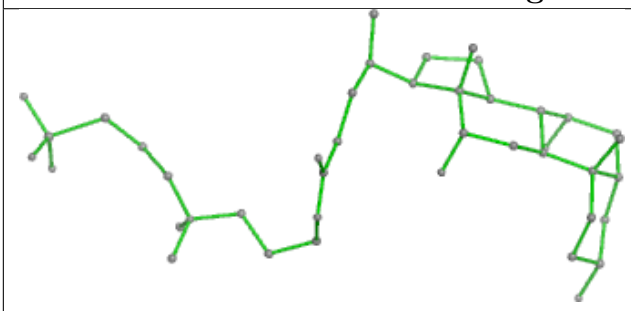


Torsions



Rings

Ligand CPS C 501



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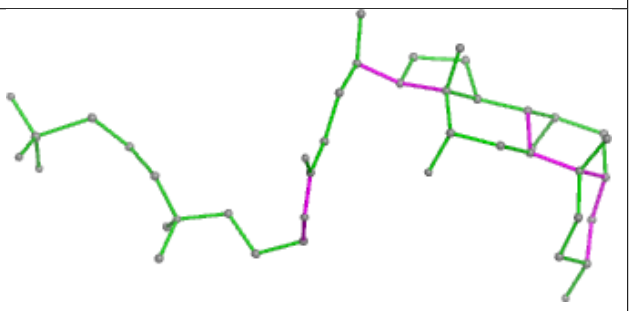

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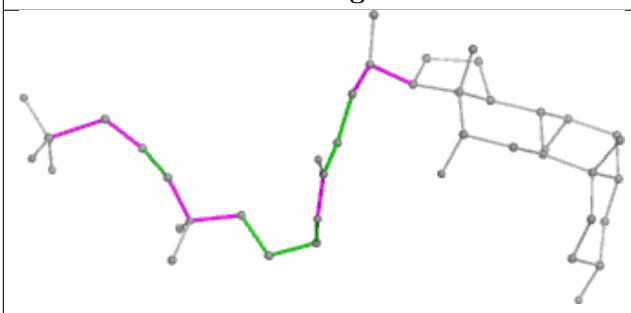

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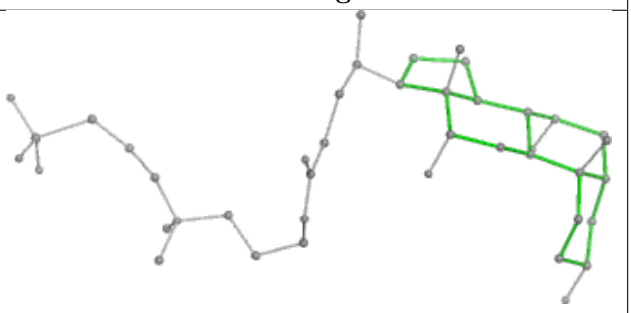
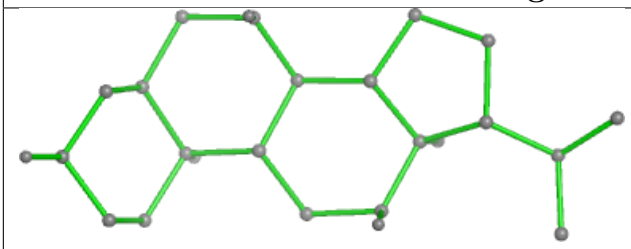


Rings

Ligand CPS E 502



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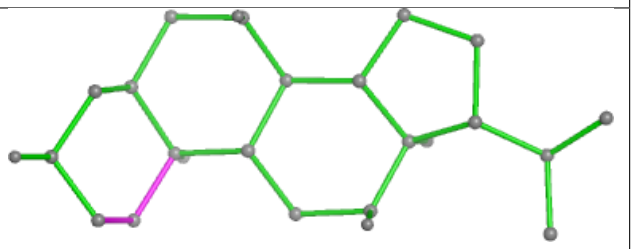
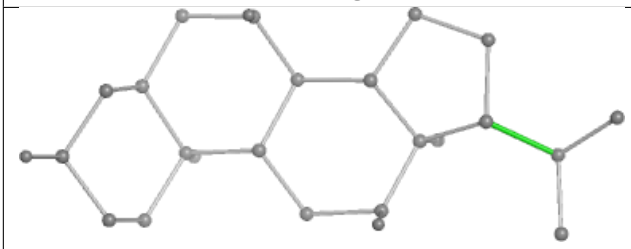


Bond angles



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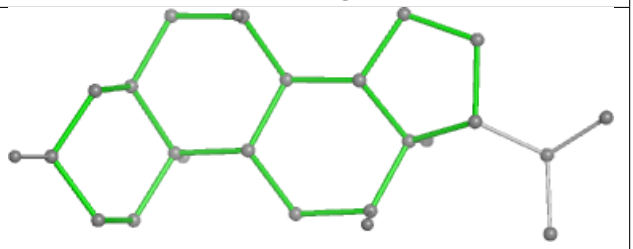
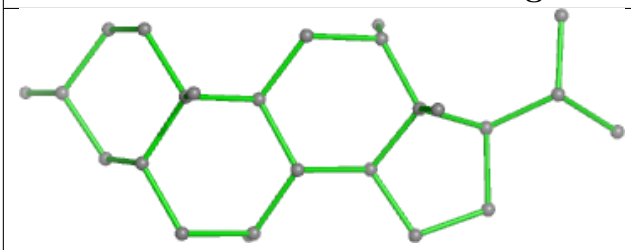


Rings

Ligand CPS H 502



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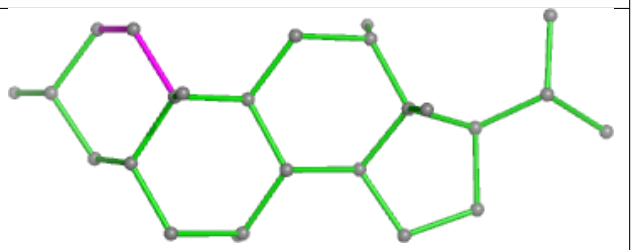
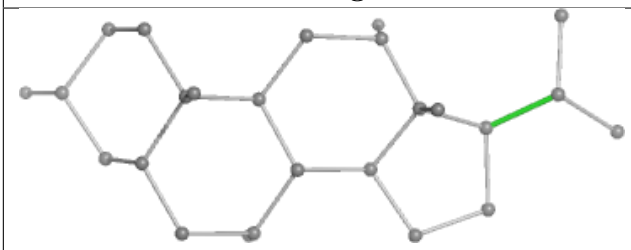
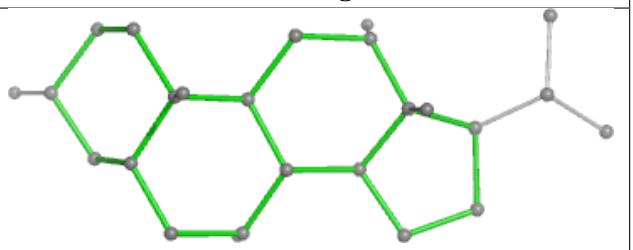


Bond angles

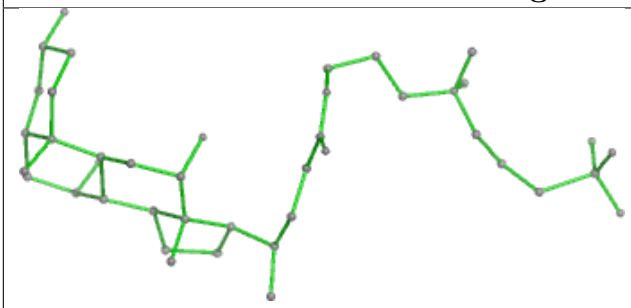


Torsions



Rings

Ligand CPS J 501



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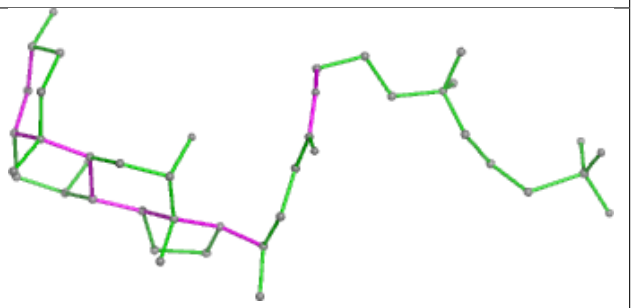
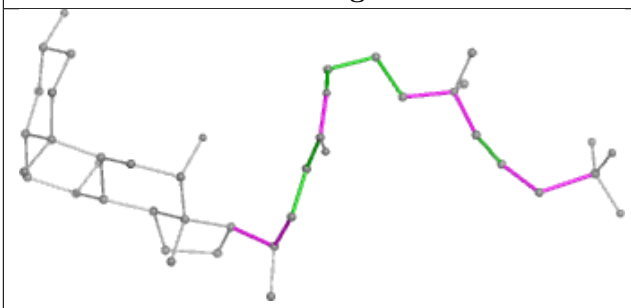


Bond angles



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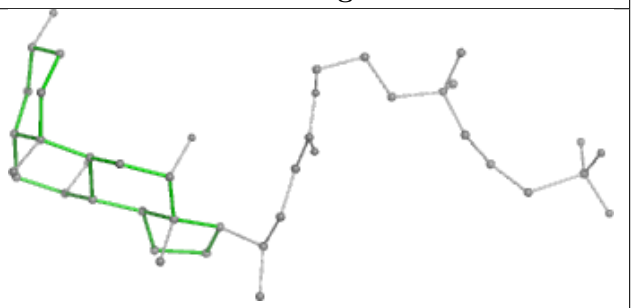
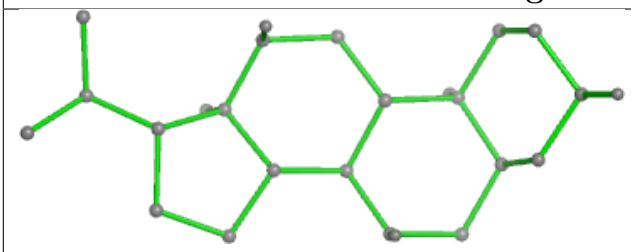


Rings

Ligand CPS O 501



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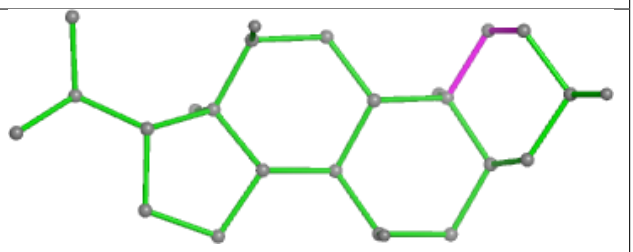

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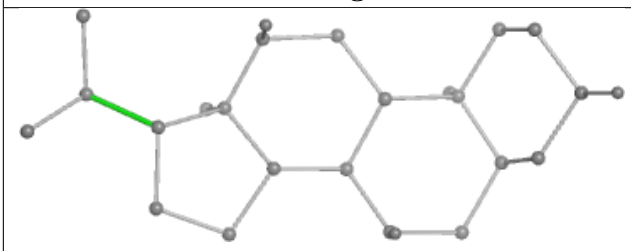

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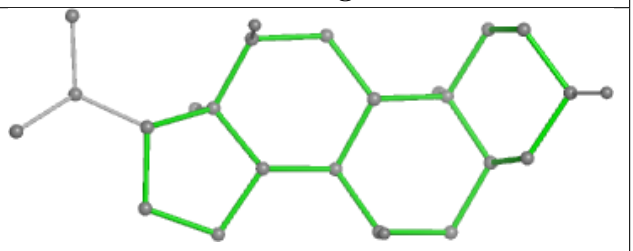
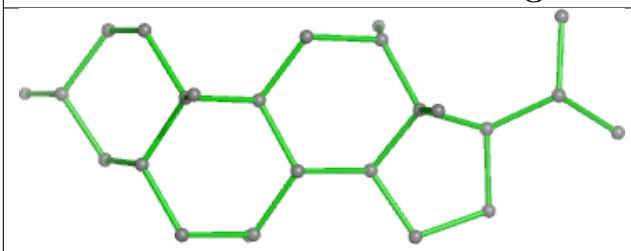


Rings

Ligand CPS K 502



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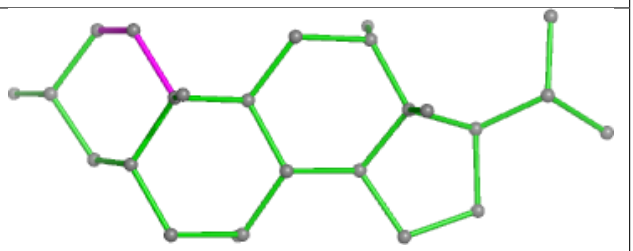
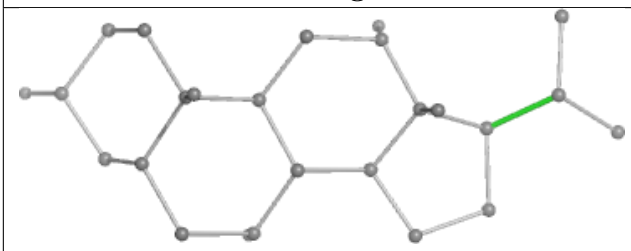


Bond angles



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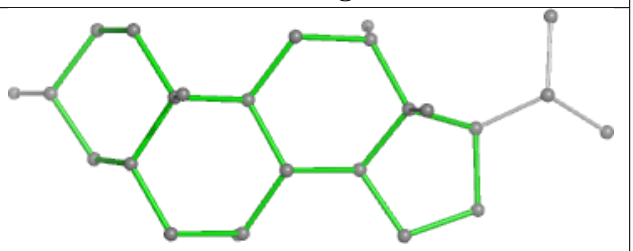
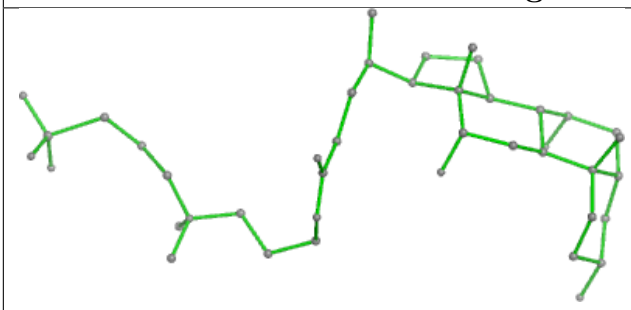


Rings

Ligand CPS A 501



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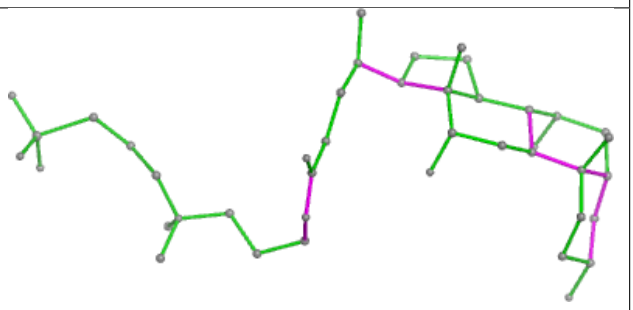

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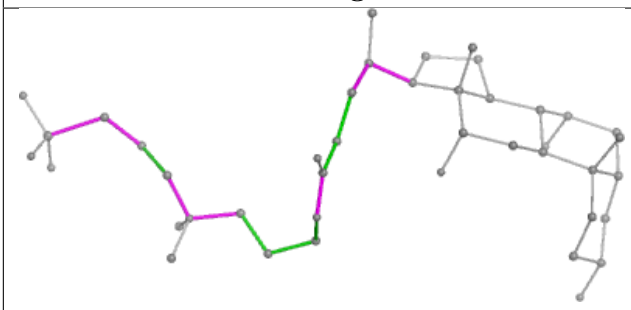

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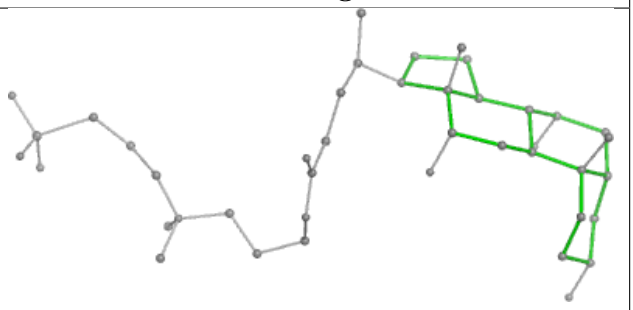
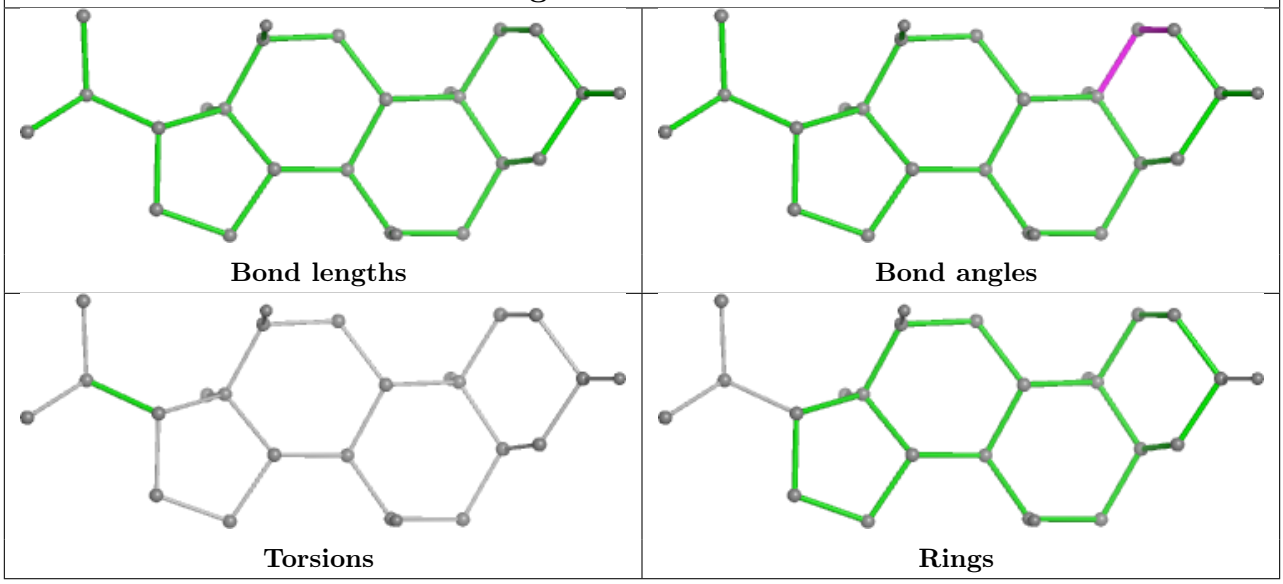
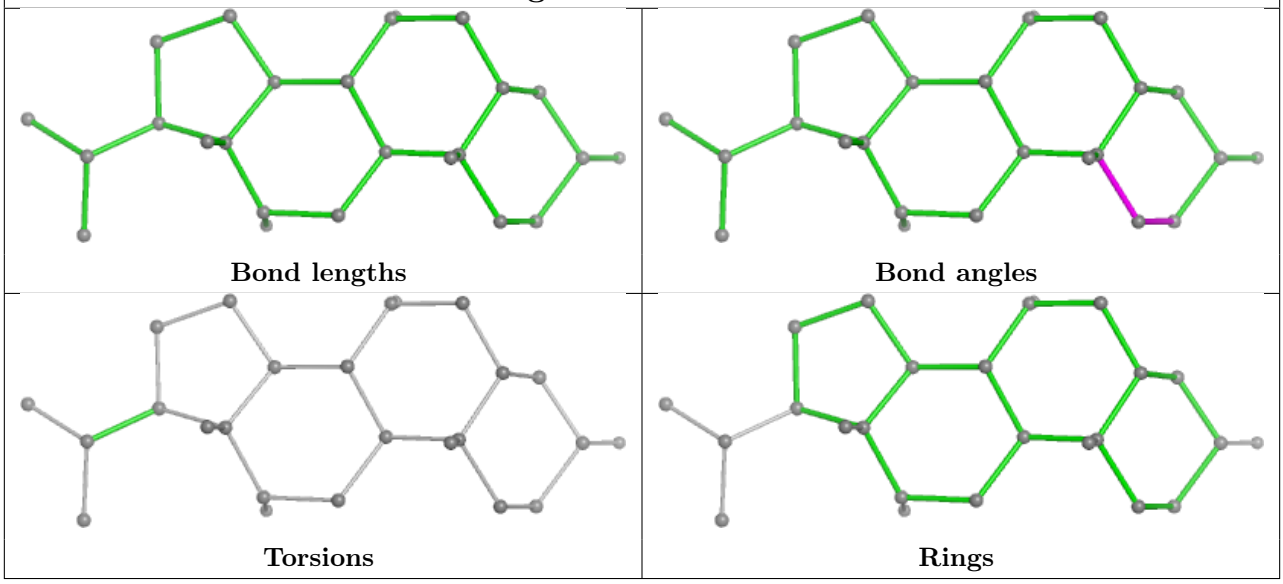


Rings

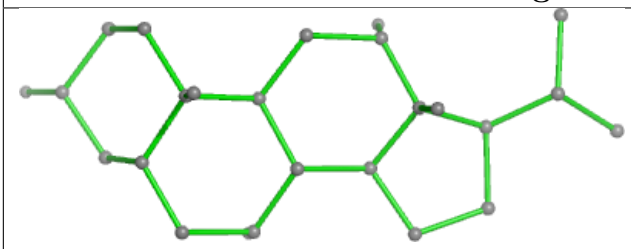
Ligand CPS L 502



Ligand CPS B 502



Ligand CPS I 502



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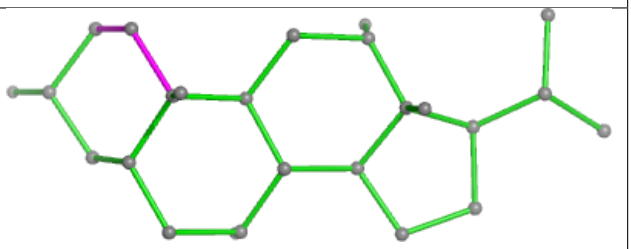
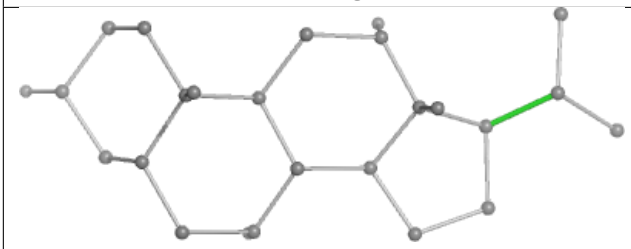
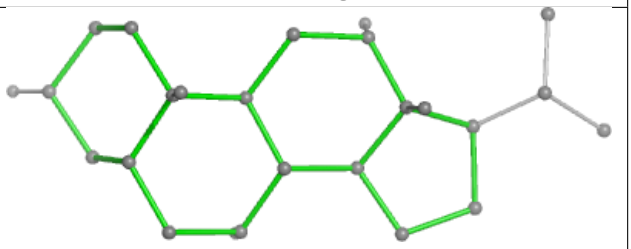


Bond angles

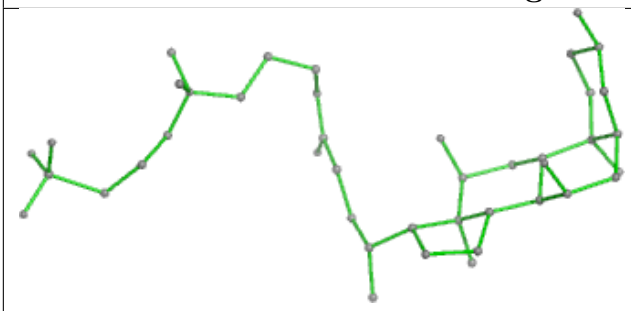


Torsions

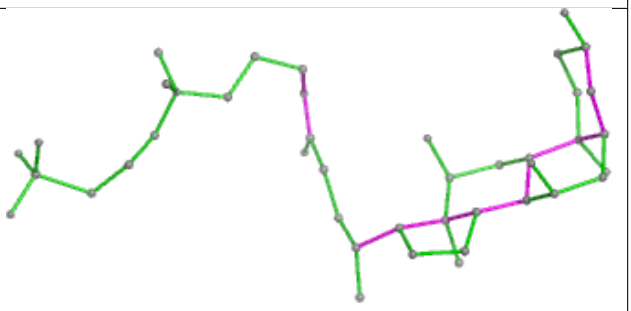


Rings

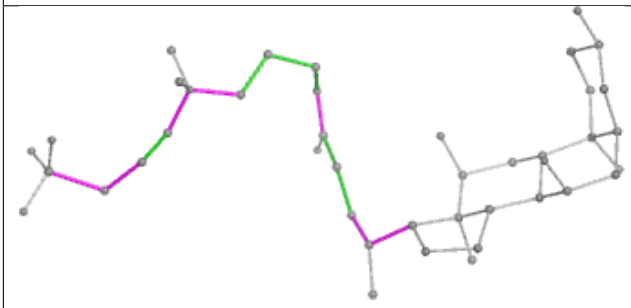
Ligand CPS G 501



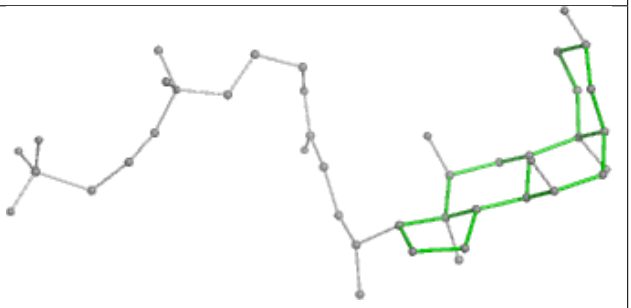
Bond lengths



Bond angles

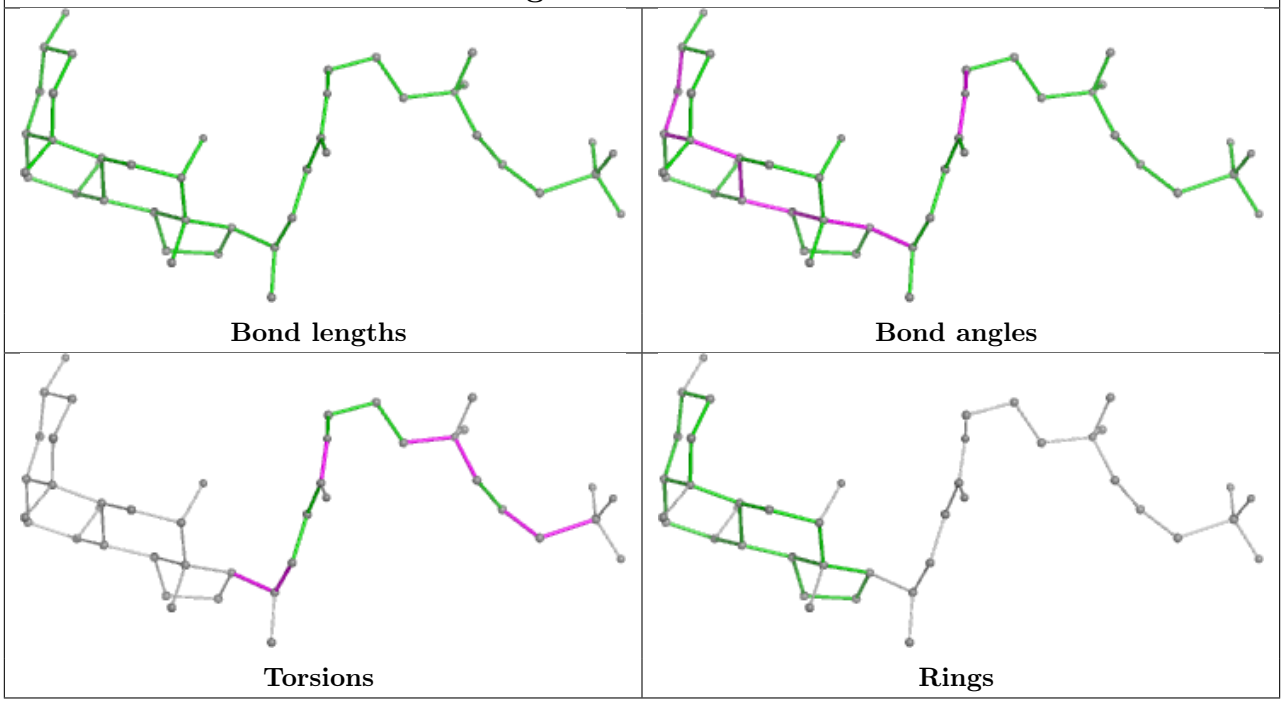


Torsions

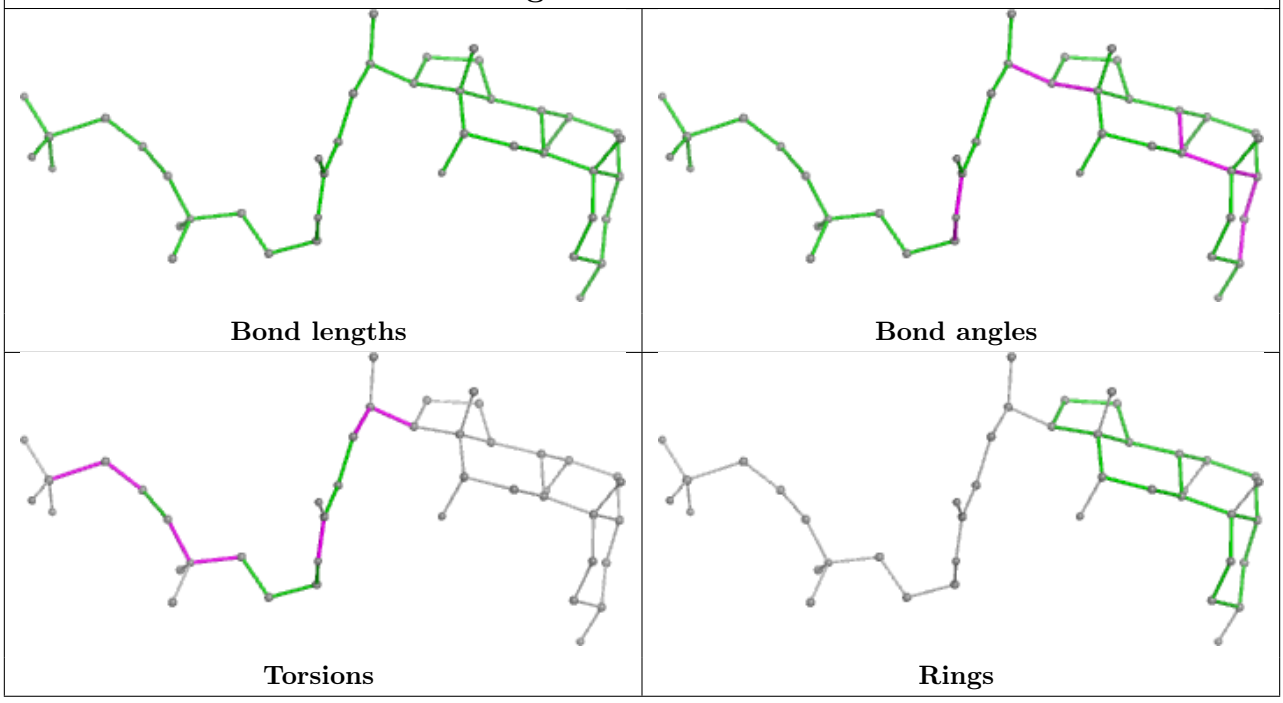


Rings

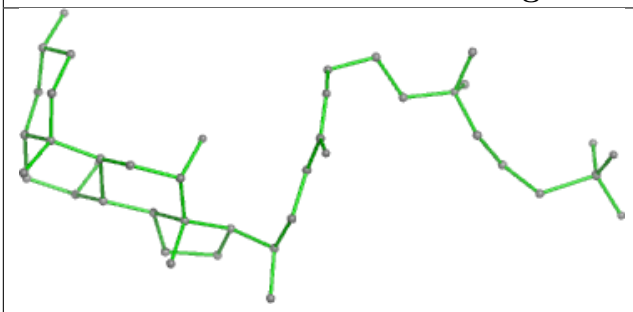
Ligand CPS H 501



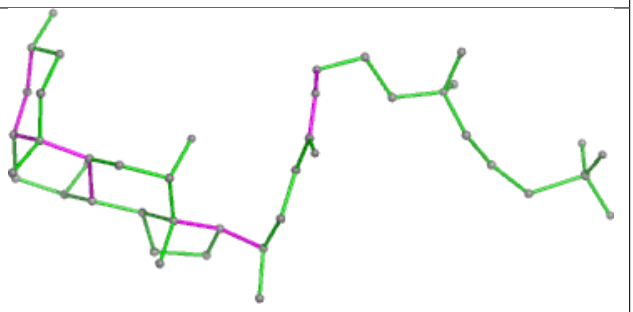
Ligand CPS D 501



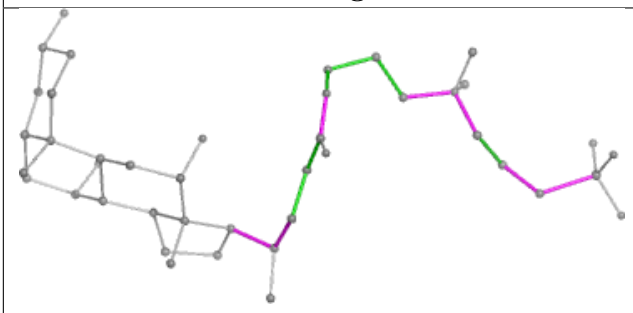
Ligand CPS M 501



Bond lengths



Bond angles



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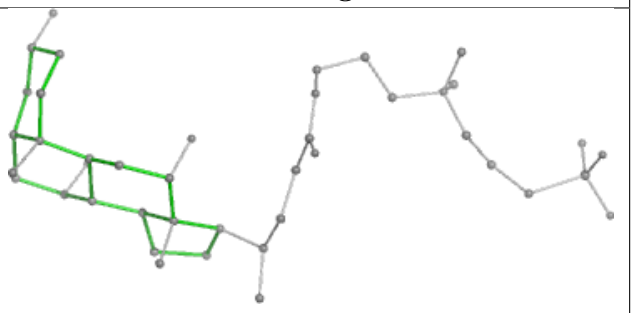
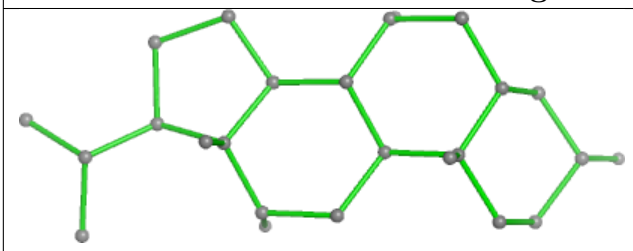


Rings

Ligand CPS J 502



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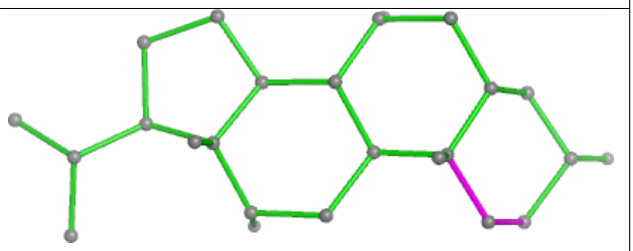
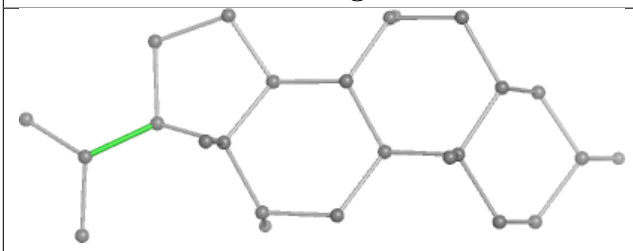


Bond angles



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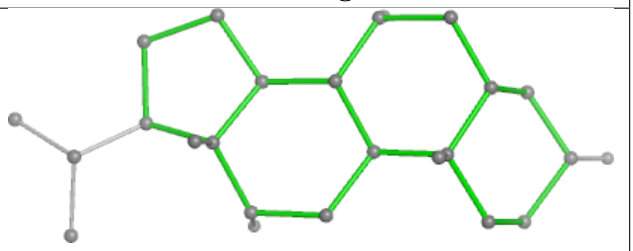
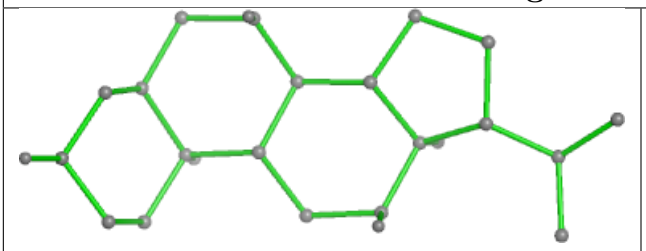


Rings

Ligand CPS C 502



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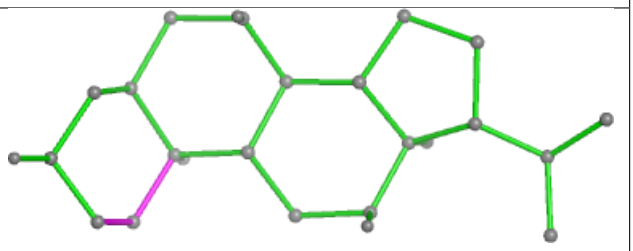
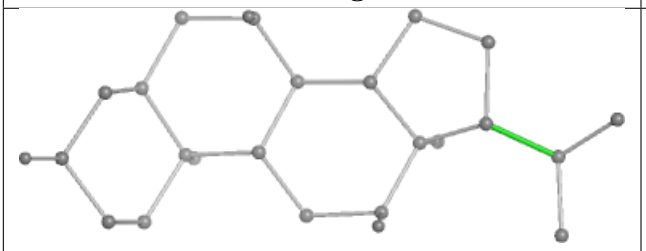


Bond angles



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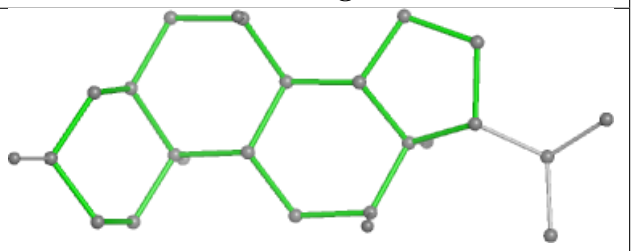
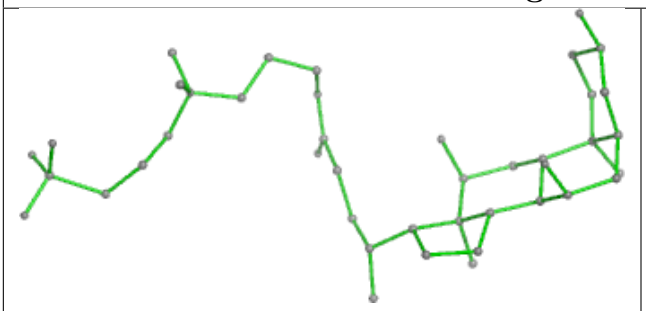


Rings

Ligand CPS O 502



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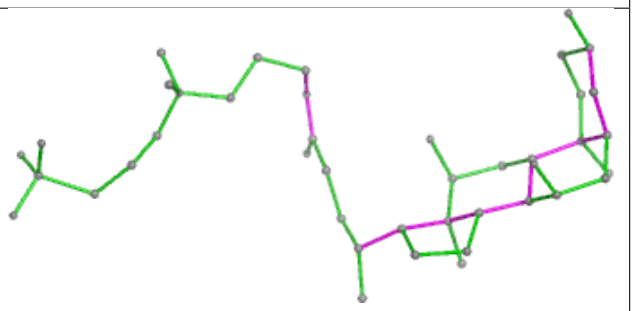
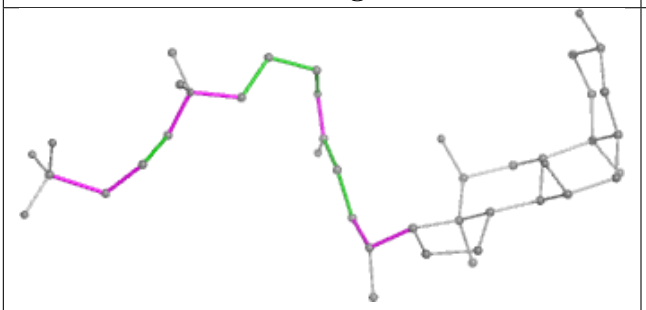
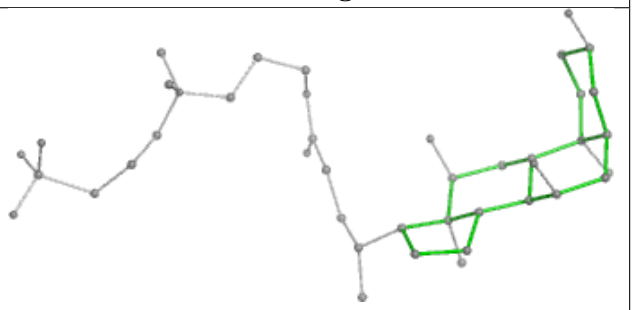


Bond angles

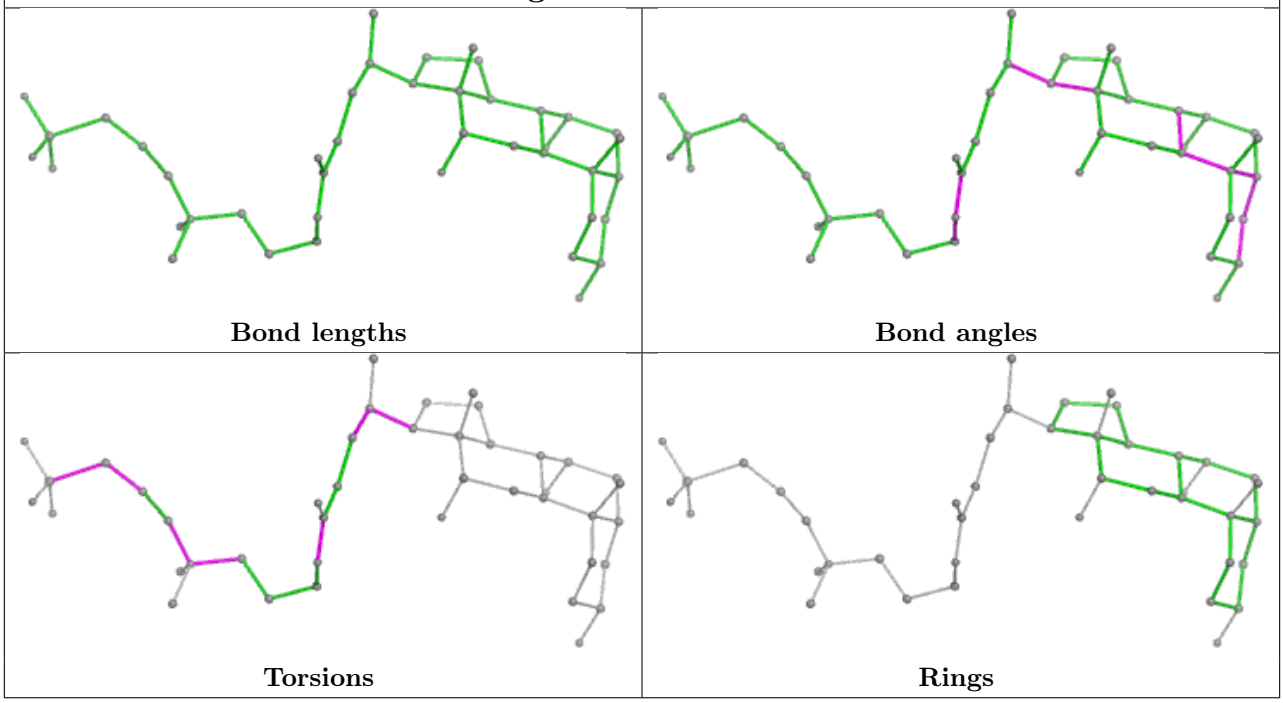


Torsions

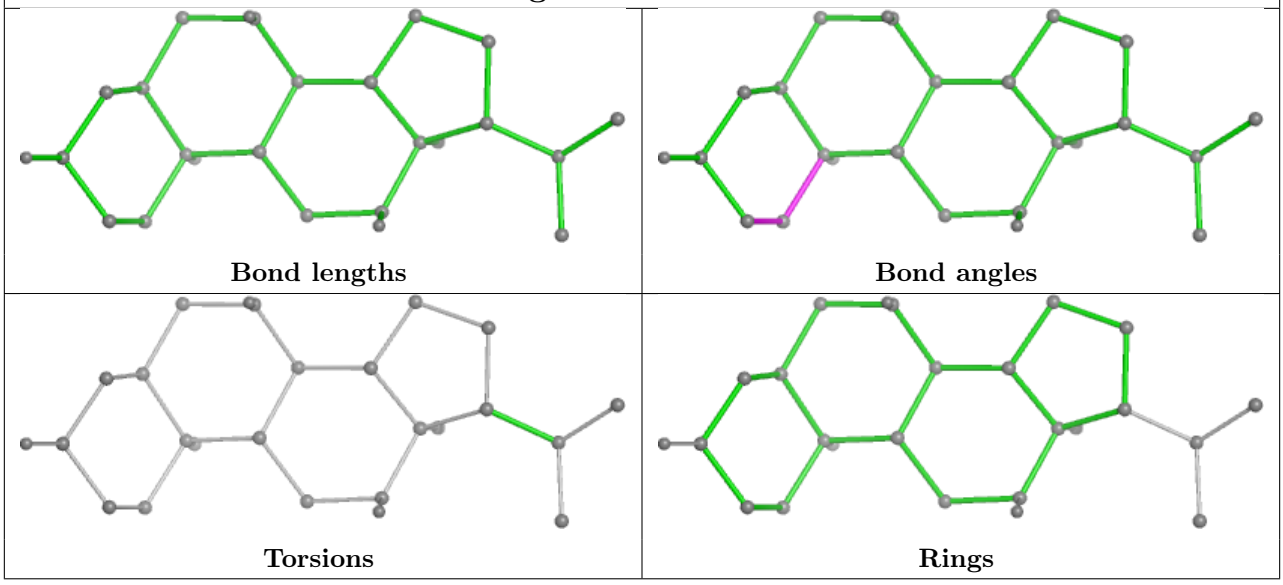


Rings

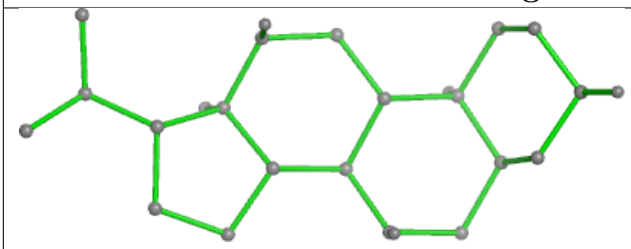
Ligand CPS B 501



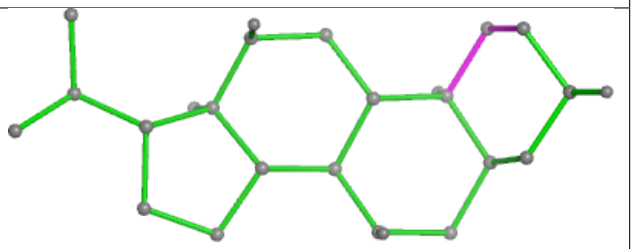
Ligand CPS F 502



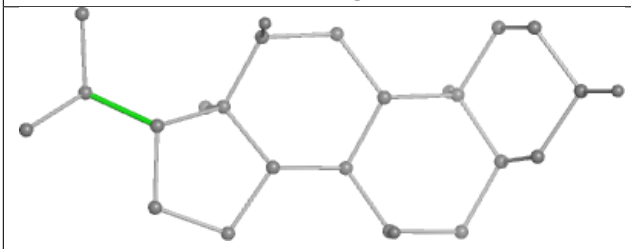
Ligand CPS M 502



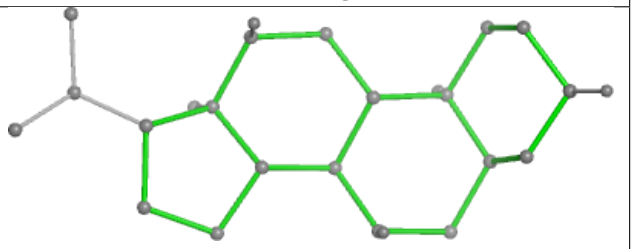
Bond lengths



Bond angles

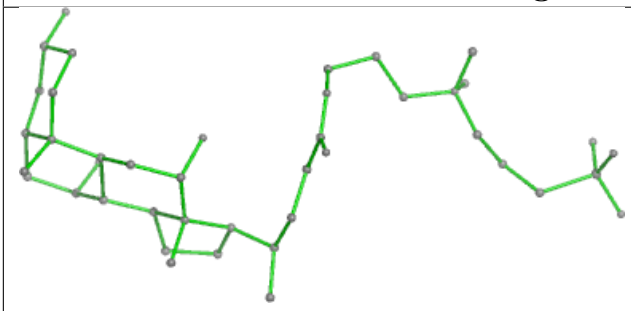


Torsions

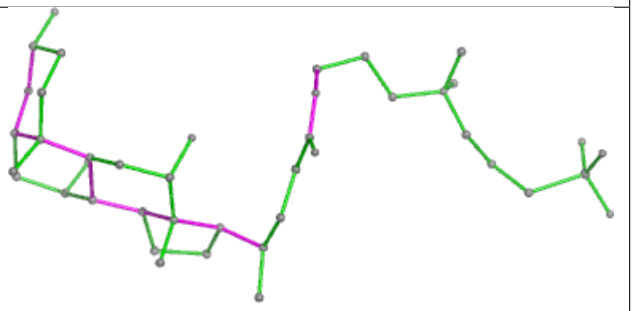


Rings

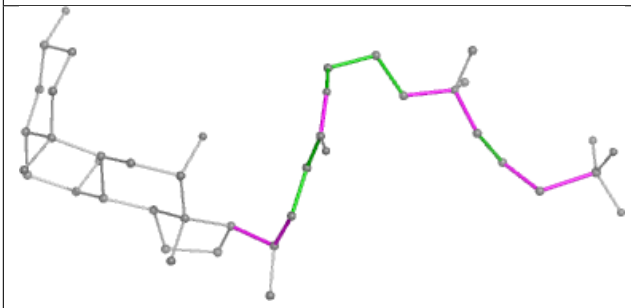
Ligand CPS I 501



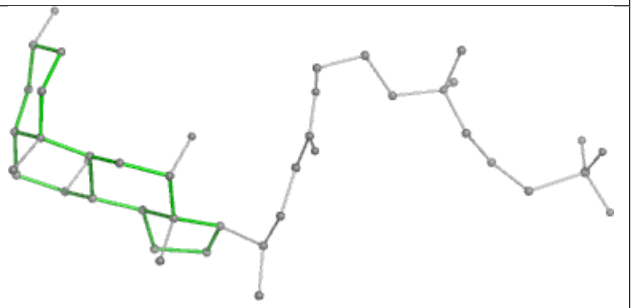
Bond lengths



Bond angles

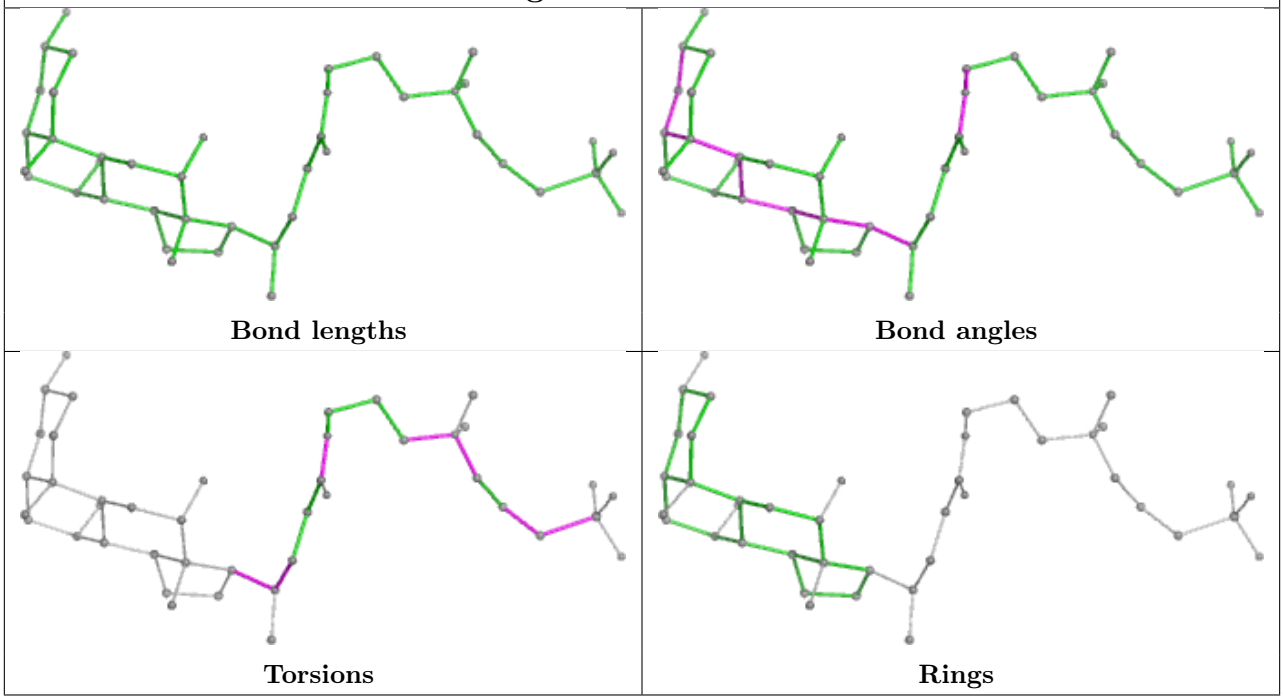


Torsions

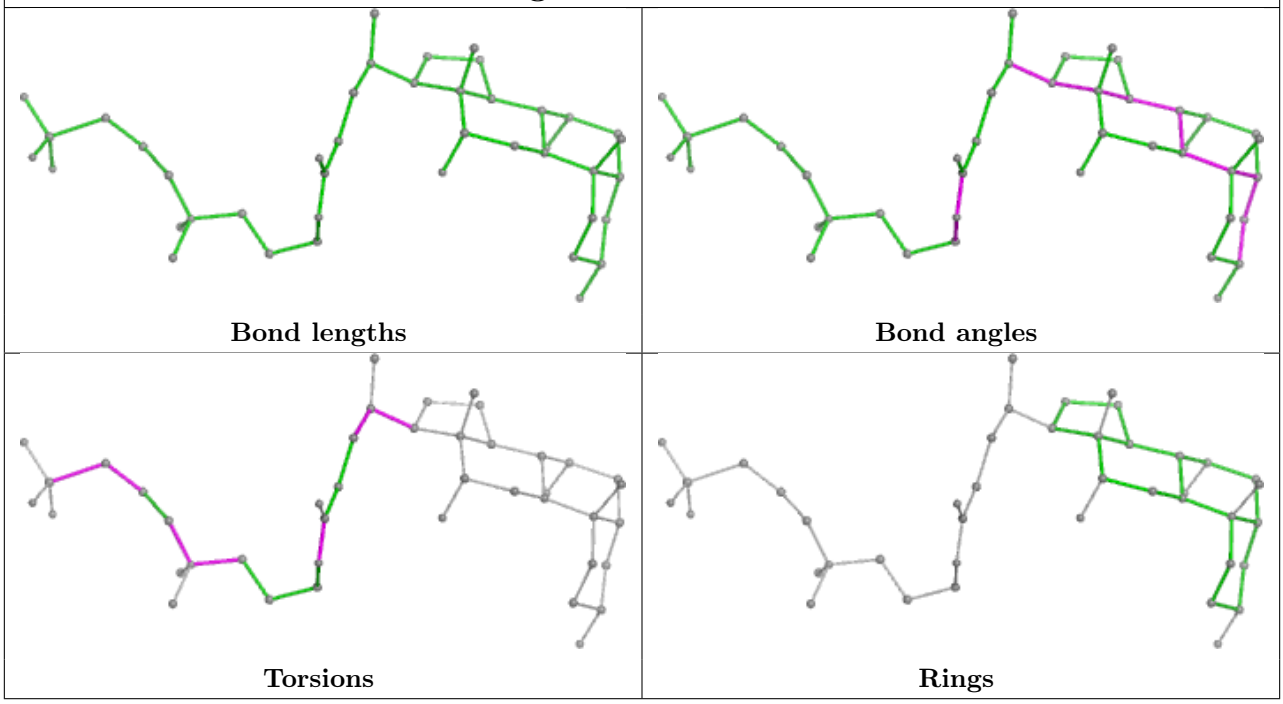


Rings

Ligand CPS K 501



Ligand CPS F 501



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.

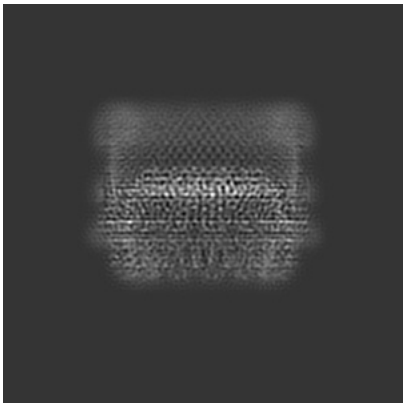
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12874. These allow visual inspection of the internal detail of the map and identification of artifacts.

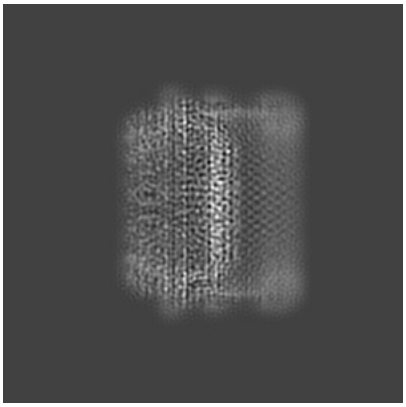
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

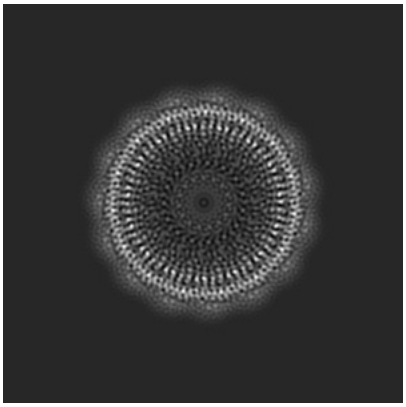
6.1.1 Primary map



X



Y

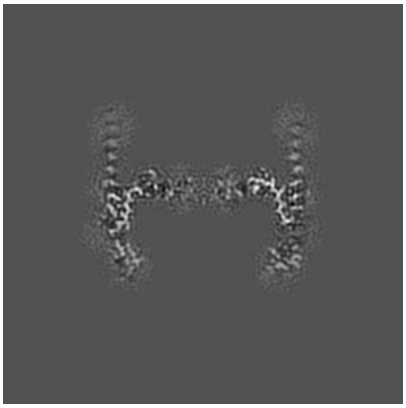


Z

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

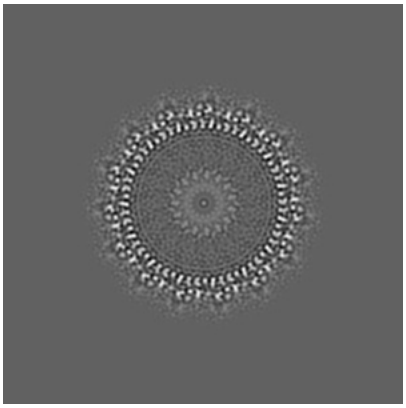
6.2 Central slices

6.2.1 Primary map



X Index: 112

Y Index: 112

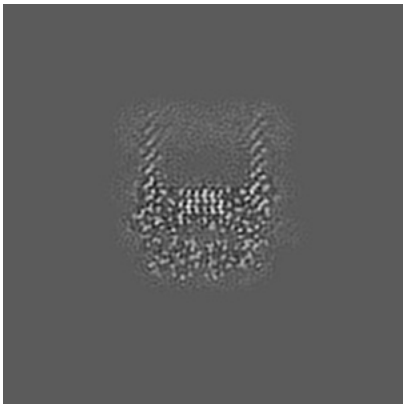


Z Index: 112

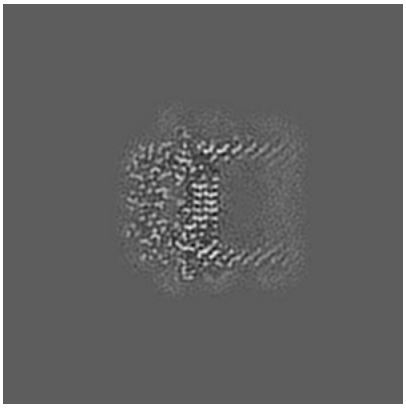
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

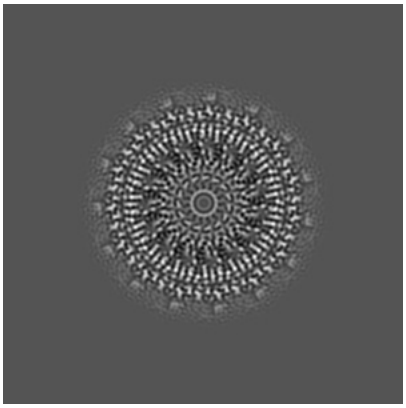
6.3.1 Primary map



X Index: 154



Y Index: 70

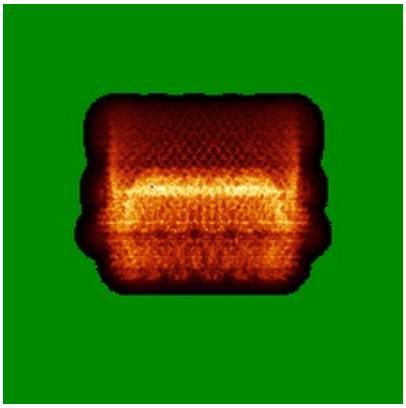


Z Index: 119

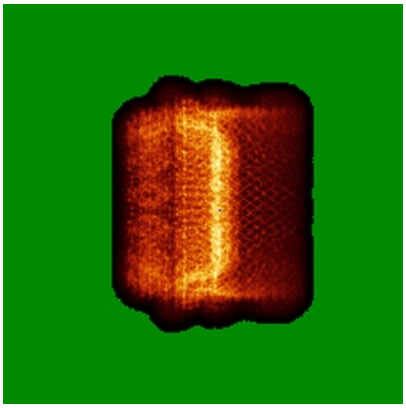
The images above show the largest variance slices of the map in three orthogonal directions.

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

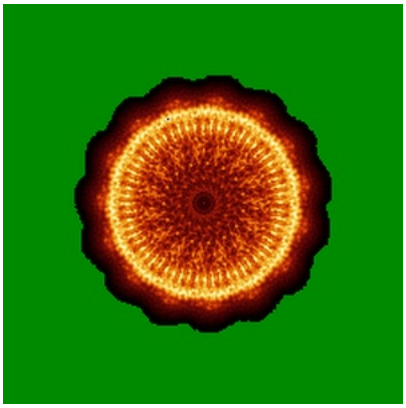
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

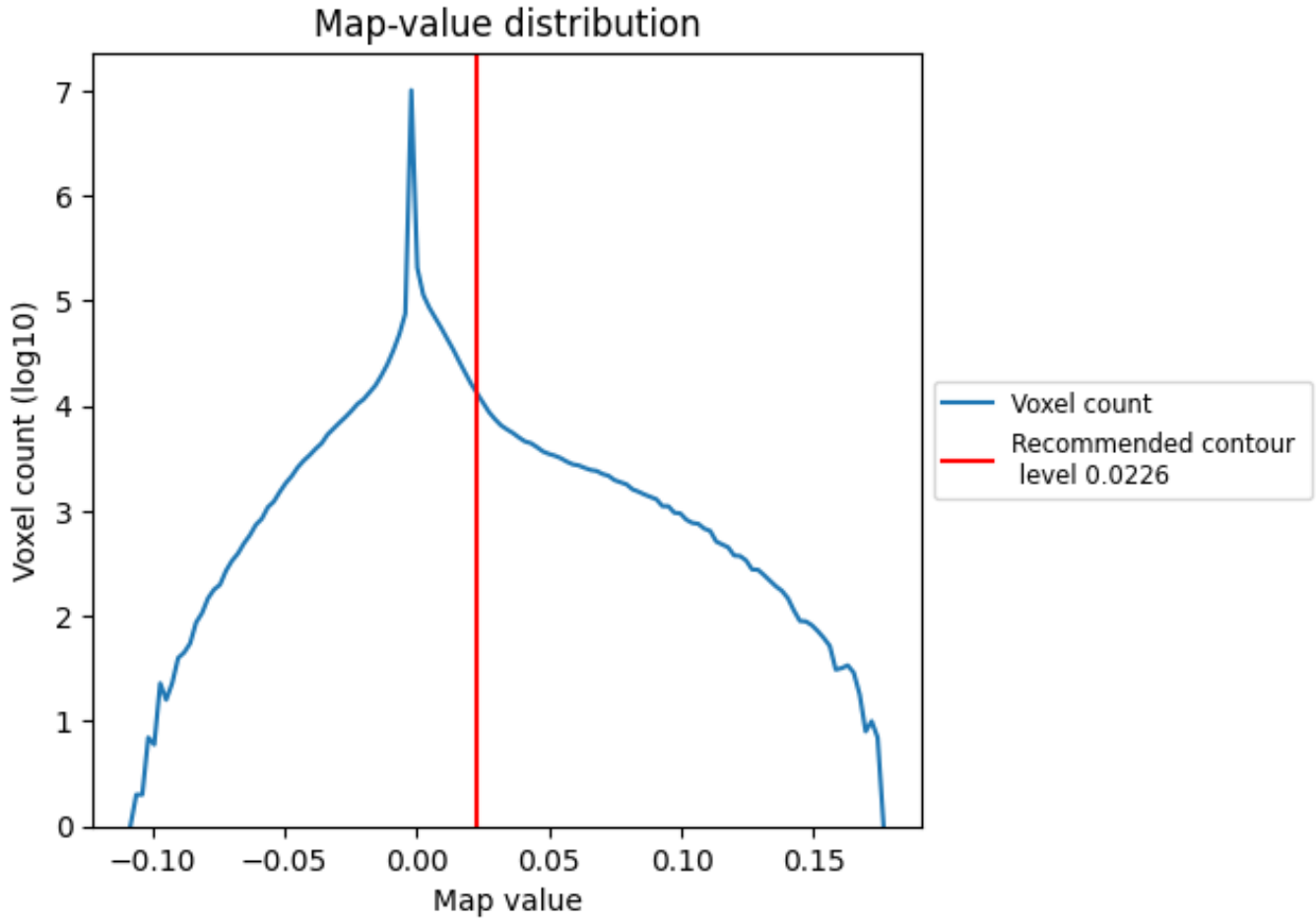
6.6 Mask visualisation (i)

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

7 Map analysis

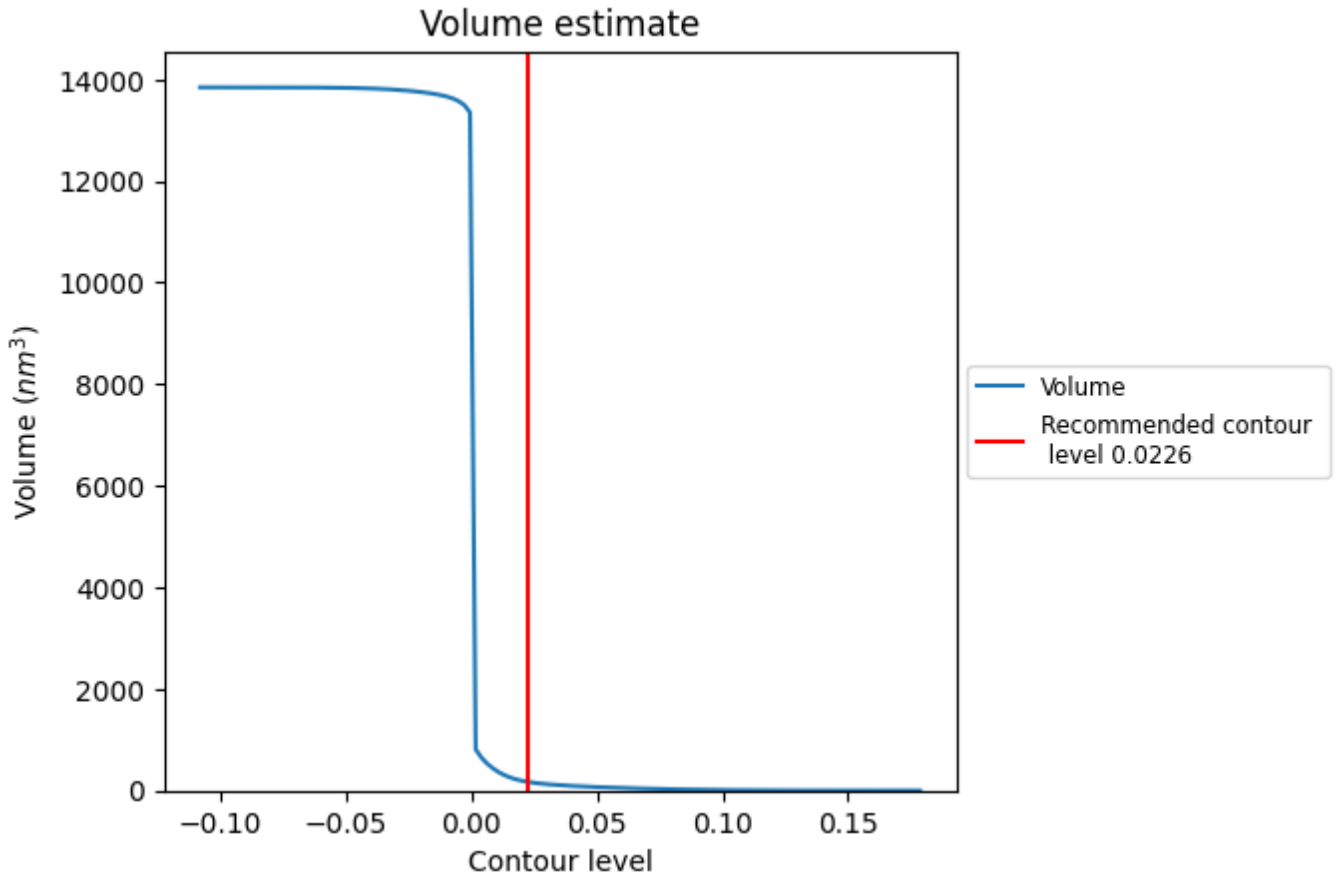
This section contains the results of statistical analysis of the map.

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.

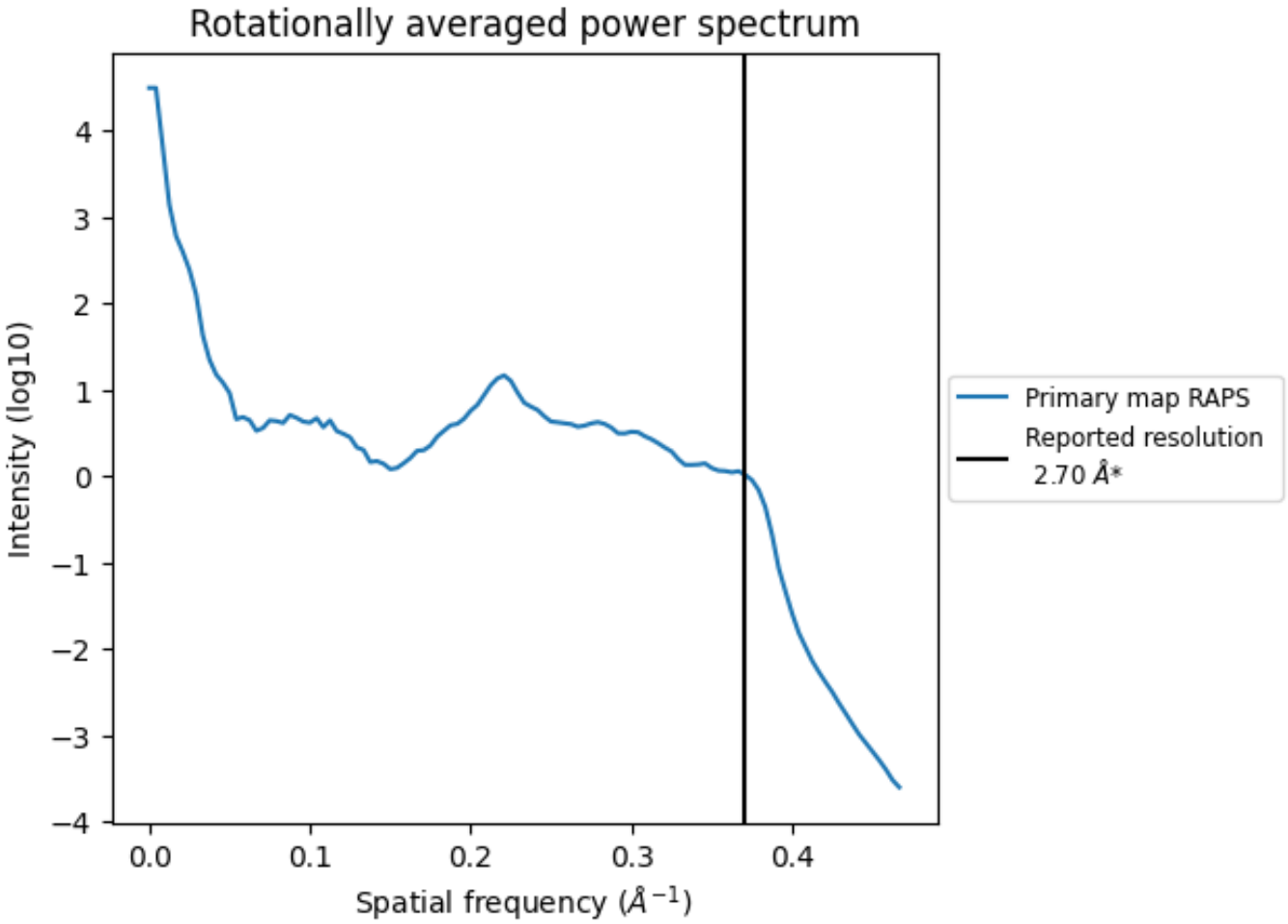
7.2 Volume estimate



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 153 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

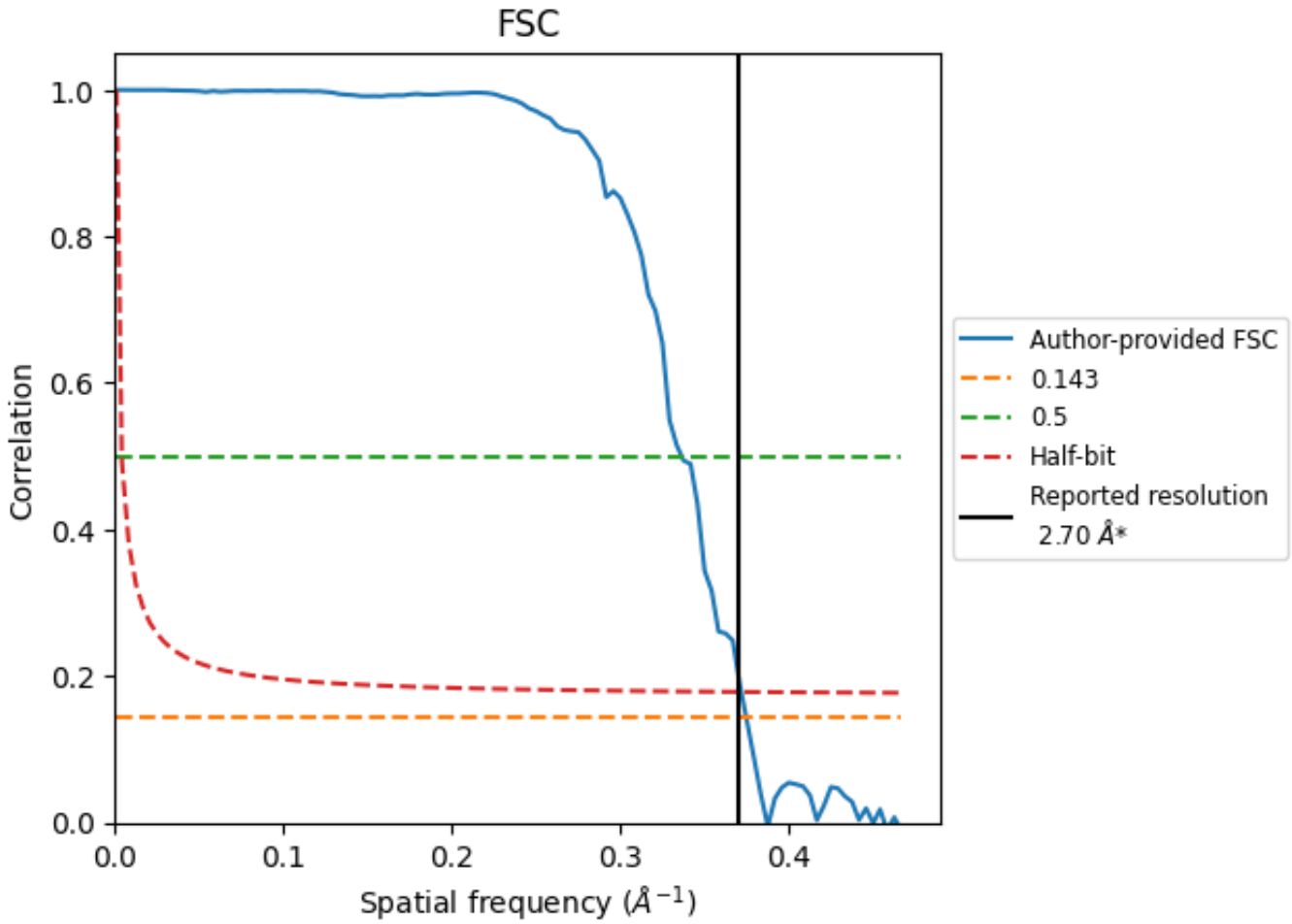


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

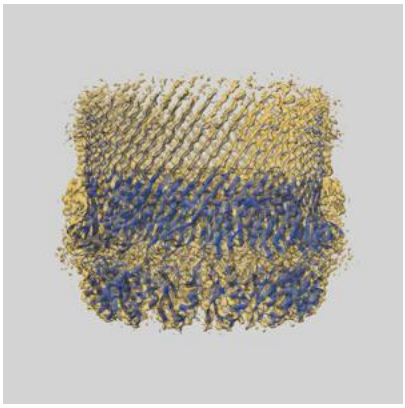
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	2.98	2.69
Unmasked-calculated*	-	-	-

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

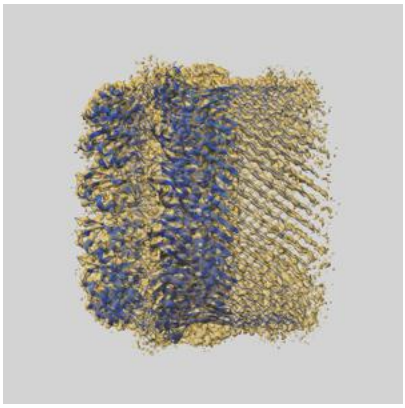
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12874 and PDB model 7OFH. Per-residue inclusion information can be found in section 3 on page 12.

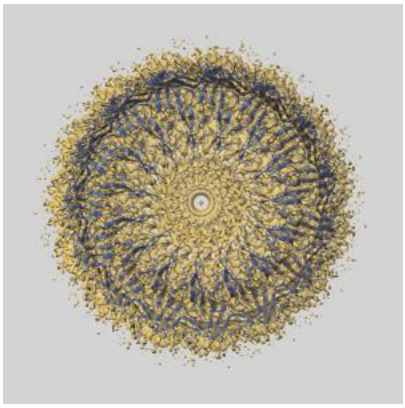
9.1 Map-model overlay



X



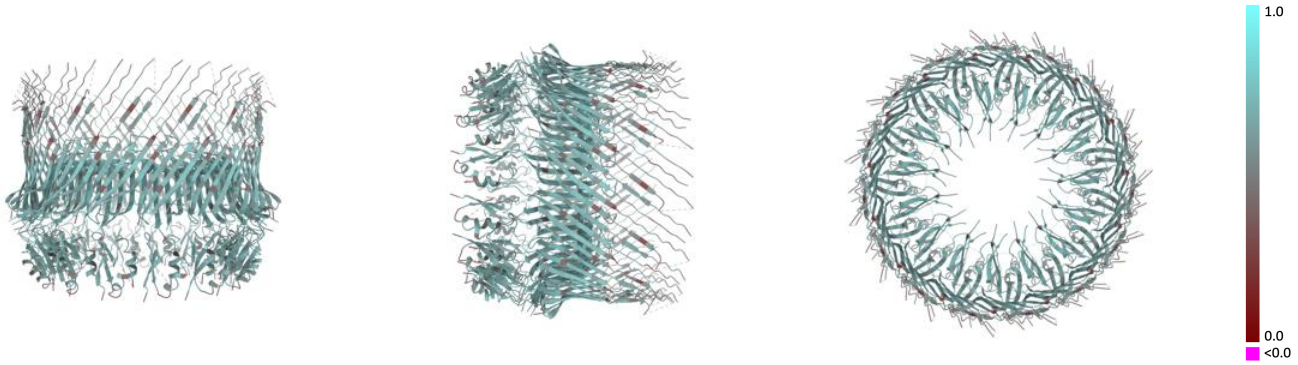
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

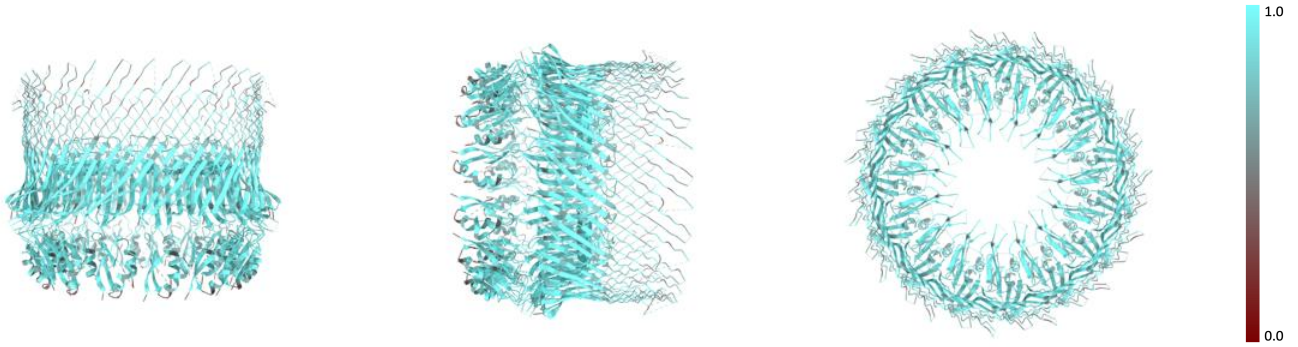
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

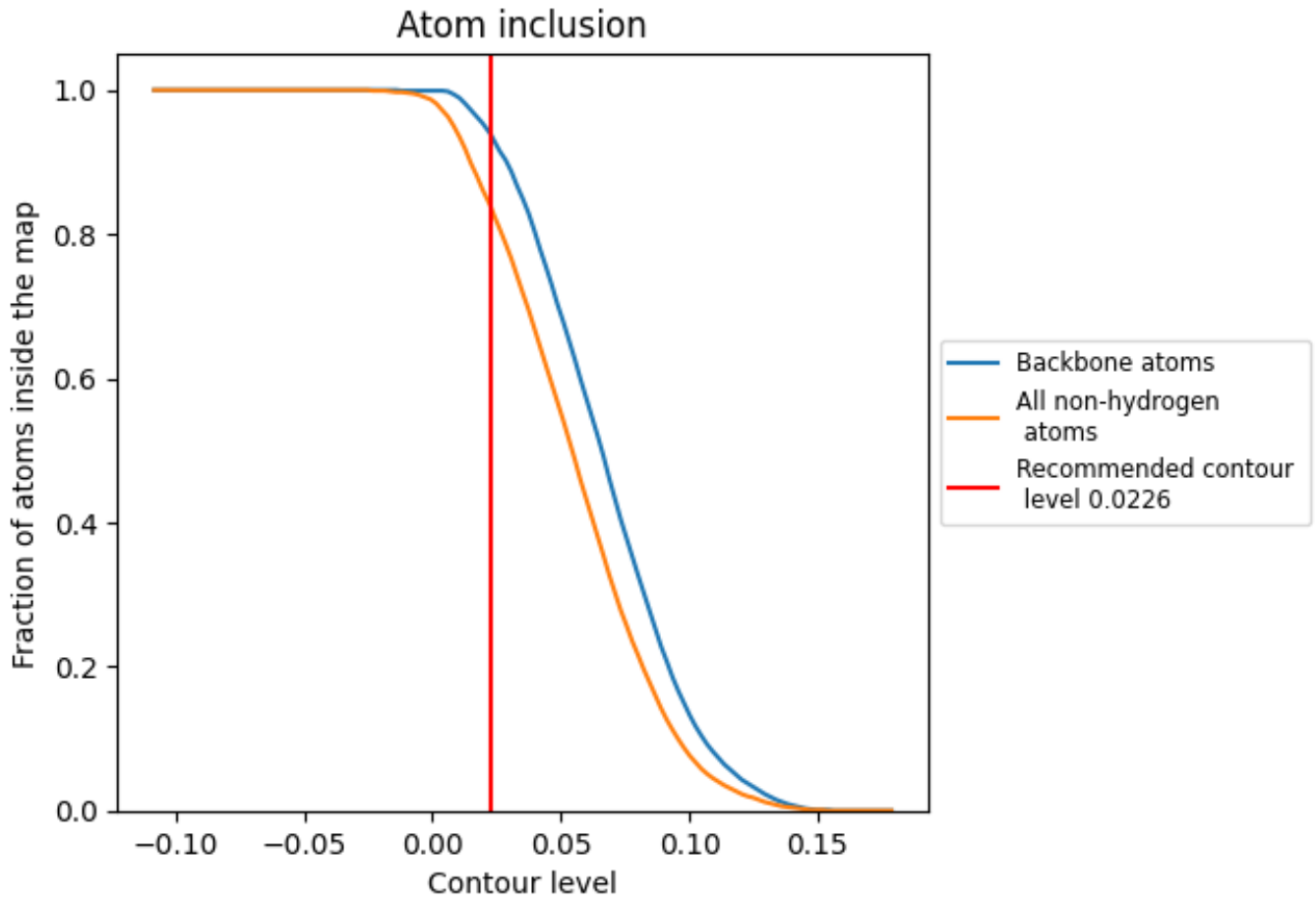
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0226).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.5780
A	0.8420	0.5780
B	0.8390	0.5760
C	0.8390	0.5780
D	0.8360	0.5770
E	0.8400	0.5780
F	0.8450	0.5780
G	0.8360	0.5780
H	0.8370	0.5780
I	0.8370	0.5770
J	0.8390	0.5770
K	0.8380	0.5790
L	0.8390	0.5820
M	0.8430	0.5790
N	0.8400	0.5790
O	0.8350	0.5760