Full wwPDB EM Validation Report ⓘ

Mar 20, 2023 – 07:33 pm GMT

PDB ID	:	8AOW
EMDB ID	:	EMD-15554
Title	:	CryoEM structure of the Chikungunya virus nsP1 capping pores in complex with m7GTP and SAH ligands
Authors	:	Jones, R.; Hons, M.; Reguera, J.
Deposited on	:	2022-08-08
Resolution	:	2.70 Å(reported)
Based on initial model	:	6Z0V

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:

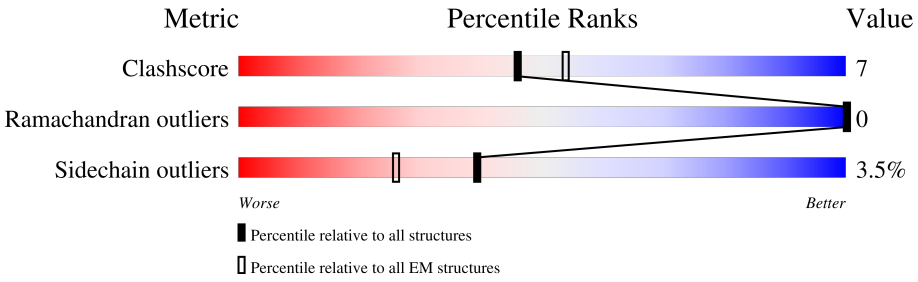
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



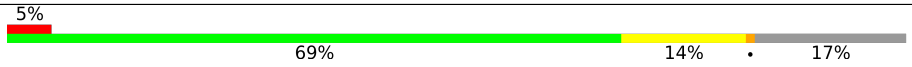
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	543	68% 14% • 17%
1	C	543	67% 15% • 17%
1	E	543	68% 14% • 17%
1	G	543	68% 13% • 17%
1	I	543	70% 12% • 17%
1	K	543	68% 15% • 17%
1	M	543	69% 13% • 17%
1	O	543	67% 15% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	543	
1	S	543	
1	V	543	
1	X	543	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43632 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 mRNA-capping enzyme nsP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	C	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	E	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	G	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	I	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	K	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	M	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	O	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	Q	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	S	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	V	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		
1	X	451	Total	C	N	O	S	4	0
			3547	2239	618	659	31		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	536	ALA	-	expression tag	UNP Q8JUX6
A	537	ALA	-	expression tag	UNP Q8JUX6
A	538	HIS	-	expression tag	UNP Q8JUX6
A	539	HIS	-	expression tag	UNP Q8JUX6
A	540	HIS	-	expression tag	UNP Q8JUX6
A	541	HIS	-	expression tag	UNP Q8JUX6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	HIS	-	expression tag	UNP Q8JUX6
A	543	HIS	-	expression tag	UNP Q8JUX6
C	536	ALA	-	expression tag	UNP Q8JUX6
C	537	ALA	-	expression tag	UNP Q8JUX6
C	538	HIS	-	expression tag	UNP Q8JUX6
C	539	HIS	-	expression tag	UNP Q8JUX6
C	540	HIS	-	expression tag	UNP Q8JUX6
C	541	HIS	-	expression tag	UNP Q8JUX6
C	542	HIS	-	expression tag	UNP Q8JUX6
C	543	HIS	-	expression tag	UNP Q8JUX6
E	536	ALA	-	expression tag	UNP Q8JUX6
E	537	ALA	-	expression tag	UNP Q8JUX6
E	538	HIS	-	expression tag	UNP Q8JUX6
E	539	HIS	-	expression tag	UNP Q8JUX6
E	540	HIS	-	expression tag	UNP Q8JUX6
E	541	HIS	-	expression tag	UNP Q8JUX6
E	542	HIS	-	expression tag	UNP Q8JUX6
E	543	HIS	-	expression tag	UNP Q8JUX6
G	536	ALA	-	expression tag	UNP Q8JUX6
G	537	ALA	-	expression tag	UNP Q8JUX6
G	538	HIS	-	expression tag	UNP Q8JUX6
G	539	HIS	-	expression tag	UNP Q8JUX6
G	540	HIS	-	expression tag	UNP Q8JUX6
G	541	HIS	-	expression tag	UNP Q8JUX6
G	542	HIS	-	expression tag	UNP Q8JUX6
G	543	HIS	-	expression tag	UNP Q8JUX6
I	536	ALA	-	expression tag	UNP Q8JUX6
I	537	ALA	-	expression tag	UNP Q8JUX6
I	538	HIS	-	expression tag	UNP Q8JUX6
I	539	HIS	-	expression tag	UNP Q8JUX6
I	540	HIS	-	expression tag	UNP Q8JUX6
I	541	HIS	-	expression tag	UNP Q8JUX6
I	542	HIS	-	expression tag	UNP Q8JUX6
I	543	HIS	-	expression tag	UNP Q8JUX6
K	536	ALA	-	expression tag	UNP Q8JUX6
K	537	ALA	-	expression tag	UNP Q8JUX6
K	538	HIS	-	expression tag	UNP Q8JUX6
K	539	HIS	-	expression tag	UNP Q8JUX6
K	540	HIS	-	expression tag	UNP Q8JUX6
K	541	HIS	-	expression tag	UNP Q8JUX6
K	542	HIS	-	expression tag	UNP Q8JUX6
K	543	HIS	-	expression tag	UNP Q8JUX6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	536	ALA	-	expression tag	UNP Q8JUX6
M	537	ALA	-	expression tag	UNP Q8JUX6
M	538	HIS	-	expression tag	UNP Q8JUX6
M	539	HIS	-	expression tag	UNP Q8JUX6
M	540	HIS	-	expression tag	UNP Q8JUX6
M	541	HIS	-	expression tag	UNP Q8JUX6
M	542	HIS	-	expression tag	UNP Q8JUX6
M	543	HIS	-	expression tag	UNP Q8JUX6
O	536	ALA	-	expression tag	UNP Q8JUX6
O	537	ALA	-	expression tag	UNP Q8JUX6
O	538	HIS	-	expression tag	UNP Q8JUX6
O	539	HIS	-	expression tag	UNP Q8JUX6
O	540	HIS	-	expression tag	UNP Q8JUX6
O	541	HIS	-	expression tag	UNP Q8JUX6
O	542	HIS	-	expression tag	UNP Q8JUX6
O	543	HIS	-	expression tag	UNP Q8JUX6
Q	536	ALA	-	expression tag	UNP Q8JUX6
Q	537	ALA	-	expression tag	UNP Q8JUX6
Q	538	HIS	-	expression tag	UNP Q8JUX6
Q	539	HIS	-	expression tag	UNP Q8JUX6
Q	540	HIS	-	expression tag	UNP Q8JUX6
Q	541	HIS	-	expression tag	UNP Q8JUX6
Q	542	HIS	-	expression tag	UNP Q8JUX6
Q	543	HIS	-	expression tag	UNP Q8JUX6
S	536	ALA	-	expression tag	UNP Q8JUX6
S	537	ALA	-	expression tag	UNP Q8JUX6
S	538	HIS	-	expression tag	UNP Q8JUX6
S	539	HIS	-	expression tag	UNP Q8JUX6
S	540	HIS	-	expression tag	UNP Q8JUX6
S	541	HIS	-	expression tag	UNP Q8JUX6
S	542	HIS	-	expression tag	UNP Q8JUX6
S	543	HIS	-	expression tag	UNP Q8JUX6
V	536	ALA	-	expression tag	UNP Q8JUX6
V	537	ALA	-	expression tag	UNP Q8JUX6
V	538	HIS	-	expression tag	UNP Q8JUX6
V	539	HIS	-	expression tag	UNP Q8JUX6
V	540	HIS	-	expression tag	UNP Q8JUX6
V	541	HIS	-	expression tag	UNP Q8JUX6
V	542	HIS	-	expression tag	UNP Q8JUX6
V	543	HIS	-	expression tag	UNP Q8JUX6
X	536	ALA	-	expression tag	UNP Q8JUX6
X	537	ALA	-	expression tag	UNP Q8JUX6

Continued on next page...

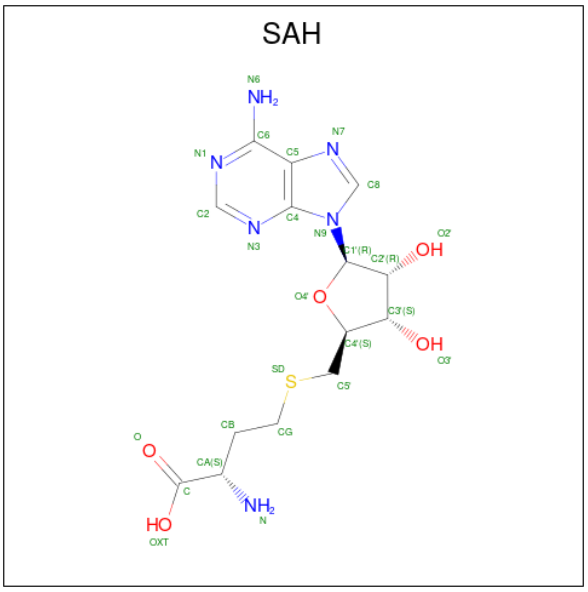
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	538	HIS	-	expression tag	UNP Q8JUX6
X	539	HIS	-	expression tag	UNP Q8JUX6
X	540	HIS	-	expression tag	UNP Q8JUX6
X	541	HIS	-	expression tag	UNP Q8JUX6
X	542	HIS	-	expression tag	UNP Q8JUX6
X	543	HIS	-	expression tag	UNP Q8JUX6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

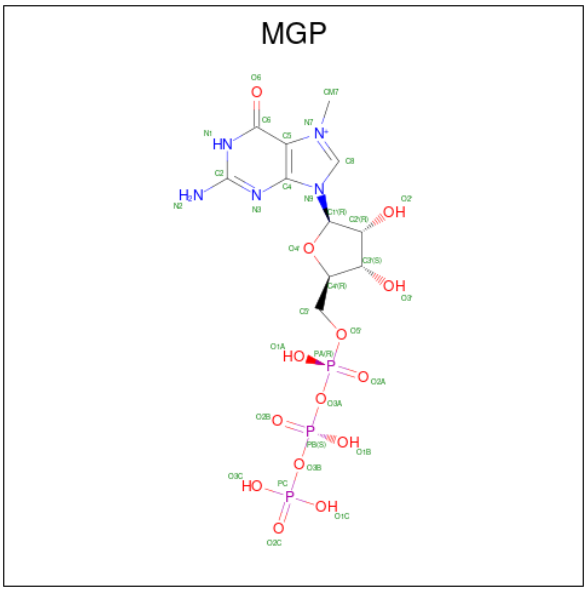
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	E	1	Total Zn 1 1	0
2	G	1	Total Zn 1 1	0
2	I	1	Total Zn 1 1	0
2	K	1	Total Zn 1 1	0
2	M	1	Total Zn 1 1	0
2	O	1	Total Zn 1 1	0
2	Q	1	Total Zn 1 1	0
2	S	1	Total Zn 1 1	0
2	V	1	Total Zn 1 1	0
2	X	1	Total Zn 1 1	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	C	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	E	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	G	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	I	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	K	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	M	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	O	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	Q	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	S	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	V	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	X	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 4 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: MGP) (formula: $C_{11}H_{19}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	C	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	E	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	G	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	I	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	K	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	M	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	O	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	Q	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	S	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	V	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	X	1	Total	C	N	O	P	0
			33	11	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Mg 2 2	0
5	C	2	Total Mg 2 2	0
5	E	2	Total Mg 2 2	0
5	G	2	Total Mg 2 2	0
5	I	2	Total Mg 2 2	0
5	K	2	Total Mg 2 2	0
5	M	2	Total Mg 2 2	0
5	O	2	Total Mg 2 2	0
5	Q	2	Total Mg 2 2	0
5	S	2	Total Mg 2 2	0
5	V	2	Total Mg 2 2	0
5	X	2	Total Mg 2 2	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	27	Total O 27 27	0
6	C	27	Total O 27 27	0
6	E	27	Total O 27 27	0
6	G	27	Total O 27 27	0
6	I	27	Total O 27 27	0
6	K	27	Total O 27 27	0
6	M	27	Total O 27 27	0
6	O	27	Total O 27 27	0

Continued on next page...

Continued from previous page...

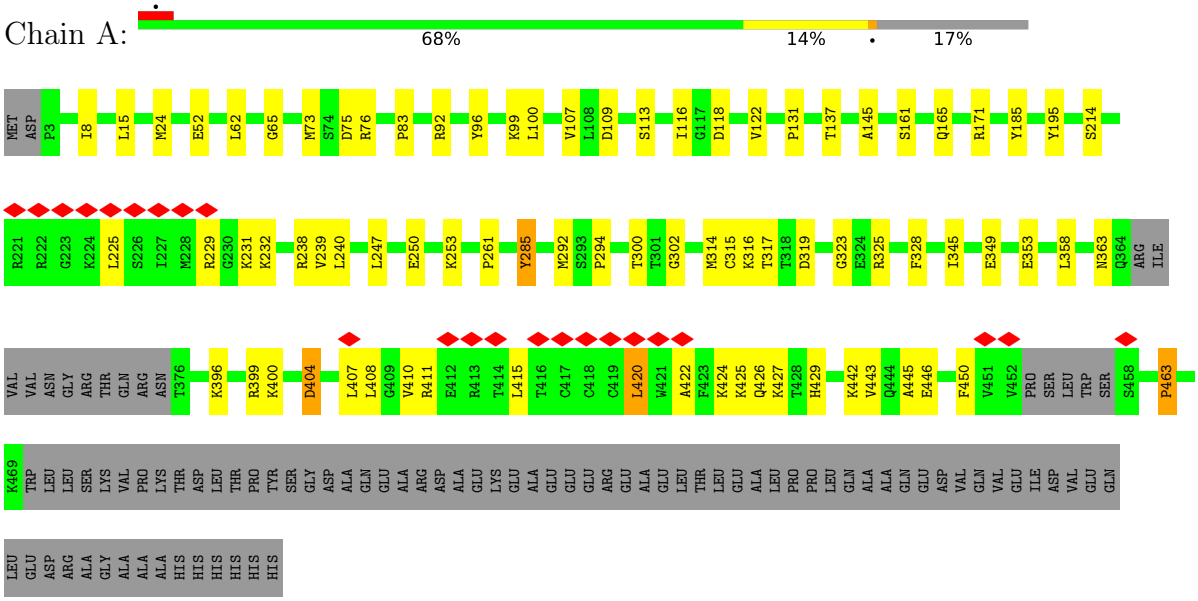
Mol	Chain	Residues	Atoms	AltConf
6	Q	27	Total O 27 27	0
6	S	27	Total O 27 27	0
6	V	27	Total O 27 27	0
6	X	27	Total O 27 27	0

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.

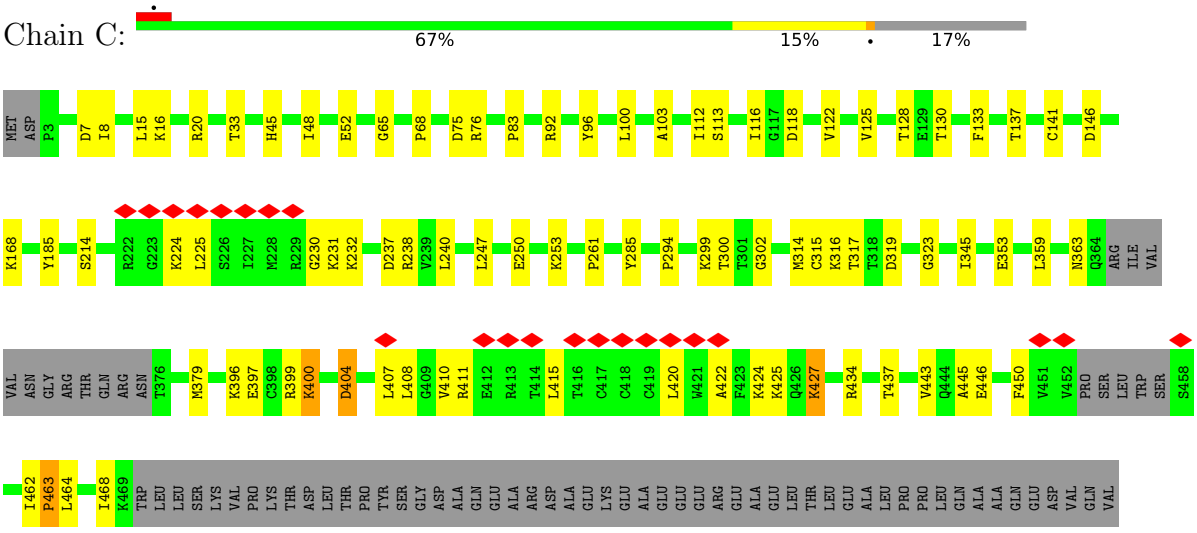
• Molecule 1: mRNA-capping enzyme nsP1

Chain A:



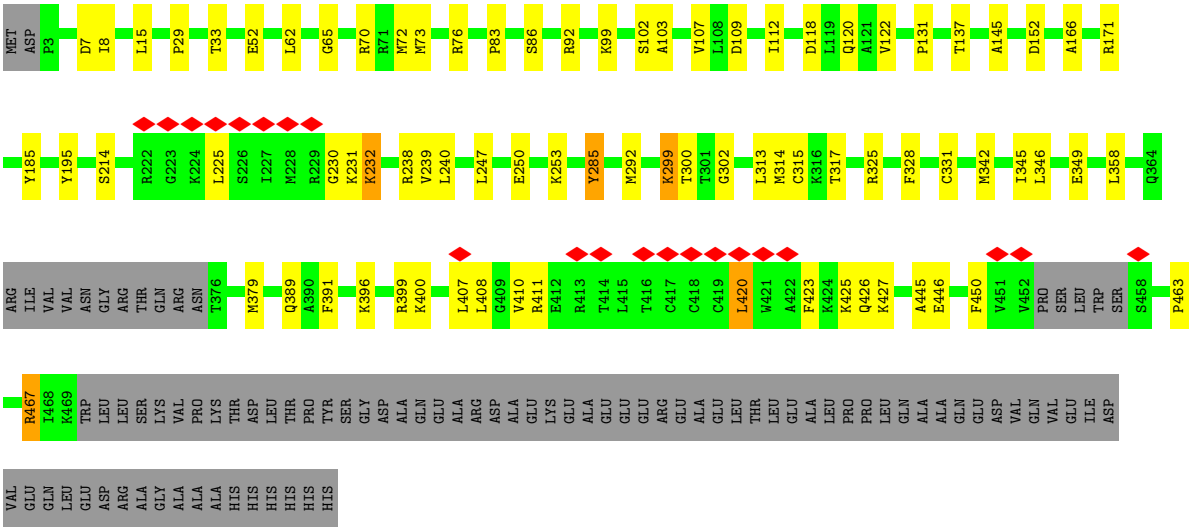
• Molecule 1: mRNA-capping enzyme nsP1

Chain C:



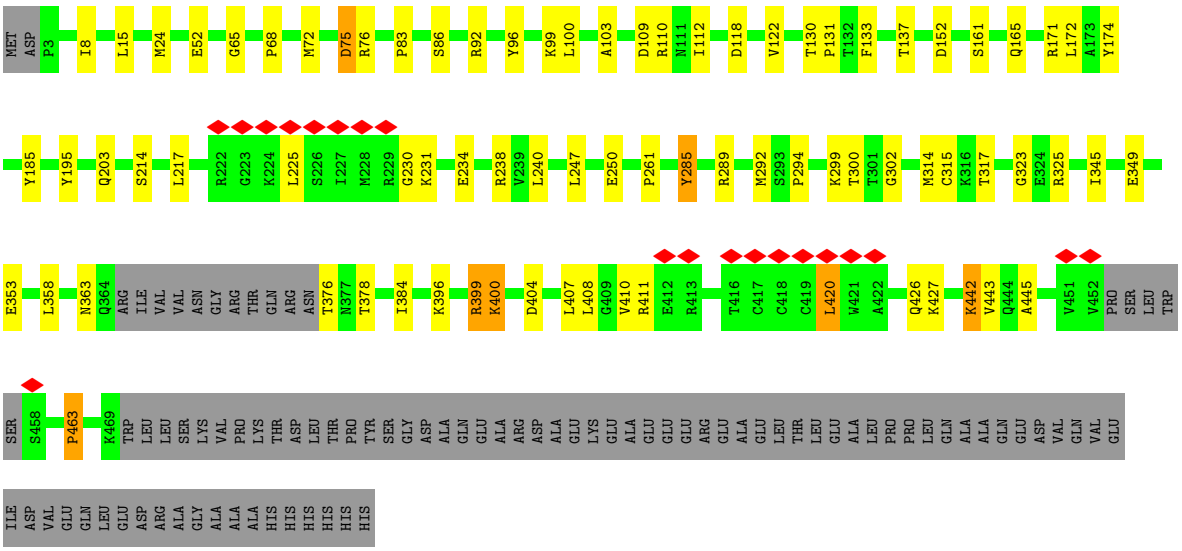
• Molecule 1: mRNA-capping enzyme nsP1

Chain E:



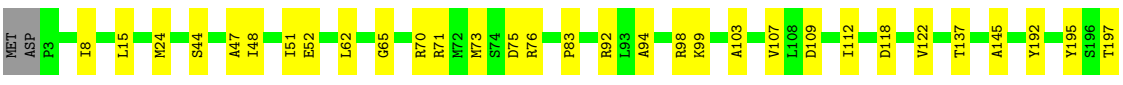
• Molecule 1: mRNA-capping enzyme nsP1

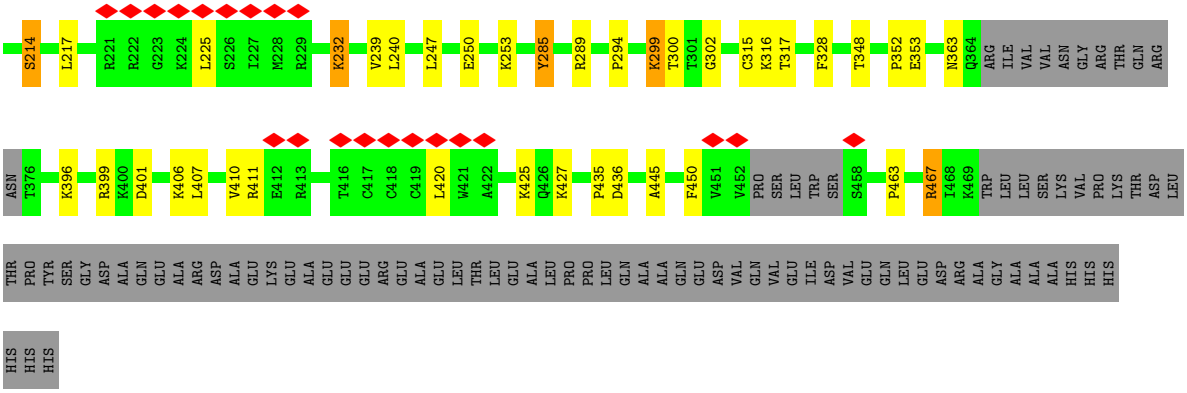
Chain G:



• Molecule 1: mRNA-capping enzyme nsP1

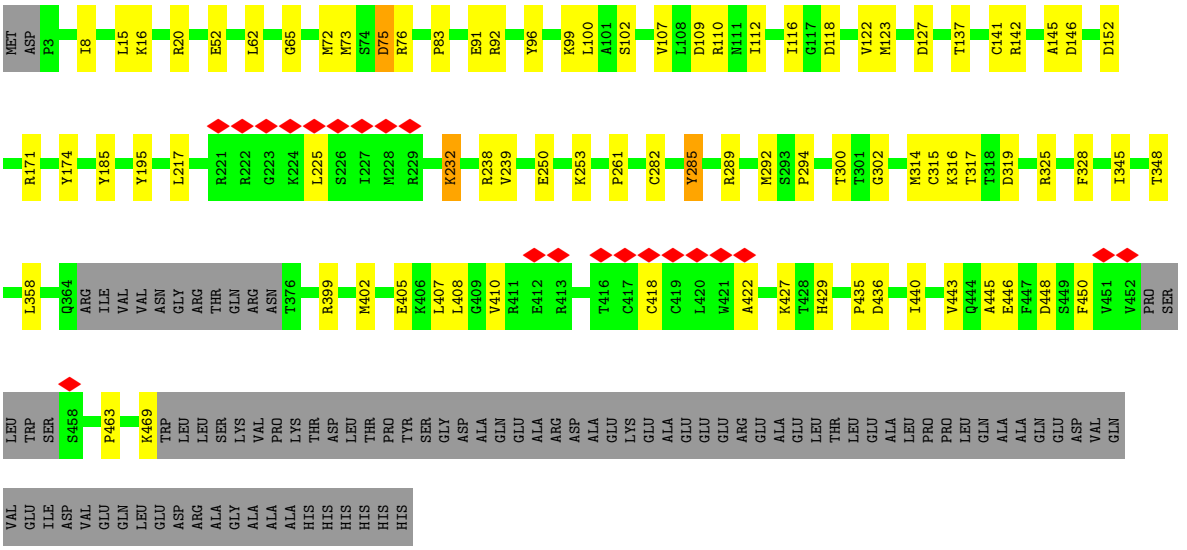
Chain I:





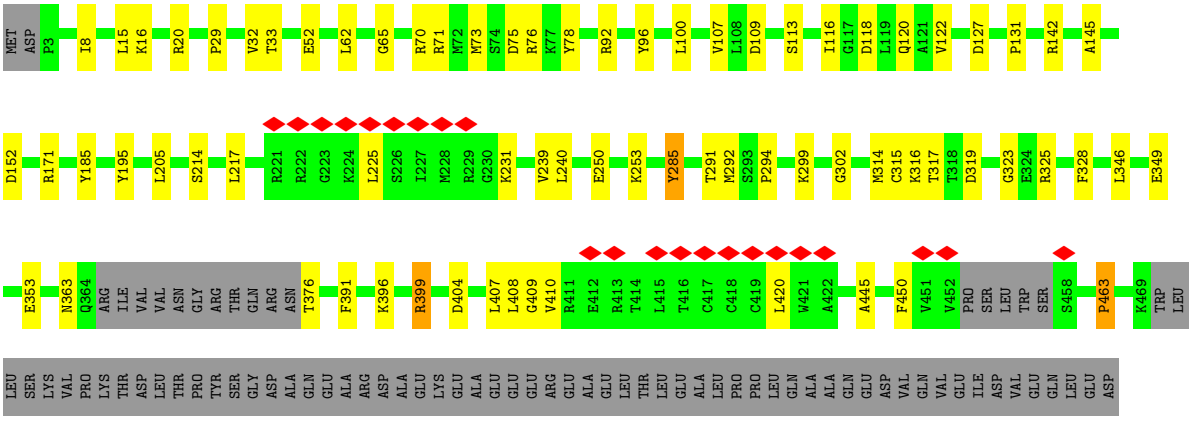
• Molecule 1: mRNA-capping enzyme nsP1

Chain K:



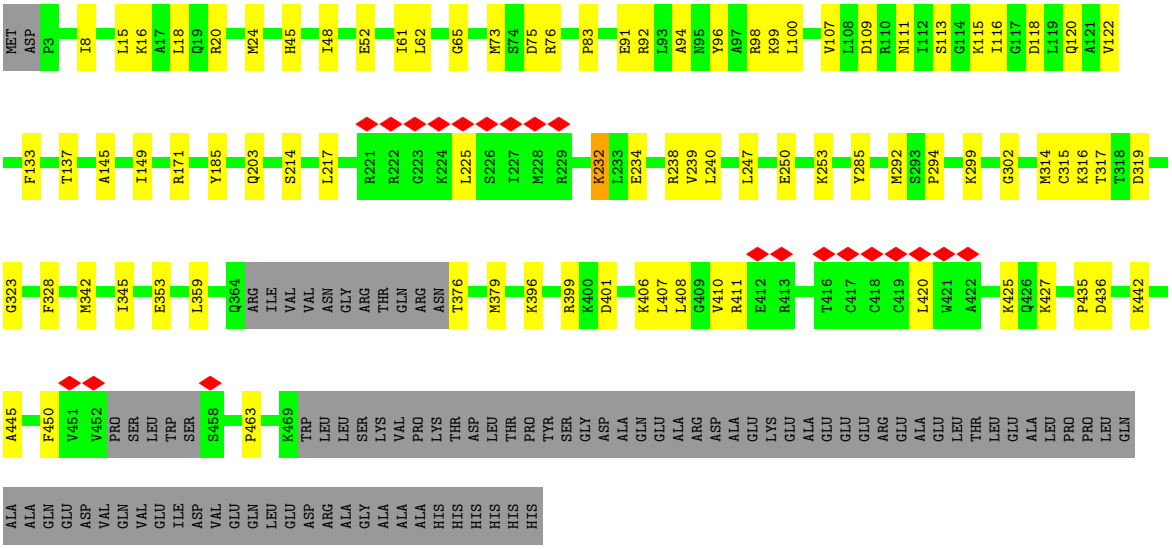
• Molecule 1: mRNA-capping enzyme nsP1

Chain M:



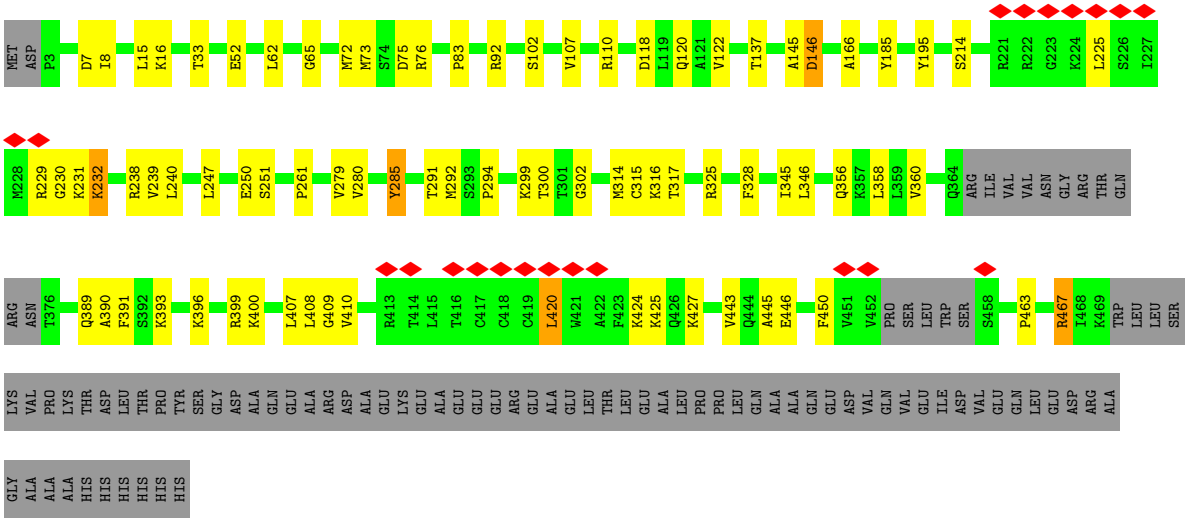
• Molecule 1: mRNA-capping enzyme nsP1

Chain O:



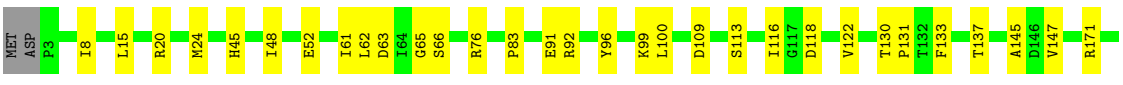
• Molecule 1: mRNA-capping enzyme nsP1

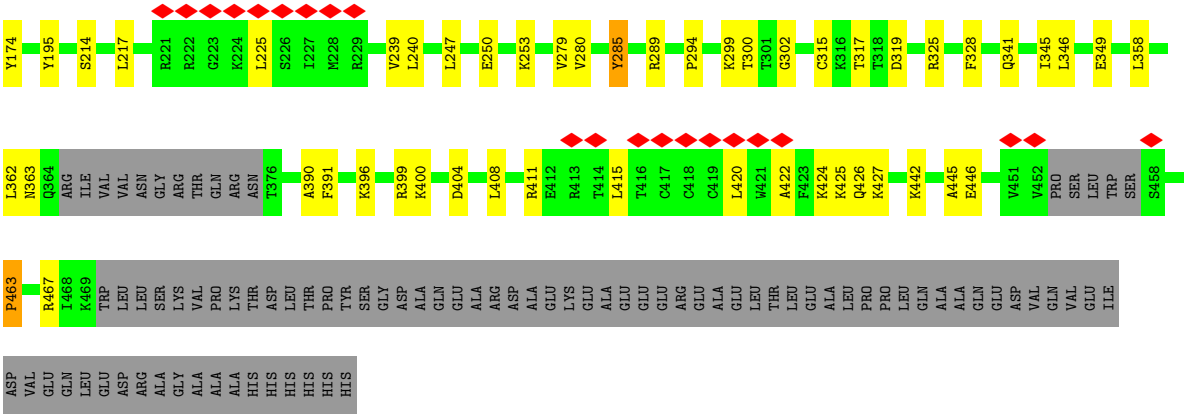
Chain Q:



• Molecule 1: mRNA-capping enzyme nsP1

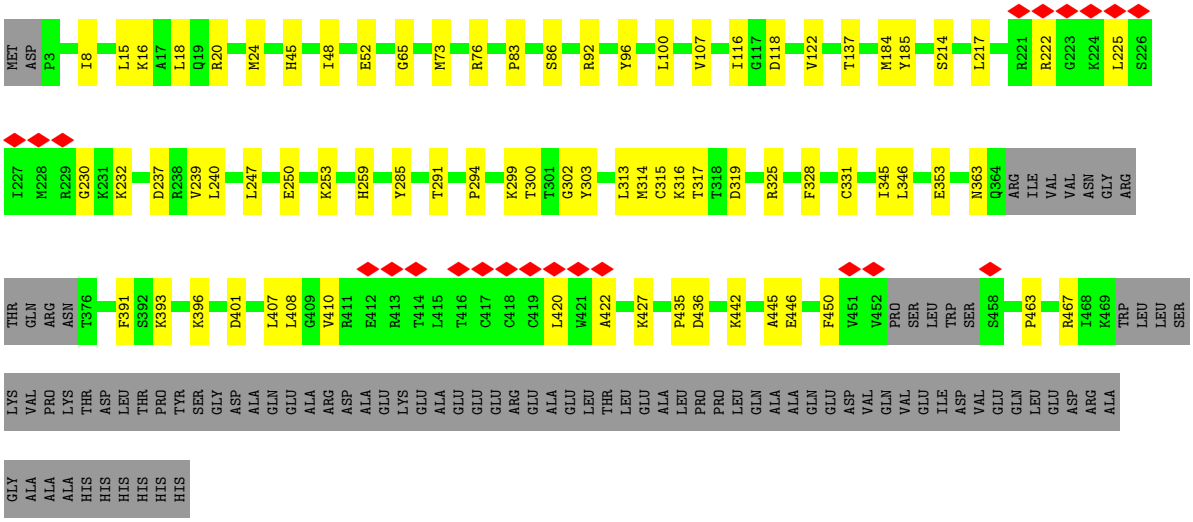
Chain S:





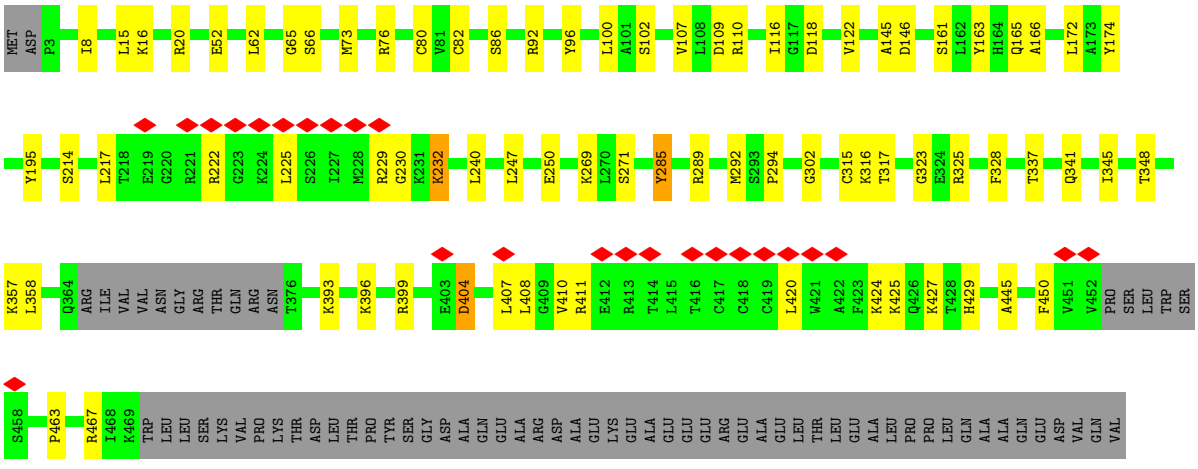
• Molecule 1: mRNA-capping enzyme nsP1

Chain V:



• Molecule 1: mRNA-capping enzyme nsP1

Chain X:



GLU
ILE
ASP
VAL
GLU
GLN
LEU
GLU
ASP
ARG
ALA
GLY
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	253384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83900005, 0.83900005, 0.83900005	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MGP, SAH, ZN

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	0.36	1/3629 (0.0%)	0.60	4/4911 (0.1%)
1	C	0.55	3/3629 (0.1%)	0.80	5/4911 (0.1%)
1	E	0.30	0/3629	0.53	0/4911
1	G	0.36	1/3629 (0.0%)	0.60	3/4911 (0.1%)
1	I	0.30	0/3629	0.52	0/4911
1	K	0.30	0/3629	0.52	0/4911
1	M	0.34	1/3629 (0.0%)	0.58	2/4911 (0.0%)
1	O	0.30	0/3629	0.52	0/4911
1	Q	0.30	0/3629	0.54	1/4911 (0.0%)
1	S	0.37	1/3629 (0.0%)	0.60	3/4911 (0.1%)
1	V	0.30	0/3629	0.52	0/4911
1	X	0.30	0/3629	0.54	1/4911 (0.0%)
All	All	0.35	7/43548 (0.0%)	0.58	19/58932 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	463	PRO	CG-CD	-25.16	0.67	1.50
1	S	463	PRO	CG-CD	-12.13	1.10	1.50
1	G	463	PRO	CG-CD	-11.62	1.12	1.50
1	A	463	PRO	CG-CD	-11.31	1.13	1.50
1	C	463	PRO	CB-CG	9.02	1.95	1.50
1	M	463	PRO	CG-CD	-7.90	1.24	1.50
1	C	463	PRO	N-CA	5.67	1.56	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	463	PRO	N-CD-CG	-33.42	53.07	103.20
1	C	463	PRO	CA-CB-CG	-18.57	68.72	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	463	PRO	N-CD-CG	-15.04	80.65	103.20
1	G	463	PRO	N-CD-CG	-14.89	80.87	103.20
1	A	463	PRO	N-CD-CG	-14.40	81.60	103.20
1	C	463	PRO	N-CA-CB	-12.32	88.51	103.30
1	M	463	PRO	CA-N-CD	-11.18	95.85	111.50
1	A	463	PRO	CA-N-CD	-10.98	96.13	111.50
1	S	463	PRO	CA-N-CD	-10.56	96.71	111.50
1	M	463	PRO	N-CD-CG	-10.47	87.50	103.20
1	G	463	PRO	CA-N-CD	-10.07	97.40	111.50
1	S	463	PRO	CA-CB-CG	-7.57	89.61	104.00
1	G	463	PRO	CA-CB-CG	-7.46	89.82	104.00
1	A	463	PRO	CA-CB-CG	-7.25	90.22	104.00
1	C	463	PRO	CA-N-CD	-6.44	102.48	111.50
1	X	404	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	404	ASP	CB-CG-OD2	5.64	123.38	118.30
1	Q	420	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	404	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3547	0	3556	61	0
1	C	3547	0	3556	65	0
1	E	3547	0	3556	56	0
1	G	3547	0	3556	58	0
1	I	3547	0	3556	53	0
1	K	3547	0	3556	65	0
1	M	3547	0	3556	55	0
1	O	3547	0	3556	64	0
1	Q	3547	0	3556	63	0
1	S	3547	0	3556	54	0
1	V	3547	0	3556	52	0
1	X	3547	0	3556	62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
2	M	1	0	0	0	0
2	O	1	0	0	0	0
2	Q	1	0	0	0	0
2	S	1	0	0	0	0
2	V	1	0	0	0	0
2	X	1	0	0	0	0
3	A	26	0	19	2	0
3	C	26	0	19	1	0
3	E	26	0	19	1	0
3	G	26	0	19	1	0
3	I	26	0	19	2	0
3	K	26	0	19	2	0
3	M	26	0	19	1	0
3	O	26	0	19	1	0
3	Q	26	0	19	1	0
3	S	26	0	19	1	0
3	V	26	0	19	1	0
3	X	26	0	19	2	0
4	A	33	0	15	2	0
4	C	33	0	15	2	0
4	E	33	0	15	2	0
4	G	33	0	15	2	0
4	I	33	0	15	2	0
4	K	33	0	15	2	0
4	M	33	0	15	2	0
4	O	33	0	15	2	0
4	Q	33	0	15	2	0
4	S	33	0	15	2	0
4	V	33	0	15	2	0
4	X	33	0	15	2	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
5	G	2	0	0	0	0
5	I	2	0	0	0	0
5	K	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	2	0	0	0	0
5	O	2	0	0	0	0
5	Q	2	0	0	0	0
5	S	2	0	0	0	0
5	V	2	0	0	0	0
5	X	2	0	0	0	0
6	A	27	0	0	1	0
6	C	27	0	0	1	0
6	E	27	0	0	2	0
6	G	27	0	0	1	0
6	I	27	0	0	2	0
6	K	27	0	0	1	0
6	M	27	0	0	2	0
6	O	27	0	0	1	0
6	Q	27	0	0	1	0
6	S	27	0	0	1	0
6	V	27	0	0	1	0
6	X	27	0	0	1	0
All	All	43632	0	43080	571	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 7.

All (571) 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:E:8:ILE:HD11	1:E:15:LEU:HD13	1.59	0.84
1:O:316[A]:LYS:HD2	1:Q:408:LEU:HD13	1.60	0.83
1:K:316[A]:LYS:HD2	1:M:408:LEU:HD13	1.60	0.83
1:O:316[A]:LYS:HE2	1:Q:408:LEU:HD22	1.63	0.81
1:A:408:LEU:HD13	1:X:316[A]:LYS:HD2	1.62	0.79
1:I:316[A]:LYS:HD2	1:K:408:LEU:HD13	1.64	0.78
1:Q:316[A]:LYS:HD2	1:S:408:LEU:HD13	1.67	0.77
1:O:8:ILE:HD11	1:O:15:LEU:HD13	1.66	0.76
1:S:8:ILE:HD11	1:S:15:LEU:HD13	1.68	0.76
1:C:8:ILE:HD11	1:C:15:LEU:HD13	1.68	0.76
1:I:8:ILE:HD11	1:I:15:LEU:HD13	1.66	0.75
1:A:8:ILE:HD11	1:A:15:LEU:HD13	1.70	0.74
1:A:316[A]:LYS:HD2	1:C:408:LEU:HD13	1.70	0.74
1:G:8:ILE:HD11	1:G:15:LEU:HD13	1.69	0.73
1:Q:8:ILE:HD11	1:Q:15:LEU:HD13	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:316[A]:LYS:HD2	1:O:408:LEU:HD13	1.69	0.73
1:O:353:GLU:HG2	1:Q:399:ARG:HH21	1.54	0.73
1:A:408:LEU:HD22	1:X:316[A]:LYS:HE2	1.71	0.72
1:V:316[A]:LYS:HD2	1:X:408:LEU:HD13	1.71	0.70
1:V:353:GLU:HG2	1:X:399:ARG:HH21	1.55	0.70
1:K:8:ILE:HD11	1:K:15:LEU:HD13	1.74	0.69
1:I:316[A]:LYS:HE2	1:K:408:LEU:HD22	1.76	0.68
1:Q:52:GLU:O	1:Q:76:ARG:NH2	2.28	0.67
1:V:8:ILE:HD11	1:V:15:LEU:HD13	1.76	0.66
1:X:8:ILE:HD11	1:X:15:LEU:HD13	1.78	0.66
1:X:52:GLU:O	1:X:76:ARG:NH2	2.29	0.66
1:K:316[A]:LYS:HE2	1:M:408:LEU:HD22	1.79	0.65
1:G:463:PRO:HB2	1:I:294:PRO:HB2	1.77	0.65
1:C:463:PRO:HG3	1:C:464:LEU:H	1.62	0.65
1:I:92:ARG:NH2	6:I:702:HOH:O	2.30	0.65
1:A:316[A]:LYS:HE2	1:C:408:LEU:HD22	1.78	0.64
1:A:353:GLU:HG2	1:C:399:ARG:HH21	1.62	0.64
1:O:225:LEU:HD23	1:Q:420:LEU:HB3	1.78	0.64
1:G:323:GLY:HA3	1:I:425:LYS:HD2	1.80	0.64
1:V:316[A]:LYS:HE2	1:X:408:LEU:HD22	1.79	0.64
1:K:92:ARG:NH2	6:K:702:HOH:O	2.30	0.64
1:M:92:ARG:NH2	6:M:702:HOH:O	2.31	0.64
1:C:92:ARG:NH2	6:C:702:HOH:O	2.30	0.63
1:S:52:GLU:O	1:S:76:ARG:NH2	2.32	0.63
1:G:353:GLU:HG2	1:I:399:ARG:HH21	1.64	0.63
1:K:123:MET:HB3	1:K:469:LYS:HE3	1.81	0.63
1:M:225:LEU:HD23	1:O:420:LEU:HB3	1.79	0.63
1:I:52:GLU:O	1:I:76:ARG:NH2	2.32	0.62
1:M:52:GLU:O	1:M:76:ARG:NH2	2.32	0.62
1:Q:92:ARG:NH2	6:Q:702:HOH:O	2.31	0.62
1:A:92:ARG:NH2	6:A:1101:HOH:O	2.31	0.62
1:S:92:ARG:NH2	6:S:702:HOH:O	2.33	0.62
1:E:92:ARG:NH2	6:E:702:HOH:O	2.31	0.62
1:O:92:ARG:NH2	6:O:702:HOH:O	2.32	0.62
1:G:92:ARG:NH2	6:G:702:HOH:O	2.32	0.62
1:G:225:LEU:HD23	1:I:420:LEU:HB3	1.80	0.62
1:V:92:ARG:NH2	6:V:702:HOH:O	2.33	0.61
1:C:397:GLU:HG2	1:C:427:LYS:HE2	1.83	0.61
1:V:118:ASP:O	1:V:122:VAL:HG23	2.01	0.61
1:E:52:GLU:O	1:E:76:ARG:NH2	2.34	0.61
1:K:52:GLU:O	1:K:76:ARG:NH2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:ASP:O	1:I:122:VAL:HG23	2.01	0.61
1:O:118:ASP:O	1:O:122:VAL:HG23	2.01	0.61
1:Q:232:LYS:H	1:Q:232:LYS:HD3	1.66	0.61
1:M:8:ILE:HD11	1:M:15:LEU:HD13	1.82	0.60
1:C:300:THR:OG1	1:C:446:GLU:OE2	2.19	0.60
1:C:52:GLU:O	1:C:76:ARG:NH2	2.34	0.60
1:G:75:ASP:OD1	1:G:75:ASP:N	2.34	0.60
1:V:52:GLU:O	1:V:76:ARG:NH2	2.34	0.60
1:I:316[B]:LYS:NZ	1:K:405:GLU:OE2	2.29	0.60
1:C:316[A]:LYS:HE2	1:E:408:LEU:HD22	1.84	0.59
1:X:66:SER:OG	1:X:82:CYS:SG	2.60	0.59
1:E:300:THR:OG1	1:E:446:GLU:OE2	2.20	0.59
1:V:100:LEU:HD22	1:V:116:ILE:HG23	1.85	0.59
1:C:75:ASP:OD2	1:C:75:ASP:N	2.34	0.59
1:O:73:MET:HE1	1:O:107:VAL:HG11	1.84	0.59
1:I:353:GLU:HG2	1:K:399:ARG:HH21	1.66	0.59
1:O:52:GLU:O	1:O:76:ARG:NH2	2.37	0.58
1:X:250:GLU:OE2	4:X:604:MGP:N2	2.36	0.58
1:Q:316[A]:LYS:HE2	1:S:408:LEU:HD22	1.85	0.58
1:C:353:GLU:HG2	1:E:399:ARG:HH21	1.69	0.58
1:M:316[A]:LYS:HE2	1:O:408:LEU:HD22	1.85	0.58
1:A:52:GLU:O	1:A:76:ARG:NH2	2.36	0.58
1:S:300:THR:OG1	1:S:446:GLU:OE2	2.21	0.58
1:K:118:ASP:O	1:K:122:VAL:HG23	2.04	0.57
1:S:130:THR:OG1	1:S:133:PHE:O	2.22	0.57
1:X:65:GLY:O	3:X:603:SAH:N	2.37	0.57
1:I:225:LEU:HG	1:K:422:ALA:HB2	1.86	0.57
1:Q:467:ARG:HD2	1:S:171:ARG:HE	1.68	0.57
1:C:118:ASP:O	1:C:122:VAL:HG23	2.05	0.57
1:K:100:LEU:HD22	1:K:116:ILE:HG13	1.87	0.57
1:C:323:GLY:HA3	1:E:425:LYS:HD2	1.87	0.56
1:O:75:ASP:OD1	1:O:75:ASP:N	2.32	0.56
1:C:316[A]:LYS:HE2	1:E:408:LEU:HD13	1.87	0.56
1:O:65:GLY:O	3:O:603:SAH:N	2.39	0.56
1:X:240:LEU:HD12	1:X:247:LEU:HD11	1.89	0.55
1:I:70:ARG:NH1	6:I:704:HOH:O	2.40	0.55
1:A:250:GLU:OE2	4:A:1003:MGP:N1	2.40	0.55
1:E:65:GLY:O	3:E:603:SAH:N	2.38	0.55
1:G:52:GLU:O	1:G:76:ARG:NH2	2.40	0.55
1:Q:238:ARG:HH22	1:S:299:LYS:NZ	2.04	0.55
1:I:65:GLY:O	3:I:603:SAH:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:345:ILE:H	1:Q:345:ILE:HD12	1.72	0.55
1:C:250:GLU:OE2	4:C:604:MGP:N1	2.40	0.54
1:I:250:GLU:OE2	4:I:604:MGP:N2	2.38	0.54
1:X:92:ARG:NH2	6:X:702:HOH:O	2.41	0.54
1:S:65:GLY:O	3:S:603:SAH:N	2.41	0.54
1:S:279:VAL:HG23	1:S:280:VAL:HG23	1.89	0.54
1:E:238:ARG:HH22	1:G:299:LYS:NZ	2.06	0.54
1:O:328:PHE:HA	1:Q:408:LEU:HD11	1.90	0.54
1:M:353:GLU:OE1	1:O:399:ARG:NH2	2.41	0.54
1:G:250:GLU:OE2	4:G:604:MGP:N1	2.40	0.54
1:E:72:MET:HE3	1:E:73:MET:SD	2.48	0.54
1:M:250:GLU:OE2	4:M:604:MGP:N2	2.37	0.54
1:V:217:LEU:HD13	1:X:316[A]:LYS:HE3	1.89	0.53
1:E:250:GLU:OE2	4:E:604:MGP:N1	2.40	0.53
1:A:65:GLY:O	3:A:1002:SAH:N	2.40	0.53
1:A:425:LYS:HD2	1:X:323:GLY:HA3	1.91	0.53
1:M:323:GLY:HA3	1:O:425:LYS:HD2	1.90	0.53
1:M:65:GLY:O	3:M:603:SAH:N	2.42	0.53
1:E:467:ARG:HD2	1:G:171:ARG:HH11	1.74	0.53
1:X:161:SER:O	1:X:165:GLN:HG2	2.09	0.53
1:E:73:MET:HE1	1:E:107:VAL:HG11	1.90	0.53
1:O:250:GLU:OE2	4:O:604:MGP:N1	2.40	0.53
1:I:94:ALA:O	1:I:98:ARG:HG2	2.09	0.53
1:G:65:GLY:O	3:G:603:SAH:N	2.42	0.53
1:G:118:ASP:O	1:G:122:VAL:HG23	2.09	0.53
1:S:463:PRO:HB2	1:V:294:PRO:HB2	1.90	0.52
1:V:225:LEU:HB3	1:X:420:LEU:HD21	1.91	0.52
1:S:250:GLU:OE2	4:S:604:MGP:N1	2.40	0.52
1:A:349:GLU:HG2	1:A:399:ARG:HD3	1.92	0.52
1:E:118:ASP:O	1:E:122:VAL:HG23	2.09	0.52
1:K:250:GLU:OE2	4:K:604:MGP:N1	2.39	0.52
1:V:65:GLY:O	3:V:603:SAH:N	2.42	0.52
1:E:328:PHE:HA	1:G:408:LEU:HD11	1.92	0.52
1:K:75:ASP:OD2	1:K:75:ASP:N	2.34	0.52
1:O:83:PRO:HB3	1:O:137:THR:HG22	1.92	0.52
1:C:250:GLU:OE2	4:C:604:MGP:N2	2.41	0.52
1:K:171:ARG:HD3	1:K:292:MET:O	2.09	0.52
1:O:16:LYS:HB3	1:O:20:ARG:HH12	1.74	0.52
1:A:316[A]:LYS:CD	1:C:408:LEU:HD13	2.39	0.52
1:V:250:GLU:OE2	4:V:604:MGP:N2	2.40	0.52
1:A:408:LEU:HD11	1:X:328:PHE:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:94:ALA:O	1:O:98:ARG:HG2	2.10	0.52
1:Q:325:ARG:NH1	1:S:426:GLN:OE1	2.43	0.52
1:V:16:LYS:HB3	1:V:20:ARG:HH12	1.75	0.51
1:V:225:LEU:HD12	1:V:225:LEU:H	1.75	0.51
1:A:118:ASP:O	1:A:122:VAL:HG23	2.10	0.51
1:C:463:PRO:CG	1:C:464:LEU:N	2.73	0.51
1:C:65:GLY:O	3:C:603:SAH:N	2.42	0.51
1:K:195:TYR:OH	1:K:282:CYS:O	2.20	0.51
1:K:328:PHE:HA	1:M:408:LEU:HD11	1.93	0.51
1:O:316[A]:LYS:CD	1:Q:408:LEU:HD13	2.36	0.51
1:Q:225:LEU:HG	1:S:422:ALA:HB2	1.93	0.51
1:X:96:TYR:CZ	1:X:100:LEU:HD11	2.46	0.51
1:A:328:PHE:HA	1:C:408:LEU:HD11	1.93	0.51
1:M:250:GLU:OE2	4:M:604:MGP:N1	2.44	0.51
1:K:65:GLY:O	3:K:603:SAH:N	2.44	0.51
1:K:73:MET:HE1	1:K:107:VAL:HG11	1.92	0.51
1:E:240:LEU:HD12	1:E:247:LEU:HD11	1.93	0.51
1:O:323:GLY:HA3	1:Q:425:LYS:HD2	1.91	0.51
1:G:230:GLY:O	1:I:411:ARG:NE	2.41	0.50
1:Q:328:PHE:HA	1:S:408:LEU:HD11	1.93	0.50
1:E:463:PRO:HB2	1:G:294:PRO:HB2	1.93	0.50
1:Q:118:ASP:O	1:Q:122:VAL:HG23	2.12	0.50
1:K:225:LEU:HD23	1:M:420:LEU:HB3	1.94	0.50
1:K:463:PRO:HB2	1:M:294:PRO:HB2	1.94	0.50
1:G:250:GLU:OE2	4:G:604:MGP:N2	2.43	0.50
1:Q:230:GLY:O	1:S:411:ARG:NE	2.44	0.50
1:G:363:ASN:HD22	1:G:384:ILE:HD11	1.75	0.50
1:A:250:GLU:OE2	4:A:1003:MGP:N2	2.44	0.50
1:A:411:ARG:NE	1:X:230:GLY:O	2.42	0.50
1:Q:250:GLU:OE2	4:Q:604:MGP:N1	2.41	0.50
1:A:424:LYS:HE2	1:A:425:LYS:O	2.12	0.49
1:V:250:GLU:OE2	4:V:604:MGP:N1	2.45	0.49
1:K:152:ASP:OD1	1:K:285:TYR:OH	2.30	0.49
1:M:463:PRO:HB2	1:O:294:PRO:HB2	1.94	0.49
1:O:250:GLU:OE2	4:O:604:MGP:N2	2.45	0.49
1:I:250:GLU:OE2	4:I:604:MGP:N1	2.46	0.49
1:X:118:ASP:O	1:X:122:VAL:HG23	2.11	0.49
1:E:345:ILE:HG12	1:E:358:LEU:HD23	1.95	0.49
1:Q:65:GLY:O	3:Q:603:SAH:N	2.46	0.49
1:E:250:GLU:OE2	4:E:604:MGP:N2	2.45	0.49
1:E:302:GLY:HA2	1:E:445:ALA:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:250:GLU:OE2	4:X:604:MGP:N1	2.45	0.49
1:M:73:MET:HE1	1:M:107:VAL:HG11	1.95	0.48
1:M:316[A]:LYS:CD	1:O:408:LEU:HD13	2.41	0.48
1:K:239:VAL:HG23	1:K:250:GLU:HB2	1.96	0.48
1:S:345:ILE:HG21	1:S:358:LEU:HD13	1.94	0.48
1:Q:250:GLU:OE2	4:Q:604:MGP:N2	2.46	0.48
1:S:174:TYR:CE1	1:S:289:ARG:HG3	2.49	0.48
1:A:161:SER:O	1:A:165:GLN:HG2	2.14	0.48
1:C:240:LEU:HD12	1:C:247:LEU:HD11	1.94	0.48
1:K:250:GLU:OE2	4:K:604:MGP:N2	2.47	0.48
1:O:342:MET:HA	1:O:345:ILE:HD13	1.95	0.48
1:X:302:GLY:HA2	1:X:445:ALA:HB2	1.95	0.48
1:Q:73:MET:HE1	1:Q:110:ARG:HG2	1.96	0.48
1:V:96:TYR:CZ	1:V:100:LEU:HD11	2.49	0.48
1:X:73:MET:HE1	1:X:107:VAL:HG11	1.96	0.48
1:O:99:LYS:HB3	1:O:99:LYS:HE3	1.66	0.48
1:I:217:LEU:HD13	1:K:316[A]:LYS:HE3	1.95	0.48
1:X:232:LYS:H	1:X:232:LYS:HD3	1.78	0.48
1:A:83:PRO:HB3	1:A:137:THR:HG22	1.95	0.48
1:M:349:GLU:HG3	1:M:399:ARG:HD3	1.95	0.48
1:S:118:ASP:OD1	1:S:131:PRO:HD2	2.14	0.48
1:I:73:MET:HE1	1:I:107:VAL:HG11	1.94	0.47
1:M:96:TYR:CZ	1:M:100:LEU:HD11	2.49	0.47
1:M:127:ASP:OD2	1:M:142:ARG:NH2	2.38	0.47
1:M:171:ARG:HD3	1:M:292:MET:O	2.14	0.47
1:E:83:PRO:HB3	1:E:137:THR:HG22	1.95	0.47
1:G:217:LEU:HD13	1:I:316[A]:LYS:HE3	1.96	0.47
1:V:240:LEU:HD12	1:V:247:LEU:HD11	1.96	0.47
1:V:328:PHE:HA	1:X:408:LEU:HD11	1.95	0.47
1:I:47:ALA:O	1:I:51:ILE:HG13	2.13	0.47
1:M:118:ASP:O	1:M:122:VAL:HG23	2.14	0.47
1:M:316[A]:LYS:HD3	1:M:316[A]:LYS:HA	1.64	0.47
1:G:174:TYR:CE1	1:G:289:ARG:HG3	2.50	0.47
1:V:225:LEU:HB3	1:X:420:LEU:CD2	2.44	0.47
1:C:261:PRO:HG3	1:C:443:VAL:HG23	1.95	0.47
1:E:230:GLY:O	1:G:411:ARG:NE	2.42	0.47
1:O:353:GLU:HG2	1:Q:399:ARG:NH2	2.28	0.47
1:V:237:ASP:OD1	1:V:253:LYS:HG3	2.15	0.47
1:A:463:PRO:HB2	1:C:294:PRO:HB2	1.95	0.47
1:C:434:ARG:O	1:C:437:THR:OG1	2.22	0.47
1:C:463:PRO:HG3	1:C:464:LEU:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:LEU:HD12	1:G:247:LEU:HD11	1.95	0.47
1:I:48:ILE:HG12	1:I:71:ARG:NH1	2.30	0.47
1:Q:279:VAL:HG23	1:Q:280:VAL:HG23	1.96	0.47
1:Q:316[A]:LYS:HA	1:Q:316[A]:LYS:HD3	1.67	0.47
1:S:83:PRO:HB3	1:S:137:THR:HG22	1.97	0.47
1:A:426:GLN:HG3	1:X:325:ARG:HB2	1.97	0.47
1:K:16:LYS:HB3	1:K:20:ARG:HH12	1.79	0.47
1:K:302:GLY:HA2	1:K:445:ALA:HB2	1.96	0.47
1:M:328:PHE:HA	1:O:408:LEU:HD11	1.97	0.47
1:S:91:GLU:HG3	1:V:291:THR:HG21	1.97	0.47
1:G:363:ASN:OD1	1:G:378:THR:N	2.47	0.47
1:K:100:LEU:HD23	1:K:112:ILE:HG23	1.97	0.46
1:M:70:ARG:NH1	6:M:704:HOH:O	2.47	0.46
1:S:96:TYR:CZ	1:S:100:LEU:HD11	2.50	0.46
1:M:302:GLY:HA2	1:M:445:ALA:HB2	1.97	0.46
1:O:239:VAL:HG23	1:O:250:GLU:HB2	1.97	0.46
1:O:302:GLY:HA2	1:O:445:ALA:HB2	1.96	0.46
1:O:345:ILE:HD12	1:O:345:ILE:H	1.80	0.46
1:K:83:PRO:HB3	1:K:137:THR:HG22	1.96	0.46
1:M:32:VAL:HG23	1:M:33:THR:HG23	1.97	0.46
1:A:316[A]:LYS:HE3	1:X:217:LEU:HD13	1.97	0.46
1:C:237:ASP:OD1	1:C:253:LYS:HG3	2.15	0.46
1:S:118:ASP:O	1:S:122:VAL:HG23	2.15	0.46
1:X:393:LYS:HD3	1:X:429:HIS:HB3	1.98	0.46
1:A:294:PRO:HB2	1:X:463:PRO:HB2	1.98	0.46
1:C:103:ALA:O	1:C:112:ILE:HG21	2.15	0.46
1:Q:73:MET:HE1	1:Q:107:VAL:HG11	1.97	0.46
1:A:325:ARG:HD3	1:C:404:ASP:O	2.16	0.46
1:I:217:LEU:CD1	1:K:316[A]:LYS:HE3	2.46	0.46
1:Q:166:ALA:HB2	1:Q:292:MET:SD	2.55	0.46
1:Q:240:LEU:HD12	1:Q:247:LEU:HD11	1.98	0.46
1:V:302:GLY:HA2	1:V:445:ALA:HB2	1.98	0.46
1:A:238:ARG:HH22	1:C:299:LYS:NZ	2.14	0.46
1:A:400:LYS:NZ	1:A:427:LYS:HB3	2.30	0.46
1:C:302:GLY:HA2	1:C:445:ALA:HB2	1.97	0.46
1:I:302:GLY:HA2	1:I:445:ALA:HB2	1.97	0.46
1:M:217:LEU:HB3	1:O:316[A]:LYS:HE3	1.98	0.46
1:S:99:LYS:HB3	1:S:99:LYS:HE3	1.61	0.46
1:S:250:GLU:OE2	4:S:604:MGP:N2	2.45	0.46
1:A:427:LYS:HE2	1:A:427:LYS:HA	1.97	0.46
1:G:103:ALA:O	1:G:112:ILE:HG21	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:302:GLY:HA2	1:Q:445:ALA:HB2	1.98	0.46
1:V:407:LEU:O	1:V:410:VAL:HG22	2.16	0.46
1:C:464:LEU:O	1:C:468:ILE:HG12	2.16	0.46
1:E:232:LYS:HD3	1:E:232:LYS:H	1.81	0.46
1:G:161:SER:O	1:G:165:GLN:HG2	2.16	0.46
1:I:240:LEU:HD12	1:I:247:LEU:HD11	1.98	0.46
1:A:302:GLY:HA2	1:A:445:ALA:HB2	1.98	0.45
1:G:83:PRO:HB3	1:G:137:THR:HG22	1.97	0.45
1:I:463:PRO:HB2	1:K:294:PRO:HB2	1.99	0.45
1:M:16:LYS:HB3	1:M:20:ARG:HH12	1.80	0.45
1:K:232:LYS:HA	1:M:409:GLY:O	2.17	0.45
1:Q:316[A]:LYS:CD	1:S:408:LEU:HD13	2.40	0.45
1:V:230:GLY:O	1:X:411:ARG:NE	2.48	0.45
1:K:62:LEU:HG	1:K:145:ALA:HB3	1.98	0.45
1:O:407:LEU:O	1:O:410:VAL:HG22	2.16	0.45
1:V:396:LYS:HE3	1:V:396:LYS:HB3	1.80	0.45
1:K:96:TYR:CZ	1:K:100:LEU:HD11	2.51	0.45
1:V:222:ARG:NH1	1:X:424:LYS:HB2	2.31	0.45
1:A:113:SER:O	1:A:116:ILE:HG13	2.16	0.45
1:A:404:ASP:O	1:X:325:ARG:HD3	2.16	0.45
1:I:348:THR:HG22	1:I:399:ARG:NH2	2.30	0.45
1:I:467:ARG:HD2	1:K:171:ARG:HD2	1.99	0.45
1:O:113:SER:O	1:O:116:ILE:HG13	2.17	0.45
1:A:195:TYR:CZ	1:A:285:TYR:HB2	2.52	0.45
1:C:113:SER:O	1:C:116:ILE:HG13	2.16	0.45
1:C:125:VAL:O	1:C:128:THR:HG22	2.17	0.45
1:G:426:GLN:H	1:G:426:GLN:HG2	1.53	0.45
1:M:239:VAL:HG23	1:M:250:GLU:HB2	1.99	0.45
1:Q:346:LEU:HD21	1:Q:391:PHE:HB3	1.99	0.45
1:A:238:ARG:HH22	1:C:299:LYS:HZ2	1.63	0.45
1:C:345:ILE:HD12	1:C:345:ILE:H	1.82	0.45
1:K:83:PRO:HG3	3:K:603:SAH:C4	2.47	0.45
1:O:345:ILE:HD12	1:O:345:ILE:N	2.31	0.45
1:I:232:LYS:H	1:I:232:LYS:HD3	1.82	0.45
1:O:463:PRO:HB2	1:Q:294:PRO:HB2	1.98	0.45
1:S:217:LEU:HD13	1:V:316[A]:LYS:HE3	1.99	0.45
1:S:225:LEU:HG	1:V:422:ALA:HB2	1.99	0.45
1:V:73:MET:HE1	1:V:107:VAL:HG11	1.99	0.45
1:X:316[A]:LYS:HA	1:X:316[A]:LYS:HD3	1.77	0.45
1:I:328:PHE:HA	1:K:408:LEU:HD11	1.99	0.45
1:O:91:GLU:HG3	1:Q:291:THR:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:62:LEU:HG	1:Q:145:ALA:HB3	1.99	0.45
1:Q:299:LYS:HB2	1:Q:299:LYS:HE2	1.72	0.45
1:S:315[A]:CYS:SG	1:S:390:ALA:HA	2.57	0.45
1:G:171:ARG:HD3	1:G:292:MET:O	2.17	0.44
1:A:99:LYS:HB3	1:A:99:LYS:HE3	1.62	0.44
1:C:225:LEU:HD23	1:E:420:LEU:HB3	1.99	0.44
1:C:238:ARG:HH22	1:E:299:LYS:NZ	2.16	0.44
1:I:407:LEU:O	1:I:410:VAL:HG22	2.17	0.44
1:Q:356:GLN:O	1:Q:360:VAL:HG23	2.17	0.44
1:S:302:GLY:HA2	1:S:445:ALA:HB2	1.98	0.44
1:V:316[A]:LYS:HA	1:V:316[A]:LYS:HD3	1.62	0.44
1:X:166:ALA:HB2	1:X:292:MET:SD	2.57	0.44
1:X:407:LEU:O	1:X:410:VAL:HG22	2.17	0.44
1:C:122:VAL:HG21	1:C:133:PHE:HD2	1.82	0.44
1:K:217:LEU:HD13	1:M:316[A]:LYS:HE3	1.99	0.44
1:M:217:LEU:HD13	1:O:316[A]:LYS:HE3	1.99	0.44
1:X:174:TYR:CE1	1:X:289:ARG:HG3	2.53	0.44
1:G:217:LEU:HB3	1:I:316[A]:LYS:HE3	1.99	0.44
1:V:185:TYR:HB3	1:V:314:MET:SD	2.58	0.44
1:X:16:LYS:O	1:X:20:ARG:HG3	2.18	0.44
1:E:426:GLN:H	1:E:426:GLN:HG2	1.62	0.44
1:G:302:GLY:HA2	1:G:445:ALA:HB2	1.99	0.44
1:G:442:LYS:HB2	1:G:442:LYS:HE3	1.76	0.44
1:X:345:ILE:HG21	1:X:358:LEU:HD13	1.99	0.44
1:C:16:LYS:HB3	1:C:20:ARG:HH12	1.83	0.44
1:E:396:LYS:HE3	1:E:396:LYS:HB3	1.69	0.44
1:G:99:LYS:HE3	1:G:99:LYS:HB3	1.67	0.44
1:K:345:ILE:HD12	1:K:345:ILE:H	1.83	0.44
1:V:239:VAL:HG23	1:V:250:GLU:HB2	2.00	0.44
1:K:72:MET:HE1	1:K:99:LYS:HE3	2.00	0.44
1:K:348:THR:HG22	1:K:399:ARG:NH2	2.32	0.44
1:O:16:LYS:HB3	1:O:20:ARG:NH1	2.33	0.44
1:X:62:LEU:HG	1:X:145:ALA:HB3	2.00	0.44
1:A:118:ASP:OD1	1:A:131:PRO:HD2	2.18	0.44
1:G:195:TYR:CZ	1:G:285:TYR:HB2	2.53	0.44
1:K:195:TYR:CZ	1:K:285:TYR:HB2	2.53	0.44
1:K:217:LEU:CD1	1:M:316[A]:LYS:HE3	2.48	0.44
1:V:463:PRO:HB2	1:X:294:PRO:HB2	2.00	0.44
1:C:231:LYS:HD2	1:E:411:ARG:O	2.18	0.44
1:E:7:ASP:OD2	1:E:33:THR:OG1	2.35	0.44
1:E:99:LYS:HE3	1:E:99:LYS:HB3	1.78	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316[A]:LYS:HA	1:A:316[A]:LYS:HD3	1.68	0.43
1:A:415:LEU:HD11	1:X:229:ARG:HH22	1.83	0.43
1:E:349:GLU:HG3	1:E:399:ARG:HG3	1.99	0.43
1:I:239:VAL:HG23	1:I:250:GLU:HB2	2.00	0.43
1:K:99:LYS:HE3	1:K:99:LYS:HB3	1.64	0.43
1:Q:463:PRO:HB2	1:S:294:PRO:HB2	1.99	0.43
1:C:141:CYS:SG	1:C:168:LYS:NZ	2.91	0.43
1:Q:195:TYR:CZ	1:Q:285:TYR:HB2	2.53	0.43
1:X:424:LYS:HE2	1:X:425:LYS:O	2.18	0.43
1:A:316[A]:LYS:HE3	1:X:217:LEU:CD1	2.48	0.43
1:E:70:ARG:NH1	6:E:704:HOH:O	2.51	0.43
1:E:239:VAL:HG23	1:E:250:GLU:HB2	1.99	0.43
1:M:205:LEU:HD11	1:M:240:LEU:HD23	2.00	0.43
1:S:349:GLU:HG3	1:S:399:ARG:HD3	2.00	0.43
1:A:225:LEU:HG	1:C:422:ALA:HB2	1.99	0.43
1:A:420:LEU:HB3	1:X:225:LEU:HD23	2.01	0.43
1:S:113:SER:O	1:S:116:ILE:HG13	2.18	0.43
1:V:303:TYR:CE1	1:V:442:LYS:HE3	2.53	0.43
1:X:396:LYS:HB3	1:X:396:LYS:HE3	1.75	0.43
1:E:325:ARG:HD3	1:G:404:ASP:O	2.18	0.43
1:K:174:TYR:CE1	1:K:289:ARG:HG3	2.53	0.43
1:K:325:ARG:HD3	1:M:404:ASP:O	2.18	0.43
1:G:396:LYS:HB3	1:G:396:LYS:HE3	1.76	0.43
1:K:316[A]:LYS:HA	1:K:316[A]:LYS:HD3	1.60	0.43
1:M:15:LEU:HD21	1:M:29:PRO:HG3	2.01	0.43
1:Q:238:ARG:HH22	1:S:299:LYS:HZ2	1.66	0.43
1:E:171:ARG:HD2	1:E:292:MET:O	2.18	0.43
1:G:238:ARG:HH22	1:I:299:LYS:NZ	2.17	0.43
1:G:396:LYS:HG3	1:G:400:LYS:HE3	2.00	0.43
1:I:352:PRO:HG2	1:K:402:MET:HE1	2.00	0.43
1:M:407:LEU:O	1:M:410:VAL:HG22	2.18	0.43
1:Q:7:ASP:OD2	1:Q:33:THR:OG1	2.35	0.43
1:S:240:LEU:HD12	1:S:247:LEU:HD11	2.00	0.43
1:X:66:SER:OG	1:X:80:CYS:HB3	2.18	0.43
1:A:239:VAL:HG23	1:A:250:GLU:HB2	2.01	0.43
1:C:462:ILE:HD12	1:C:462:ILE:H	1.84	0.43
1:K:73:MET:HE1	1:K:110:ARG:HG2	2.01	0.43
1:M:62:LEU:HG	1:M:145:ALA:HB3	2.01	0.43
1:M:152:ASP:OD1	1:M:285:TYR:OH	2.31	0.43
1:S:239:VAL:HG23	1:S:250:GLU:HB2	2.01	0.43
1:S:325:ARG:HE	1:V:401:ASP:HA	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:424:LYS:HE2	1:S:425:LYS:O	2.19	0.43
1:A:396:LYS:HB3	1:A:396:LYS:HE3	1.79	0.43
1:E:185:TYR:HB3	1:E:314:MET:SD	2.59	0.43
1:Q:146:ASP:OD2	1:Q:146:ASP:N	2.51	0.43
1:Q:239:VAL:HG23	1:Q:250:GLU:HB2	2.01	0.43
1:A:73:MET:HE1	1:A:107:VAL:HG11	2.00	0.42
1:A:407:LEU:O	1:A:410:VAL:HG22	2.19	0.42
1:A:408:LEU:HD13	1:X:316[A]:LYS:CD	2.43	0.42
1:I:103:ALA:O	1:I:112:ILE:HG21	2.19	0.42
1:I:396:LYS:HB3	1:I:396:LYS:HE3	1.73	0.42
1:S:299:LYS:HG2	1:S:300:THR:N	2.34	0.42
1:S:396:LYS:HB3	1:S:396:LYS:HE3	1.78	0.42
1:X:345:ILE:HD12	1:X:345:ILE:H	1.84	0.42
1:C:224:LYS:HG3	1:E:423:PHE:CZ	2.54	0.42
1:E:118:ASP:OD2	1:E:131:PRO:HD2	2.19	0.42
1:E:62:LEU:HG	1:E:145:ALA:HB3	2.00	0.42
1:I:299:LYS:HG2	1:I:300:THR:N	2.33	0.42
1:M:195:TYR:CZ	1:M:285:TYR:HB2	2.54	0.42
1:O:96:TYR:CZ	1:O:100:LEU:HD11	2.54	0.42
1:O:217:LEU:CD1	1:Q:316[A]:LYS:HE3	2.49	0.42
1:X:172:LEU:HD11	1:X:289:ARG:HD3	2.02	0.42
1:A:62:LEU:HG	1:A:145:ALA:HB3	2.01	0.42
1:C:83:PRO:HB3	1:C:137:THR:HG22	2.01	0.42
1:E:238:ARG:HH22	1:G:299:LYS:HZ1	1.66	0.42
1:G:172:LEU:HD11	1:G:289:ARG:HD3	2.02	0.42
1:I:62:LEU:HG	1:I:145:ALA:HB3	2.02	0.42
1:V:45:HIS:O	1:V:48:ILE:HG22	2.19	0.42
1:V:345:ILE:H	1:V:345:ILE:HD12	1.83	0.42
1:A:240:LEU:HD12	1:A:247:LEU:HD11	2.01	0.42
1:A:345:ILE:HG21	1:A:358:LEU:HD13	2.01	0.42
1:C:299:LYS:HG2	1:C:300:THR:N	2.34	0.42
1:C:359:LEU:HD22	1:C:379[A]:MET:HE1	2.02	0.42
1:E:195:TYR:CZ	1:E:285:TYR:HB2	2.54	0.42
1:O:232:LYS:HA	1:Q:409:GLY:O	2.20	0.42
1:Q:83:PRO:HB3	1:Q:137:THR:HG22	2.00	0.42
1:S:63:ASP:HB3	1:S:66:SER:HB2	2.01	0.42
1:V:442:LYS:HE3	1:V:442:LYS:HB2	1.84	0.42
1:A:96:TYR:CZ	1:A:100:LEU:HD11	2.55	0.42
1:A:171:ARG:HD2	1:A:292:MET:O	2.19	0.42
1:A:185:TYR:HB3	1:A:314:MET:SD	2.60	0.42
1:E:342:MET:HA	1:E:345:ILE:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:ASN:O	1:O:115:LYS:HD2	2.19	0.42
1:O:240:LEU:HD12	1:O:247:LEU:HD11	2.02	0.42
1:C:185:TYR:HB3	1:C:314:MET:SD	2.60	0.42
1:O:171:ARG:HD2	1:O:292:MET:O	2.19	0.42
1:Q:261:PRO:HG3	1:Q:443:VAL:HG23	2.00	0.42
1:Q:407:LEU:O	1:Q:410:VAL:HG22	2.20	0.42
1:S:195:TYR:CZ	1:S:285:TYR:HB2	2.55	0.42
1:S:328:PHE:HA	1:V:408:LEU:HD11	2.01	0.42
1:E:152:ASP:OD1	1:E:285:TYR:OH	2.33	0.42
1:G:68:PRO:HB2	1:G:96:TYR:CG	2.55	0.42
1:Q:424:LYS:HE2	1:Q:425:LYS:O	2.20	0.42
1:V:313:LEU:O	1:V:331:CYS:HA	2.20	0.42
1:C:407:LEU:O	1:C:410:VAL:HG22	2.19	0.42
1:C:424:LYS:HE2	1:C:425:LYS:O	2.20	0.42
1:K:146:ASP:OD2	1:K:146:ASP:N	2.53	0.42
1:O:18:LEU:HD23	1:O:18:LEU:HA	1.93	0.42
1:V:217:LEU:CD1	1:X:316[A]:LYS:HE3	2.49	0.42
1:A:261:PRO:HG3	1:A:443:VAL:HG23	2.01	0.42
1:I:192:TYR:HB2	1:I:197:THR:HB	2.02	0.42
1:K:345:ILE:HG21	1:K:358:LEU:HD13	2.01	0.42
1:O:122:VAL:HG21	1:O:133:PHE:HD2	1.85	0.42
1:O:203:GLN:NE2	1:O:234:GLU:O	2.42	0.42
1:S:217:LEU:CD1	1:V:316[A]:LYS:HE3	2.50	0.42
1:G:299:LYS:HG2	1:G:300:THR:N	2.33	0.41
1:K:127:ASP:OD2	1:K:142:ARG:NH2	2.37	0.41
1:O:396:LYS:HB3	1:O:396:LYS:HE3	1.78	0.41
1:Q:396:LYS:HG3	1:Q:400:LYS:HE2	2.01	0.41
1:X:146:ASP:OD2	1:X:146:ASP:N	2.53	0.41
1:A:229:ARG:HH22	1:C:415:LEU:HD11	1.85	0.41
1:E:345:ILE:H	1:E:345:ILE:HD12	1.84	0.41
1:G:345:ILE:HG21	1:G:358:LEU:HD13	2.01	0.41
1:I:99:LYS:HB3	1:I:99:LYS:HE3	1.66	0.41
1:K:238:ARG:HH22	1:M:299:LYS:NZ	2.18	0.41
1:K:407:LEU:O	1:K:410:VAL:HG22	2.20	0.41
1:M:113:SER:O	1:M:116:ILE:HG13	2.20	0.41
1:M:325:ARG:HE	1:O:401:ASP:HA	1.85	0.41
1:S:48:ILE:HD12	1:S:48:ILE:HA	1.91	0.41
1:X:73:MET:HE1	1:X:110:ARG:HG2	2.02	0.41
1:X:195:TYR:CZ	1:X:285:TYR:HB2	2.55	0.41
1:A:300:THR:OG1	1:A:446:GLU:OE2	2.29	0.41
1:C:16:LYS:HB3	1:C:20:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:ALA:O	1:E:112:ILE:HG21	2.20	0.41
1:E:166:ALA:HB2	1:E:292:MET:SD	2.60	0.41
1:E:407:LEU:O	1:E:410:VAL:HG22	2.20	0.41
1:G:231:LYS:HD2	1:I:411:ARG:O	2.19	0.41
1:I:214:SER:HB2	1:K:440:ILE:O	2.21	0.41
1:K:185:TYR:HB3	1:K:314:MET:SD	2.60	0.41
1:K:300:THR:OG1	1:K:446:GLU:OE2	2.24	0.41
1:M:346:LEU:HD21	1:M:391:PHE:HB3	2.03	0.41
1:O:185:TYR:HB3	1:O:314:MET:SD	2.60	0.41
1:S:61:ILE:HG23	1:S:147:VAL:HG12	2.02	0.41
1:S:62:LEU:HG	1:S:145:ALA:HB3	2.03	0.41
1:E:231:LYS:HD2	1:G:411:ARG:O	2.20	0.41
1:I:435:PRO:O	1:I:436:ASP:HB2	2.20	0.41
1:O:442:LYS:HE3	1:O:442:LYS:HB2	1.88	0.41
1:Q:231:LYS:HD2	1:S:411:ARG:O	2.21	0.41
1:Q:325:ARG:HD3	1:S:404:ASP:O	2.19	0.41
1:S:341:GLN:OE1	1:S:362:LEU:HD22	2.21	0.41
1:E:313:LEU:O	1:E:331:CYS:HA	2.20	0.41
1:E:346:LEU:HD21	1:E:391:PHE:HB3	2.03	0.41
1:G:118:ASP:OD1	1:G:131:PRO:HD2	2.20	0.41
1:G:203:GLN:NE2	1:G:234:GLU:O	2.45	0.41
1:G:261:PRO:HG3	1:G:443:VAL:HG23	2.02	0.41
1:I:195:TYR:CZ	1:I:285:TYR:HB2	2.56	0.41
1:I:316[A]:LYS:CD	1:K:408:LEU:HD13	2.45	0.41
1:Q:185:TYR:HB3	1:Q:314:MET:SD	2.61	0.41
1:Q:315[A]:CYS:SG	1:Q:390:ALA:HA	2.61	0.41
1:M:185:TYR:HB3	1:M:314:MET:SD	2.60	0.41
1:M:231:LYS:HD2	1:O:411:ARG:O	2.21	0.41
1:O:316[A]:LYS:HA	1:O:316[A]:LYS:HD3	1.86	0.41
1:V:184:MET:HG3	1:V:259:HIS:CD2	2.56	0.41
1:A:225:LEU:H	1:A:225:LEU:HD12	1.85	0.41
1:C:96:TYR:CZ	1:C:100:LEU:HD11	2.56	0.41
1:E:15:LEU:HD21	1:E:29:PRO:HG3	2.02	0.41
1:E:225:LEU:HD23	1:G:420:LEU:HB3	2.01	0.41
1:E:467:ARG:HD2	1:G:171:ARG:NH1	2.35	0.41
1:G:185:TYR:HB3	1:G:314:MET:SD	2.61	0.41
1:G:349:GLU:HG2	1:G:399:ARG:HG3	2.01	0.41
1:K:16:LYS:HB3	1:K:20:ARG:NH1	2.36	0.41
1:M:325:ARG:HD2	1:O:406:LYS:HE3	2.02	0.41
1:O:45:HIS:O	1:O:48:ILE:HG22	2.20	0.41
1:O:61:ILE:HG21	1:O:149:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:345:ILE:HG21	1:Q:358:LEU:HD13	2.02	0.41
3:X:603:SAH:H4'	3:X:603:SAH:HG2	1.92	0.41
3:A:1002:SAH:H4'	3:A:1002:SAH:HG2	1.91	0.41
1:C:118:ASP:HB3	1:C:130:THR:OG1	2.21	0.41
1:C:230:GLY:O	1:E:411:ARG:NE	2.53	0.41
1:C:400:LYS:HA	1:C:400:LYS:HD3	1.81	0.41
1:V:346:LEU:HD21	1:V:391:PHE:HB3	2.03	0.41
1:A:231:LYS:HD2	1:C:411:ARG:O	2.21	0.41
1:A:422:ALA:HB2	1:X:225:LEU:HG	2.03	0.41
1:C:396:LYS:HE3	1:C:396:LYS:HB3	1.80	0.41
1:G:325:ARG:HB3	1:I:406:LYS:HE3	2.02	0.41
1:I:83:PRO:HB3	1:I:137:THR:HG22	2.03	0.41
1:I:427:LYS:O	1:I:427:LYS:HG3	2.20	0.41
1:K:261:PRO:HG3	1:K:443:VAL:HG23	2.03	0.41
1:M:118:ASP:OD1	1:M:131:PRO:HD2	2.21	0.41
1:O:359:LEU:HD22	1:O:379[A]:MET:HE1	2.02	0.41
1:Q:72:MET:HE3	1:Q:73:MET:SD	2.60	0.41
1:S:346:LEU:HD21	1:S:391:PHE:HB3	2.02	0.41
1:V:18:LEU:HD23	1:V:18:LEU:HA	1.93	0.41
1:V:48:ILE:HD12	1:V:48:ILE:HA	1.87	0.41
1:V:325:ARG:HD3	1:X:404:ASP:O	2.21	0.41
1:V:435:PRO:O	1:V:436:ASP:HB2	2.21	0.41
1:A:323:GLY:HA3	1:C:425:LYS:HD2	2.03	0.41
1:G:152:ASP:OD1	1:G:285:TYR:OH	2.35	0.41
1:G:325:ARG:HE	1:I:401:ASP:HA	1.86	0.41
1:A:424:LYS:HB2	1:X:222:ARG:NH1	2.35	0.40
1:C:68:PRO:HB2	1:C:96:TYR:CG	2.56	0.40
1:C:146:ASP:OD2	1:C:146:ASP:N	2.54	0.40
1:O:238:ARG:NH1	1:O:238:ARG:HG2	2.35	0.40
1:Q:396:LYS:HB3	1:Q:396:LYS:HE3	1.83	0.40
1:X:348:THR:HG22	1:X:399:ARG:HH22	1.86	0.40
1:C:45:HIS:O	1:C:48:ILE:HG22	2.21	0.40
1:G:130:THR:OG1	1:G:133:PHE:O	2.33	0.40
1:G:407:LEU:O	1:G:410:VAL:HG22	2.21	0.40
1:K:91:GLU:HG3	1:M:291:THR:HG21	2.03	0.40
1:K:238:ARG:HA	1:K:238:ARG:HD3	1.96	0.40
1:Q:300:THR:OG1	1:Q:446:GLU:OE2	2.25	0.40
1:M:71:ARG:HB3	1:M:78:TYR:CD2	2.56	0.40
1:O:62:LEU:HG	1:O:145:ALA:HB3	2.03	0.40
1:C:7:ASP:OD2	1:C:33:THR:OG1	2.39	0.40
3:I:603:SAH:H4'	3:I:603:SAH:HG2	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:435:PRO:O	1:K:436:ASP:HB2	2.21	0.40
1:Q:225:LEU:HD12	1:Q:225:LEU:H	1.85	0.40
1:S:45:HIS:O	1:S:48:ILE:HG22	2.21	0.40
1:V:83:PRO:HB3	1:V:137:THR:HG22	2.03	0.40
1:X:163:TYR:OH	1:X:269:LYS:HG2	2.21	0.40
1:G:96:TYR:CZ	1:G:100:LEU:HD11	2.57	0.40
1:M:396:LYS:HB3	1:M:396:LYS:HE3	1.79	0.40
1:O:435:PRO:O	1:O:436:ASP:HB2	2.21	0.40
1:Q:229:ARG:HH22	1:S:415:LEU:HD11	1.87	0.40
1:V:300:THR:OG1	1:V:446:GLU:OE2	2.32	0.40
1:X:100:LEU:HD22	1:X:116:ILE:HG23	2.03	0.40
1:X:337:THR:O	1:X:341:GLN:HG3	2.21	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	449/543 (83%)	438 (98%)	11 (2%)	0	100	100
1	C	449/543 (83%)	437 (97%)	12 (3%)	0	100	100
1	E	449/543 (83%)	443 (99%)	6 (1%)	0	100	100
1	G	449/543 (83%)	439 (98%)	10 (2%)	0	100	100
1	I	449/543 (83%)	439 (98%)	10 (2%)	0	100	100
1	K	449/543 (83%)	438 (98%)	11 (2%)	0	100	100
1	M	449/543 (83%)	440 (98%)	9 (2%)	0	100	100
1	O	449/543 (83%)	438 (98%)	11 (2%)	0	100	100
1	Q	449/543 (83%)	440 (98%)	9 (2%)	0	100	100
1	S	449/543 (83%)	441 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	449/543 (83%)	441 (98%)	8 (2%)	0	100	100
1	X	449/543 (83%)	438 (98%)	11 (2%)	0	100	100
All	All	5388/6516 (83%)	5272 (98%)	116 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/466 (84%)	377 (96%)	14 (4%)	35	64
1	C	391/466 (84%)	381 (97%)	10 (3%)	46	75
1	E	391/466 (84%)	373 (95%)	18 (5%)	27	54
1	G	391/466 (84%)	376 (96%)	15 (4%)	33	62
1	I	391/466 (84%)	377 (96%)	14 (4%)	35	64
1	K	391/466 (84%)	377 (96%)	14 (4%)	35	64
1	M	391/466 (84%)	379 (97%)	12 (3%)	40	69
1	O	391/466 (84%)	378 (97%)	13 (3%)	38	67
1	Q	391/466 (84%)	376 (96%)	15 (4%)	33	62
1	S	391/466 (84%)	377 (96%)	14 (4%)	35	64
1	V	391/466 (84%)	377 (96%)	14 (4%)	35	64
1	X	391/466 (84%)	378 (97%)	13 (3%)	38	67
All	All	4692/5592 (84%)	4526 (96%)	166 (4%)	39	65

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	75	ASP
1	A	109	ASP
1	A	214	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	LYS
1	A	253	LYS
1	A	285	TYR
1	A	317	THR
1	A	319	ASP
1	A	363	ASN
1	A	420	LEU
1	A	429	HIS
1	A	442	LYS
1	A	450	PHE
1	C	214	SER
1	C	232	LYS
1	C	285	TYR
1	C	317	THR
1	C	319	ASP
1	C	363	ASN
1	C	400	LYS
1	C	420	LEU
1	C	427	LYS
1	C	450	PHE
1	E	86	SER
1	E	102	SER
1	E	109	ASP
1	E	120	GLN
1	E	214	SER
1	E	232	LYS
1	E	253	LYS
1	E	285	TYR
1	E	299	LYS
1	E	317	THR
1	E	379[A]	MET
1	E	379[B]	MET
1	E	389	GLN
1	E	400	LYS
1	E	420	LEU
1	E	427	LYS
1	E	450	PHE
1	E	467	ARG
1	G	24	MET
1	G	72	MET
1	G	75	ASP
1	G	86	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	109	ASP
1	G	110	ARG
1	G	214	SER
1	G	285	TYR
1	G	317	THR
1	G	376	THR
1	G	399	ARG
1	G	400	LYS
1	G	420	LEU
1	G	427	LYS
1	G	442	LYS
1	I	24	MET
1	I	44	SER
1	I	75	ASP
1	I	109	ASP
1	I	214	SER
1	I	232	LYS
1	I	253	LYS
1	I	285	TYR
1	I	289	ARG
1	I	299	LYS
1	I	317	THR
1	I	363	ASN
1	I	450	PHE
1	I	467	ARG
1	K	75	ASP
1	K	102	SER
1	K	109	ASP
1	K	141	CYS
1	K	232	LYS
1	K	253	LYS
1	K	285	TYR
1	K	317	THR
1	K	319	ASP
1	K	418	CYS
1	K	427	LYS
1	K	429	HIS
1	K	448	ASP
1	K	450	PHE
1	M	75	ASP
1	M	109	ASP
1	M	120	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	214	SER
1	M	253	LYS
1	M	285	TYR
1	M	317	THR
1	M	319	ASP
1	M	363	ASN
1	M	376	THR
1	M	399	ARG
1	M	450	PHE
1	O	24	MET
1	O	109	ASP
1	O	120	GLN
1	O	214	SER
1	O	232	LYS
1	O	253	LYS
1	O	285	TYR
1	O	299	LYS
1	O	317	THR
1	O	319	ASP
1	O	376	THR
1	O	427	LYS
1	O	450	PHE
1	Q	16	LYS
1	Q	75	ASP
1	Q	102	SER
1	Q	120	GLN
1	Q	146	ASP
1	Q	214	SER
1	Q	232	LYS
1	Q	251	SER
1	Q	285	TYR
1	Q	317	THR
1	Q	389	GLN
1	Q	393	LYS
1	Q	427	LYS
1	Q	450	PHE
1	Q	467	ARG
1	S	20	ARG
1	S	24	MET
1	S	109	ASP
1	S	214	SER
1	S	253	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	285	TYR
1	S	317	THR
1	S	319	ASP
1	S	363	ASN
1	S	400	LYS
1	S	420	LEU
1	S	427	LYS
1	S	442	LYS
1	S	467	ARG
1	V	24	MET
1	V	86	SER
1	V	214	SER
1	V	232	LYS
1	V	285	TYR
1	V	299	LYS
1	V	317	THR
1	V	319	ASP
1	V	363	ASN
1	V	393	LYS
1	V	420	LEU
1	V	427	LYS
1	V	450	PHE
1	V	467	ARG
1	X	86	SER
1	X	102	SER
1	X	109	ASP
1	X	214	SER
1	X	232	LYS
1	X	271[A]	SER
1	X	271[B]	SER
1	X	285	TYR
1	X	317	THR
1	X	357	LYS
1	X	427	LYS
1	X	450	PHE
1	X	467	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MGP	M	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	V	604	5	28,35,35	5.28	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	X	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.35	4 (13%)
3	SAH	S	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.87	4 (16%)
3	SAH	X	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.88	4 (16%)
3	SAH	M	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.84	4 (16%)
4	MGP	C	604	5	28,35,35	5.28	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	G	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.36	4 (13%)
4	MGP	E	604	5	28,35,35	5.28	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	Q	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	A	1003	5	28,35,35	5.29	15 (53%)	30,56,56	1.35	4 (13%)
3	SAH	A	1002	-	24,28,28	1.20	3 (12%)	25,40,40	1.88	4 (16%)
3	SAH	C	603	-	24,28,28	1.21	3 (12%)	25,40,40	1.86	4 (16%)
3	SAH	I	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.87	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MGP	I	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.34	4 (13%)
3	SAH	K	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.87	4 (16%)
3	SAH	O	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.86	4 (16%)
3	SAH	E	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.86	4 (16%)
4	MGP	S	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.35	4 (13%)
4	MGP	O	604	5	28,35,35	5.28	15 (53%)	30,56,56	1.35	4 (13%)
3	SAH	V	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.87	4 (16%)
3	SAH	Q	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.77	4 (16%)
4	MGP	K	604	5	28,35,35	5.29	15 (53%)	30,56,56	1.36	4 (13%)
3	SAH	G	603	-	24,28,28	1.20	3 (12%)	25,40,40	1.87	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGP	M	604	5	-	1/18/38/38	0/3/3/3
4	MGP	V	604	5	-	2/18/38/38	0/3/3/3
4	MGP	X	604	5	-	2/18/38/38	0/3/3/3
3	SAH	S	603	-	-	4/11/31/31	0/3/3/3
3	SAH	X	603	-	-	4/11/31/31	0/3/3/3
3	SAH	M	603	-	-	5/11/31/31	0/3/3/3
4	MGP	C	604	5	-	2/18/38/38	0/3/3/3
4	MGP	G	604	5	-	2/18/38/38	0/3/3/3
4	MGP	E	604	5	-	2/18/38/38	0/3/3/3
4	MGP	Q	604	5	-	1/18/38/38	0/3/3/3
4	MGP	A	1003	5	-	0/18/38/38	0/3/3/3
3	SAH	A	1002	-	-	4/11/31/31	0/3/3/3
3	SAH	C	603	-	-	4/11/31/31	0/3/3/3
3	SAH	I	603	-	-	4/11/31/31	0/3/3/3
4	MGP	I	604	5	-	3/18/38/38	0/3/3/3
3	SAH	K	603	-	-	5/11/31/31	0/3/3/3
3	SAH	O	603	-	-	4/11/31/31	0/3/3/3
3	SAH	E	603	-	-	4/11/31/31	0/3/3/3
4	MGP	S	604	5	-	1/18/38/38	0/3/3/3
4	MGP	O	604	5	-	1/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	V	603	-	-	4/11/31/31	0/3/3/3
3	SAH	Q	603	-	-	5/11/31/31	0/3/3/3
4	MGP	K	604	5	-	1/18/38/38	0/3/3/3
3	SAH	G	603	-	-	4/11/31/31	0/3/3/3

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	604	MGP	C2'-C1'	-15.01	1.31	1.53
4	G	604	MGP	C2'-C1'	-15.00	1.31	1.53
4	A	1003	MGP	C2'-C1'	-14.99	1.31	1.53
4	S	604	MGP	C2'-C1'	-14.99	1.31	1.53
4	M	604	MGP	C2'-C1'	-14.99	1.31	1.53
4	K	604	MGP	C2'-C1'	-14.99	1.31	1.53
4	I	604	MGP	C2'-C1'	-14.98	1.31	1.53
4	E	604	MGP	C2'-C1'	-14.98	1.31	1.53
4	Q	604	MGP	C2'-C1'	-14.98	1.31	1.53
4	V	604	MGP	C2'-C1'	-14.97	1.31	1.53
4	C	604	MGP	C2'-C1'	-14.96	1.31	1.53
4	O	604	MGP	C2'-C1'	-14.96	1.31	1.53
4	A	1003	MGP	O4'-C1'	13.82	1.60	1.41
4	G	604	MGP	O4'-C1'	13.82	1.60	1.41
4	M	604	MGP	O4'-C1'	13.82	1.60	1.41
4	S	604	MGP	O4'-C1'	13.82	1.60	1.41
4	Q	604	MGP	O4'-C1'	13.80	1.60	1.41
4	K	604	MGP	O4'-C1'	13.78	1.60	1.41
4	X	604	MGP	O4'-C1'	13.78	1.60	1.41
4	E	604	MGP	O4'-C1'	13.77	1.60	1.41
4	C	604	MGP	O4'-C1'	13.77	1.60	1.41
4	V	604	MGP	O4'-C1'	13.77	1.60	1.41
4	O	604	MGP	O4'-C1'	13.75	1.60	1.41
4	I	604	MGP	O4'-C1'	13.75	1.60	1.41
4	X	604	MGP	C8-N7	9.77	1.51	1.33
4	S	604	MGP	C8-N7	9.77	1.50	1.33
4	K	604	MGP	C8-N7	9.77	1.50	1.33
4	I	604	MGP	C8-N7	9.77	1.50	1.33
4	O	604	MGP	C8-N7	9.76	1.50	1.33
4	A	1003	MGP	C8-N7	9.75	1.50	1.33
4	V	604	MGP	C8-N7	9.75	1.50	1.33
4	C	604	MGP	C8-N7	9.75	1.50	1.33
4	M	604	MGP	C8-N7	9.75	1.50	1.33
4	E	604	MGP	C8-N7	9.75	1.50	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	604	MGP	C8-N7	9.74	1.50	1.33
4	Q	604	MGP	C8-N7	9.74	1.50	1.33
4	I	604	MGP	C8-N9	9.40	1.50	1.33
4	A	1003	MGP	C8-N9	9.40	1.50	1.33
4	M	604	MGP	C8-N9	9.40	1.50	1.33
4	G	604	MGP	C8-N9	9.39	1.50	1.33
4	S	604	MGP	C8-N9	9.39	1.50	1.33
4	O	604	MGP	C8-N9	9.39	1.50	1.33
4	C	604	MGP	C8-N9	9.38	1.50	1.33
4	K	604	MGP	C8-N9	9.37	1.50	1.33
4	V	604	MGP	C8-N9	9.37	1.50	1.33
4	E	604	MGP	C8-N9	9.37	1.50	1.33
4	X	604	MGP	C8-N9	9.37	1.50	1.33
4	Q	604	MGP	C8-N9	9.37	1.50	1.33
4	X	604	MGP	O4'-C4'	-6.68	1.30	1.45
4	G	604	MGP	O4'-C4'	-6.68	1.30	1.45
4	E	604	MGP	O4'-C4'	-6.67	1.30	1.45
4	K	604	MGP	O4'-C4'	-6.67	1.30	1.45
4	S	604	MGP	O4'-C4'	-6.67	1.30	1.45
4	Q	604	MGP	O4'-C4'	-6.67	1.30	1.45
4	M	604	MGP	O4'-C4'	-6.66	1.30	1.45
4	I	604	MGP	O4'-C4'	-6.66	1.30	1.45
4	A	1003	MGP	O4'-C4'	-6.65	1.30	1.45
4	O	604	MGP	O4'-C4'	-6.65	1.30	1.45
4	V	604	MGP	O4'-C4'	-6.64	1.30	1.45
4	C	604	MGP	O4'-C4'	-6.64	1.30	1.45
4	S	604	MGP	C2-N3	5.60	1.46	1.33
4	G	604	MGP	C2-N3	5.59	1.46	1.33
4	A	1003	MGP	C2-N3	5.59	1.46	1.33
4	K	604	MGP	C2-N3	5.59	1.46	1.33
4	Q	604	MGP	C2-N3	5.59	1.46	1.33
4	M	604	MGP	C2-N3	5.58	1.46	1.33
4	V	604	MGP	C2-N3	5.58	1.46	1.33
4	E	604	MGP	C2-N3	5.58	1.46	1.33
4	I	604	MGP	C2-N3	5.57	1.46	1.33
4	O	604	MGP	C2-N3	5.57	1.46	1.33
4	C	604	MGP	C2-N3	5.56	1.46	1.33
4	X	604	MGP	C2-N3	5.54	1.46	1.33
4	V	604	MGP	C2-N2	4.63	1.45	1.34
4	I	604	MGP	C2-N2	4.63	1.45	1.34
4	C	604	MGP	C2-N2	4.63	1.45	1.34
4	O	604	MGP	C2-N2	4.62	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	604	MGP	C2-N2	4.61	1.45	1.34
4	G	604	MGP	C2-N2	4.61	1.45	1.34
4	A	1003	MGP	C2-N2	4.61	1.45	1.34
4	X	604	MGP	C2-N2	4.61	1.45	1.34
4	E	604	MGP	C2-N2	4.60	1.45	1.34
4	Q	604	MGP	C2-N2	4.60	1.45	1.34
4	K	604	MGP	C2-N2	4.60	1.45	1.34
4	M	604	MGP	C2-N2	4.57	1.45	1.34
4	X	604	MGP	C6-N1	4.36	1.44	1.37
4	E	604	MGP	C6-N1	4.36	1.44	1.37
4	I	604	MGP	C6-N1	4.34	1.44	1.37
4	Q	604	MGP	C6-N1	4.34	1.44	1.37
4	V	604	MGP	C6-N1	4.34	1.44	1.37
4	K	604	MGP	C6-N1	4.34	1.44	1.37
4	O	604	MGP	C6-N1	4.34	1.44	1.37
4	C	604	MGP	C6-N1	4.33	1.44	1.37
4	A	1003	MGP	C6-N1	4.33	1.44	1.37
4	G	604	MGP	C6-N1	4.32	1.44	1.37
4	S	604	MGP	C6-N1	4.32	1.44	1.37
4	M	604	MGP	C6-N1	4.25	1.44	1.37
4	S	604	MGP	C4-N3	3.94	1.46	1.37
4	K	604	MGP	C4-N3	3.94	1.46	1.37
4	A	1003	MGP	C4-N3	3.93	1.46	1.37
4	G	604	MGP	C4-N3	3.93	1.46	1.37
4	E	604	MGP	C4-N3	3.93	1.46	1.37
4	Q	604	MGP	C4-N3	3.91	1.46	1.37
4	V	604	MGP	C4-N3	3.91	1.46	1.37
4	M	604	MGP	C4-N3	3.91	1.46	1.37
4	O	604	MGP	C4-N3	3.91	1.46	1.37
4	I	604	MGP	C4-N3	3.91	1.46	1.37
4	C	604	MGP	C4-N3	3.90	1.46	1.37
4	X	604	MGP	C4-N3	3.90	1.46	1.37
4	X	604	MGP	C2-N1	3.83	1.47	1.37
4	E	604	MGP	C2-N1	3.82	1.47	1.37
4	I	604	MGP	C2-N1	3.82	1.47	1.37
4	C	604	MGP	C2-N1	3.82	1.47	1.37
4	Q	604	MGP	C2-N1	3.81	1.47	1.37
4	V	604	MGP	C2-N1	3.81	1.47	1.37
4	O	604	MGP	C2-N1	3.81	1.47	1.37
4	K	604	MGP	C2-N1	3.81	1.47	1.37
4	A	1003	MGP	C2-N1	3.80	1.47	1.37
4	S	604	MGP	C2-N1	3.80	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	604	MGP	C2-N1	3.80	1.47	1.37
4	M	604	MGP	C2-N1	3.78	1.47	1.37
3	C	603	SAH	C2-N3	3.70	1.38	1.32
3	O	603	SAH	C2-N3	3.69	1.38	1.32
3	I	603	SAH	C2-N3	3.69	1.38	1.32
3	V	603	SAH	C2-N3	3.69	1.38	1.32
3	E	603	SAH	C2-N3	3.69	1.38	1.32
3	M	603	SAH	C2-N3	3.68	1.38	1.32
3	A	1002	SAH	C2-N3	3.67	1.38	1.32
3	Q	603	SAH	C2-N3	3.67	1.38	1.32
3	K	603	SAH	C2-N3	3.67	1.38	1.32
3	G	603	SAH	C2-N3	3.66	1.38	1.32
3	X	603	SAH	C2-N3	3.66	1.38	1.32
3	S	603	SAH	C2-N3	3.65	1.38	1.32
4	I	604	MGP	O2'-C2'	2.57	1.49	1.43
4	M	604	MGP	O2'-C2'	2.57	1.49	1.43
4	G	604	MGP	O2'-C2'	2.57	1.49	1.43
4	S	604	MGP	O2'-C2'	2.57	1.49	1.43
4	C	604	MGP	O2'-C2'	2.57	1.49	1.43
4	V	604	MGP	O2'-C2'	2.57	1.49	1.43
4	K	604	MGP	O2'-C2'	2.56	1.49	1.43
4	Q	604	MGP	O2'-C2'	2.56	1.49	1.43
4	E	604	MGP	O2'-C2'	2.56	1.49	1.43
4	O	604	MGP	O2'-C2'	2.56	1.49	1.43
4	A	1003	MGP	O2'-C2'	2.56	1.49	1.43
4	X	604	MGP	O2'-C2'	2.55	1.49	1.43
4	V	604	MGP	C5-C6	2.54	1.52	1.45
4	X	604	MGP	C5-C6	2.54	1.52	1.45
4	I	604	MGP	C5-C6	2.54	1.52	1.45
4	Q	604	MGP	C5-C6	2.54	1.52	1.45
4	C	604	MGP	C5-C6	2.54	1.52	1.45
4	O	604	MGP	C5-C6	2.53	1.52	1.45
4	E	604	MGP	C5-C6	2.53	1.52	1.45
4	K	604	MGP	C5-C6	2.53	1.52	1.45
4	S	604	MGP	C5-C6	2.53	1.52	1.45
4	A	1003	MGP	C5-C6	2.52	1.52	1.45
4	M	604	MGP	C5-C6	2.52	1.51	1.45
4	G	604	MGP	C5-C6	2.52	1.51	1.45
4	E	604	MGP	C5-C4	2.40	1.43	1.39
4	G	604	MGP	C5-C4	2.39	1.43	1.39
4	S	604	MGP	C5-C4	2.39	1.43	1.39
4	M	604	MGP	C5-C4	2.39	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	604	MGP	C5-C4	2.39	1.43	1.39
4	C	604	MGP	O3'-C3'	-2.39	1.37	1.43
4	M	604	MGP	O3'-C3'	-2.39	1.37	1.43
4	V	604	MGP	O3'-C3'	-2.39	1.37	1.43
4	A	1003	MGP	C5-C4	2.39	1.43	1.39
4	V	604	MGP	C5-C4	2.39	1.43	1.39
4	O	604	MGP	O3'-C3'	-2.38	1.37	1.43
4	I	604	MGP	O3'-C3'	-2.38	1.37	1.43
4	X	604	MGP	C5-C4	2.38	1.43	1.39
4	C	604	MGP	C5-C4	2.38	1.43	1.39
4	O	604	MGP	C5-C4	2.38	1.43	1.39
4	S	604	MGP	O3'-C3'	-2.38	1.37	1.43
4	G	604	MGP	O3'-C3'	-2.37	1.37	1.43
4	A	1003	MGP	O3'-C3'	-2.37	1.37	1.43
4	Q	604	MGP	C5-C4	2.37	1.43	1.39
4	K	604	MGP	O3'-C3'	-2.37	1.37	1.43
4	Q	604	MGP	O3'-C3'	-2.37	1.37	1.43
4	I	604	MGP	C5-C4	2.37	1.43	1.39
4	X	604	MGP	O3'-C3'	-2.37	1.37	1.43
4	E	604	MGP	O3'-C3'	-2.37	1.37	1.43
3	I	603	SAH	C2-N1	2.32	1.38	1.33
3	O	603	SAH	C2-N1	2.32	1.38	1.33
3	V	603	SAH	C2-N1	2.32	1.38	1.33
3	C	603	SAH	C2-N1	2.31	1.38	1.33
3	A	1002	SAH	C2-N1	2.30	1.38	1.33
3	E	603	SAH	C2-N1	2.30	1.38	1.33
3	X	603	SAH	C2-N1	2.30	1.38	1.33
3	Q	603	SAH	C2-N1	2.29	1.38	1.33
3	K	603	SAH	C2-N1	2.29	1.38	1.33
3	S	603	SAH	C2-N1	2.29	1.38	1.33
3	G	603	SAH	C2-N1	2.29	1.38	1.33
3	M	603	SAH	C2-N1	2.28	1.38	1.33
3	A	1002	SAH	OXT-C	-2.26	1.23	1.30
3	O	603	SAH	OXT-C	-2.26	1.23	1.30
3	G	603	SAH	OXT-C	-2.26	1.23	1.30
3	V	603	SAH	OXT-C	-2.26	1.23	1.30
3	C	603	SAH	OXT-C	-2.26	1.23	1.30
3	E	603	SAH	OXT-C	-2.26	1.23	1.30
3	M	603	SAH	OXT-C	-2.26	1.23	1.30
3	S	603	SAH	OXT-C	-2.25	1.23	1.30
3	X	603	SAH	OXT-C	-2.25	1.23	1.30
3	Q	603	SAH	OXT-C	-2.25	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	603	SAH	OXT-C	-2.25	1.23	1.30
3	K	603	SAH	OXT-C	-2.24	1.23	1.30
4	I	604	MGP	PA-O5'	2.21	1.68	1.59
4	S	604	MGP	PA-O5'	2.20	1.68	1.59
4	M	604	MGP	PA-O5'	2.20	1.68	1.59
4	C	604	MGP	PA-O5'	2.20	1.68	1.59
4	K	604	MGP	PA-O5'	2.20	1.68	1.59
4	V	604	MGP	PA-O5'	2.19	1.68	1.59
4	Q	604	MGP	PA-O5'	2.19	1.68	1.59
4	E	604	MGP	PA-O5'	2.19	1.68	1.59
4	A	1003	MGP	PA-O5'	2.19	1.68	1.59
4	O	604	MGP	PA-O5'	2.19	1.68	1.59
4	X	604	MGP	PA-O5'	2.18	1.68	1.59
4	G	604	MGP	PA-O5'	2.18	1.68	1.59

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	603	SAH	N3-C2-N1	-5.60	119.93	128.68
3	M	603	SAH	N3-C2-N1	-5.59	119.94	128.68
3	A	1002	SAH	N3-C2-N1	-5.59	119.94	128.68
3	K	603	SAH	N3-C2-N1	-5.59	119.94	128.68
3	Q	603	SAH	N3-C2-N1	-5.58	119.96	128.68
3	G	603	SAH	N3-C2-N1	-5.58	119.96	128.68
3	X	603	SAH	N3-C2-N1	-5.57	119.97	128.68
3	I	603	SAH	N3-C2-N1	-5.57	119.97	128.68
3	E	603	SAH	N3-C2-N1	-5.57	119.98	128.68
3	C	603	SAH	N3-C2-N1	-5.56	119.99	128.68
3	O	603	SAH	N3-C2-N1	-5.56	120.00	128.68
3	V	603	SAH	N3-C2-N1	-5.55	120.00	128.68
3	A	1002	SAH	C5'-SD-CG	-5.04	87.15	102.27
3	X	603	SAH	C5'-SD-CG	-5.04	87.15	102.27
3	V	603	SAH	C5'-SD-CG	-5.03	87.18	102.27
3	I	603	SAH	C5'-SD-CG	-5.02	87.20	102.27
3	G	603	SAH	C5'-SD-CG	-5.01	87.22	102.27
3	S	603	SAH	C5'-SD-CG	-4.99	87.28	102.27
3	K	603	SAH	C5'-SD-CG	-4.99	87.30	102.27
3	C	603	SAH	C5'-SD-CG	-4.91	87.54	102.27
3	O	603	SAH	C5'-SD-CG	-4.90	87.58	102.27
3	E	603	SAH	C5'-SD-CG	-4.89	87.59	102.27
3	M	603	SAH	C5'-SD-CG	-4.61	88.45	102.27
4	E	604	MGP	C3'-C2'-C1'	3.88	106.81	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	604	MGP	C3'-C2'-C1'	3.88	106.81	100.98
4	G	604	MGP	C3'-C2'-C1'	3.86	106.80	100.98
4	K	604	MGP	C3'-C2'-C1'	3.86	106.79	100.98
4	A	1003	MGP	C3'-C2'-C1'	3.85	106.77	100.98
3	Q	603	SAH	C5'-SD-CG	-3.84	90.75	102.27
4	Q	604	MGP	C3'-C2'-C1'	3.83	106.75	100.98
4	M	604	MGP	C3'-C2'-C1'	3.83	106.75	100.98
4	X	604	MGP	C3'-C2'-C1'	3.83	106.74	100.98
4	C	604	MGP	C3'-C2'-C1'	3.79	106.69	100.98
4	V	604	MGP	C3'-C2'-C1'	3.79	106.69	100.98
4	O	604	MGP	C3'-C2'-C1'	3.79	106.68	100.98
4	I	604	MGP	C3'-C2'-C1'	3.74	106.61	100.98
4	M	604	MGP	PB-O3B-PC	-3.32	121.42	132.83
4	O	604	MGP	PB-O3B-PC	-3.32	121.43	132.83
4	G	604	MGP	PB-O3B-PC	-3.31	121.47	132.83
4	A	1003	MGP	PB-O3B-PC	-3.31	121.47	132.83
4	K	604	MGP	PB-O3B-PC	-3.31	121.48	132.83
4	S	604	MGP	PB-O3B-PC	-3.29	121.54	132.83
4	C	604	MGP	PB-O3B-PC	-3.28	121.57	132.83
4	V	604	MGP	PB-O3B-PC	-3.27	121.60	132.83
4	Q	604	MGP	PB-O3B-PC	-3.23	121.74	132.83
4	X	604	MGP	PB-O3B-PC	-3.23	121.74	132.83
4	E	604	MGP	PB-O3B-PC	-3.21	121.81	132.83
4	I	604	MGP	PB-O3B-PC	-3.18	121.90	132.83
3	Q	603	SAH	OXT-C-O	-2.82	117.69	124.09
4	I	604	MGP	C2-N1-C6	-2.80	119.93	125.10
4	V	604	MGP	C2-N1-C6	-2.80	119.94	125.10
4	C	604	MGP	C2-N1-C6	-2.78	119.97	125.10
4	O	604	MGP	C2-N1-C6	-2.77	119.99	125.10
4	M	604	MGP	C2-N1-C6	-2.76	120.02	125.10
4	K	604	MGP	C2-N1-C6	-2.76	120.02	125.10
4	Q	604	MGP	C2-N1-C6	-2.75	120.03	125.10
4	X	604	MGP	C2-N1-C6	-2.75	120.04	125.10
3	E	603	SAH	OXT-C-O	-2.74	117.86	124.09
3	O	603	SAH	OXT-C-O	-2.74	117.86	124.09
3	M	603	SAH	OXT-C-O	-2.74	117.87	124.09
3	C	603	SAH	OXT-C-O	-2.74	117.88	124.09
4	E	604	MGP	C2-N1-C6	-2.74	120.06	125.10
3	X	603	SAH	OXT-C-O	-2.72	117.92	124.09
4	A	1003	MGP	C2-N1-C6	-2.72	120.10	125.10
4	S	604	MGP	C2-N1-C6	-2.72	120.10	125.10
4	G	604	MGP	C2-N1-C6	-2.71	120.10	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	603	SAH	OXT-C-O	-2.70	117.95	124.09
3	K	603	SAH	OXT-C-O	-2.70	117.95	124.09
3	S	603	SAH	OXT-C-O	-2.68	118.00	124.09
3	I	603	SAH	OXT-C-O	-2.68	118.00	124.09
3	A	1002	SAH	OXT-C-O	-2.65	118.07	124.09
3	G	603	SAH	OXT-C-O	-2.65	118.07	124.09
4	O	604	MGP	PB-O3A-PA	-2.52	124.19	132.83
4	V	604	MGP	PB-O3A-PA	-2.48	124.32	132.83
4	I	604	MGP	PB-O3A-PA	-2.48	124.33	132.83
4	C	604	MGP	PB-O3A-PA	-2.45	124.41	132.83
4	G	604	MGP	PB-O3A-PA	-2.44	124.46	132.83
4	M	604	MGP	PB-O3A-PA	-2.43	124.48	132.83
4	E	604	MGP	PB-O3A-PA	-2.41	124.54	132.83
4	Q	604	MGP	PB-O3A-PA	-2.41	124.55	132.83
4	A	1003	MGP	PB-O3A-PA	-2.41	124.55	132.83
4	X	604	MGP	PB-O3A-PA	-2.40	124.58	132.83
4	K	604	MGP	PB-O3A-PA	-2.40	124.59	132.83
4	S	604	MGP	PB-O3A-PA	-2.37	124.71	132.83
3	X	603	SAH	OXT-C-CA	2.24	121.00	113.38
3	V	603	SAH	OXT-C-CA	2.23	120.98	113.38
3	E	603	SAH	OXT-C-CA	2.21	120.90	113.38
3	K	603	SAH	OXT-C-CA	2.20	120.89	113.38
3	A	1002	SAH	OXT-C-CA	2.20	120.87	113.38
3	I	603	SAH	OXT-C-CA	2.20	120.86	113.38
3	G	603	SAH	OXT-C-CA	2.19	120.84	113.38
3	O	603	SAH	OXT-C-CA	2.18	120.81	113.38
3	S	603	SAH	OXT-C-CA	2.17	120.79	113.38
3	C	603	SAH	OXT-C-CA	2.17	120.77	113.38
3	Q	603	SAH	OXT-C-CA	2.11	120.58	113.38
3	M	603	SAH	OXT-C-CA	2.06	120.40	113.38

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	SAH	N-CA-CB-CG
3	C	603	SAH	N-CA-CB-CG
3	C	603	SAH	C-CA-CB-CG
3	E	603	SAH	N-CA-CB-CG
3	E	603	SAH	C-CA-CB-CG
3	G	603	SAH	N-CA-CB-CG
3	I	603	SAH	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	603	SAH	C-CA-CB-CG
3	K	603	SAH	N-CA-CB-CG
3	M	603	SAH	N-CA-CB-CG
3	M	603	SAH	C-CA-CB-CG
3	O	603	SAH	N-CA-CB-CG
3	O	603	SAH	C-CA-CB-CG
3	Q	603	SAH	N-CA-CB-CG
3	Q	603	SAH	C-CA-CB-CG
3	S	603	SAH	N-CA-CB-CG
3	S	603	SAH	C-CA-CB-CG
3	V	603	SAH	N-CA-CB-CG
3	X	603	SAH	N-CA-CB-CG
3	A	1002	SAH	C-CA-CB-CG
3	G	603	SAH	C-CA-CB-CG
3	K	603	SAH	C-CA-CB-CG
3	V	603	SAH	C-CA-CB-CG
3	X	603	SAH	C-CA-CB-CG
4	I	604	MGP	O4'-C4'-C5'-O5'
3	M	603	SAH	OXT-C-CA-CB
3	Q	603	SAH	OXT-C-CA-CB
4	G	604	MGP	C5'-O5'-PA-O3A
3	I	603	SAH	O-C-CA-CB
3	K	603	SAH	OXT-C-CA-CB
3	A	1002	SAH	OXT-C-CA-CB
3	C	603	SAH	OXT-C-CA-CB
3	E	603	SAH	OXT-C-CA-CB
3	G	603	SAH	O-C-CA-CB
3	G	603	SAH	OXT-C-CA-CB
3	K	603	SAH	O-C-CA-CB
3	M	603	SAH	O-C-CA-CB
3	O	603	SAH	O-C-CA-CB
3	O	603	SAH	OXT-C-CA-CB
3	Q	603	SAH	O-C-CA-CB
3	S	603	SAH	O-C-CA-CB
3	S	603	SAH	OXT-C-CA-CB
3	V	603	SAH	O-C-CA-CB
3	V	603	SAH	OXT-C-CA-CB
3	X	603	SAH	OXT-C-CA-CB
4	E	604	MGP	O4'-C4'-C5'-O5'
3	A	1002	SAH	O-C-CA-CB
3	C	603	SAH	O-C-CA-CB
3	E	603	SAH	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	603	SAH	OXT-C-CA-CB
4	X	604	MGP	O4'-C4'-C5'-O5'
3	X	603	SAH	O-C-CA-CB
4	G	604	MGP	O4'-C4'-C5'-O5'
4	Q	604	MGP	O4'-C4'-C5'-O5'
4	S	604	MGP	O4'-C4'-C5'-O5'
4	C	604	MGP	O4'-C4'-C5'-O5'
4	V	604	MGP	O4'-C4'-C5'-O5'
3	K	603	SAH	OXT-C-CA-N
4	C	604	MGP	C5'-O5'-PA-O3A
4	E	604	MGP	C5'-O5'-PA-O3A
4	I	604	MGP	C5'-O5'-PA-O3A
4	V	604	MGP	C5'-O5'-PA-O3A
4	X	604	MGP	C5'-O5'-PA-O3A
4	I	604	MGP	C3'-C4'-C5'-O5'
4	K	604	MGP	O4'-C4'-C5'-O5'
4	M	604	MGP	O4'-C4'-C5'-O5'
4	O	604	MGP	O4'-C4'-C5'-O5'
3	M	603	SAH	OXT-C-CA-N
3	Q	603	SAH	OXT-C-CA-N

There are no ring outliers.

24 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	604	MGP	2	0
4	V	604	MGP	2	0
4	X	604	MGP	2	0
3	S	603	SAH	1	0
3	X	603	SAH	2	0
3	M	603	SAH	1	0
4	C	604	MGP	2	0
4	G	604	MGP	2	0
4	E	604	MGP	2	0
4	Q	604	MGP	2	0
4	A	1003	MGP	2	0
3	A	1002	SAH	2	0
3	C	603	SAH	1	0
3	I	603	SAH	2	0
4	I	604	MGP	2	0
3	K	603	SAH	2	0
3	O	603	SAH	1	0

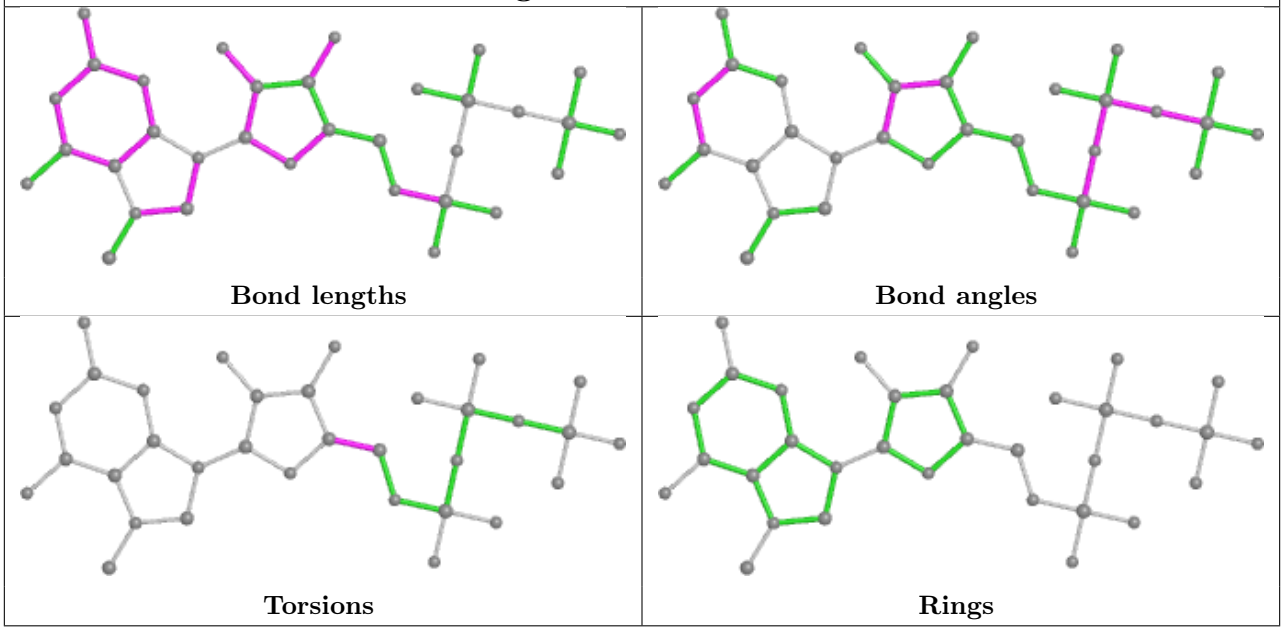
Continued on next page...

Continued from previous page...

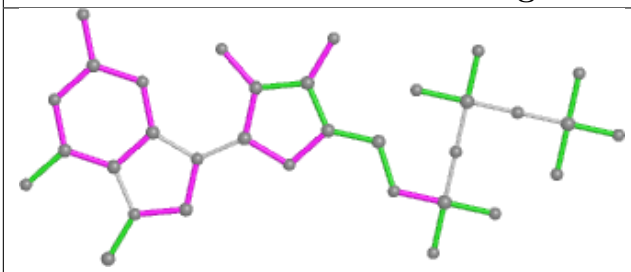
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	603	SAH	1	0
4	S	604	MGP	2	0
4	O	604	MGP	2	0
3	V	603	SAH	1	0
3	Q	603	SAH	1	0
4	K	604	MGP	2	0
3	G	603	SAH	1	0

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.

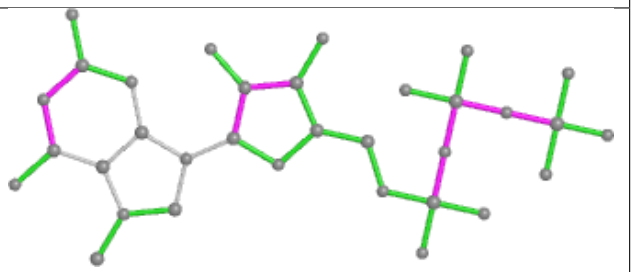
Ligand MGP M 604



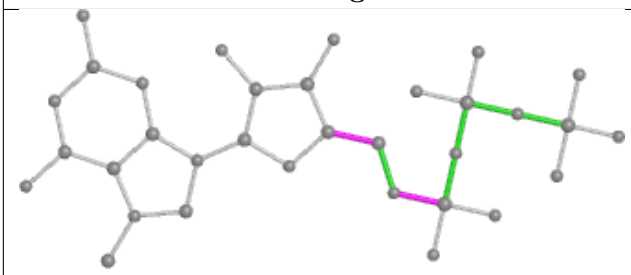
Ligand MGP V 604



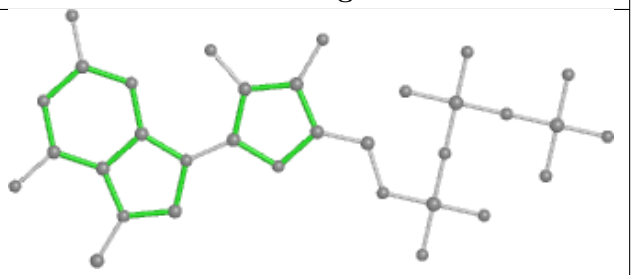
Bond lengths



Bond angles

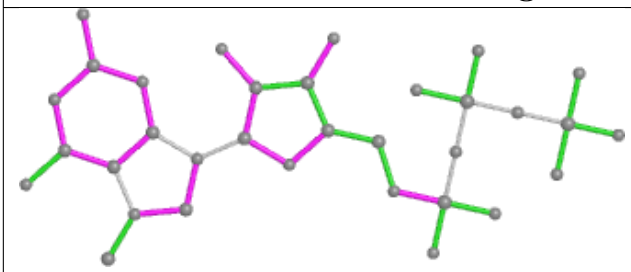


Torsions

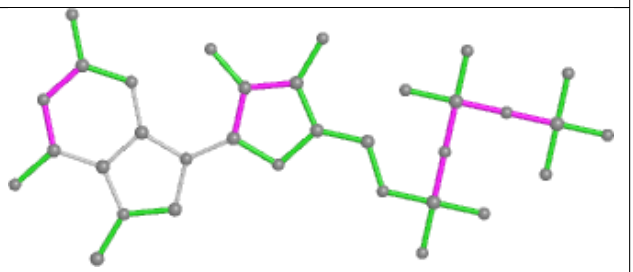


Rings

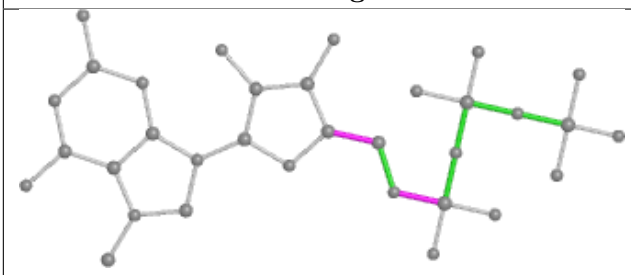
Ligand MGP X 604



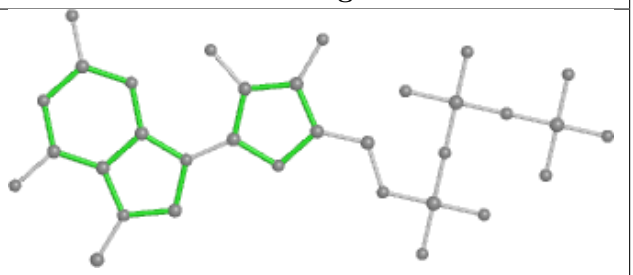
Bond lengths



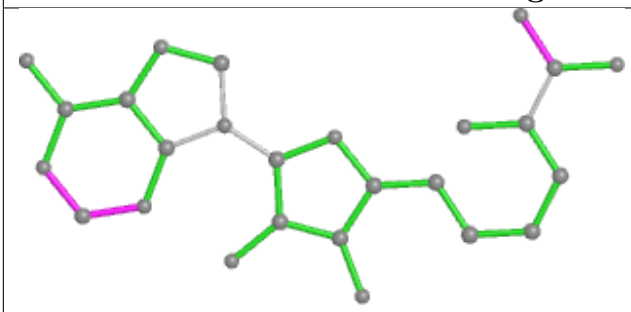
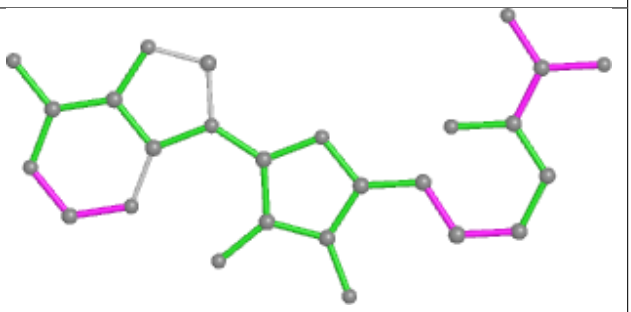
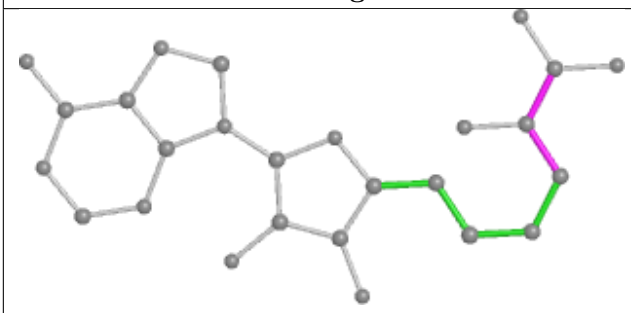
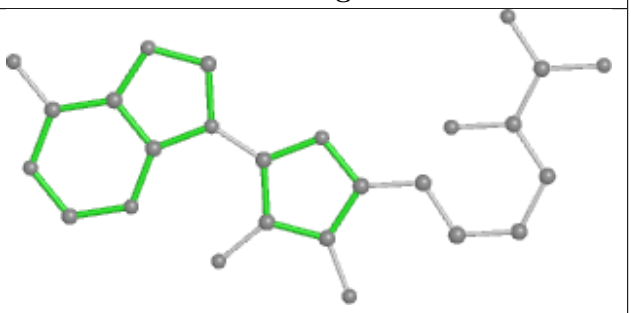
Bond angles

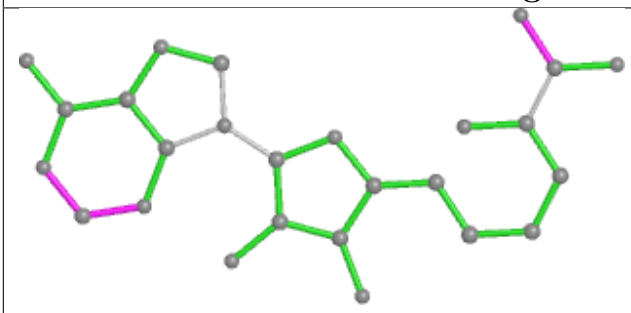
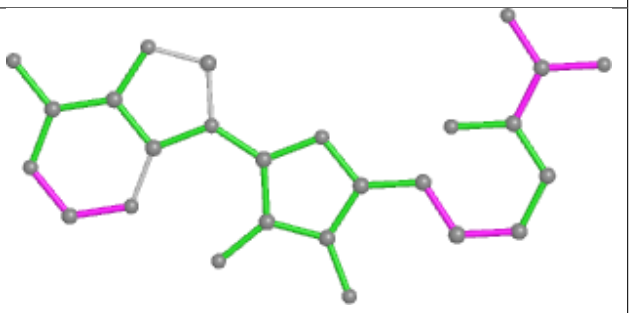
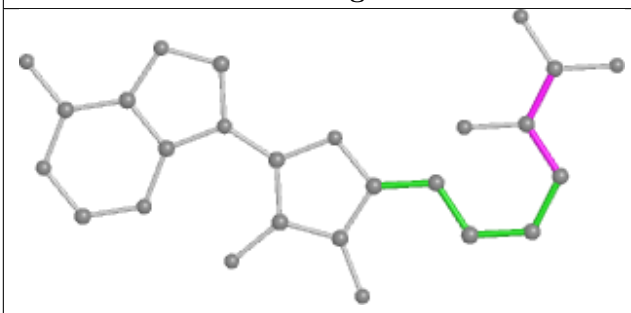
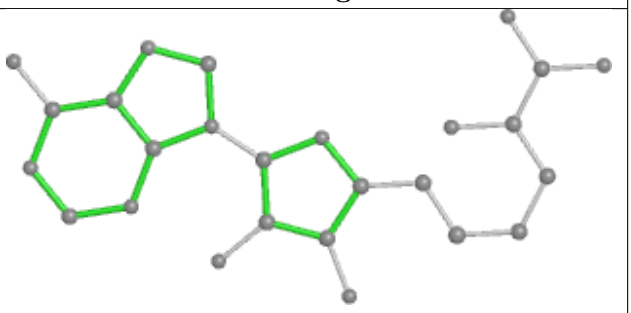


Torsions

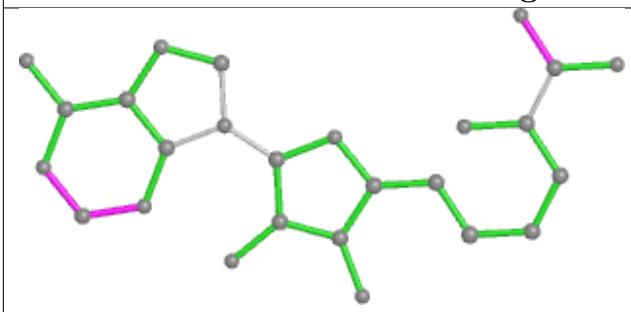


Rings

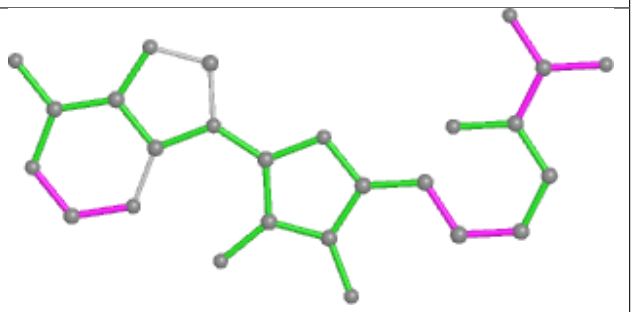
Ligand SAH S 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH X 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

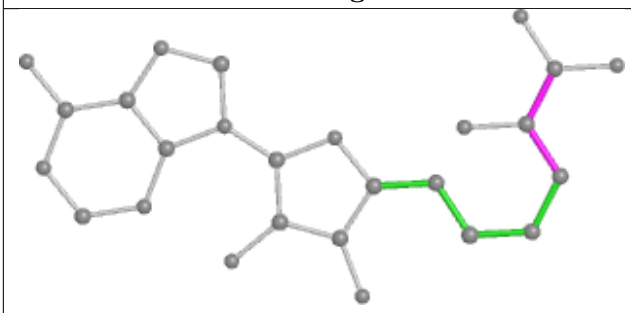
Ligand SAH M 603



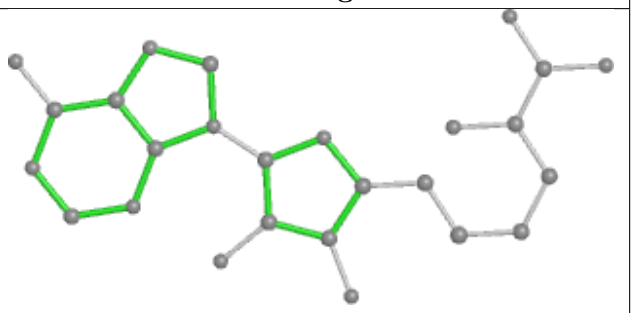
Bond lengths



Bond angles

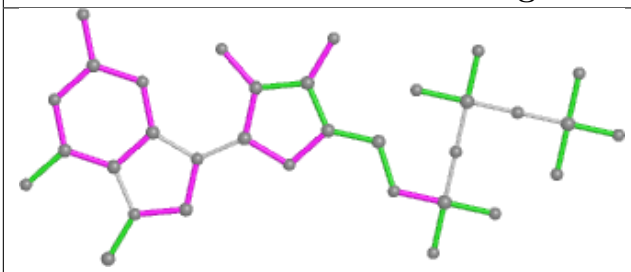


Torsions

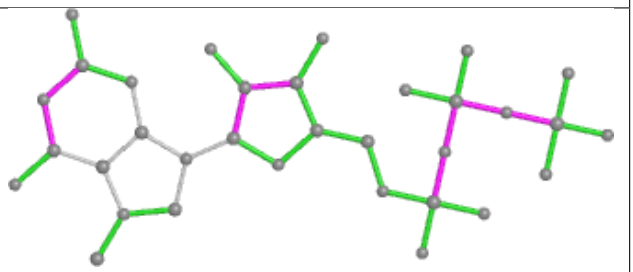


Rings

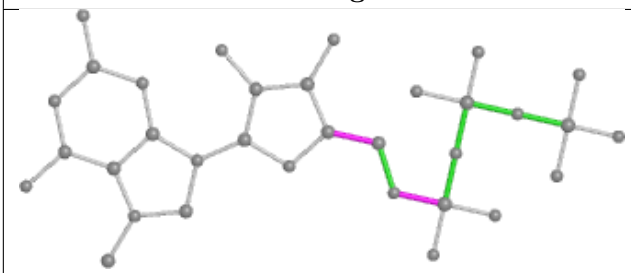
Ligand MGP C 604



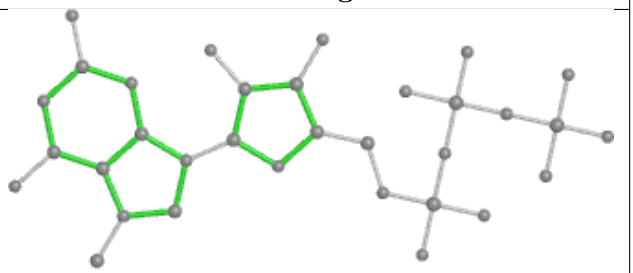
Bond lengths



Bond angles

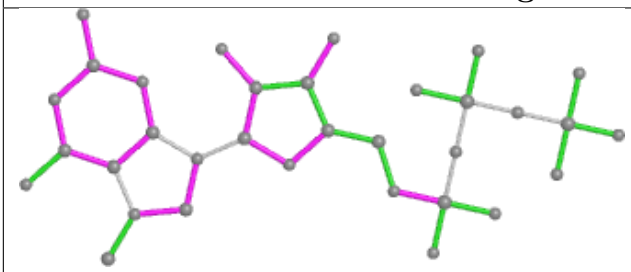


Torsions

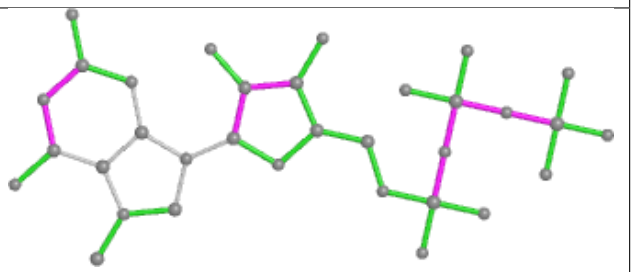


Rings

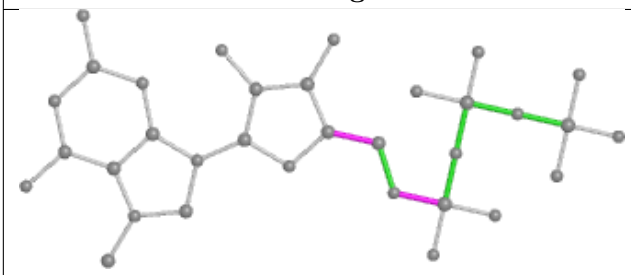
Ligand MGP G 604



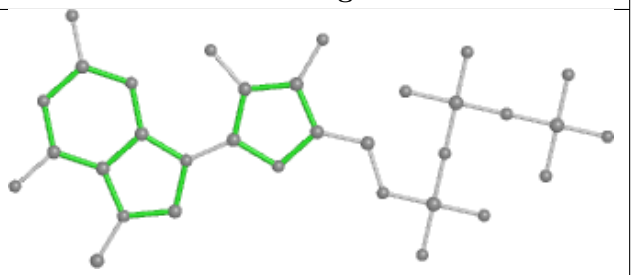
Bond lengths



Bond angles

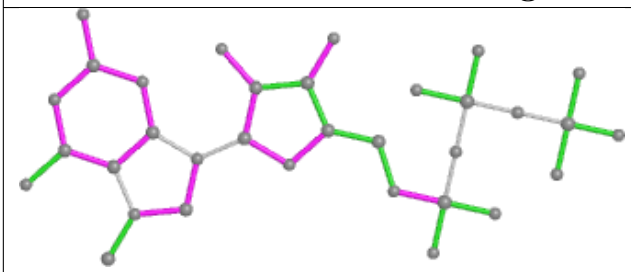


Torsions

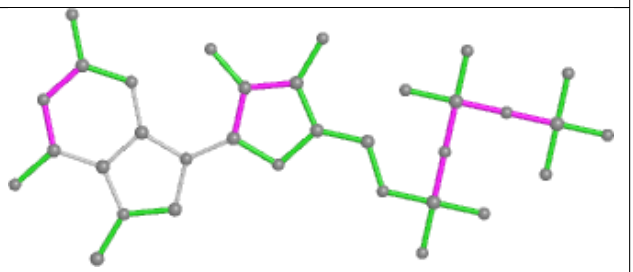


Rings

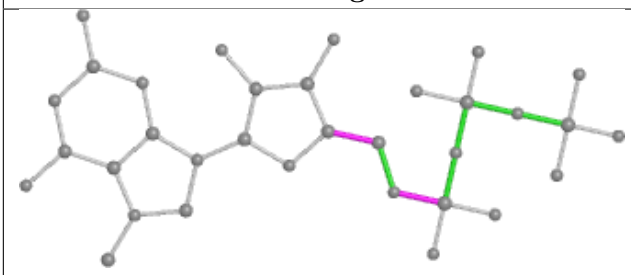
Ligand MGP E 604



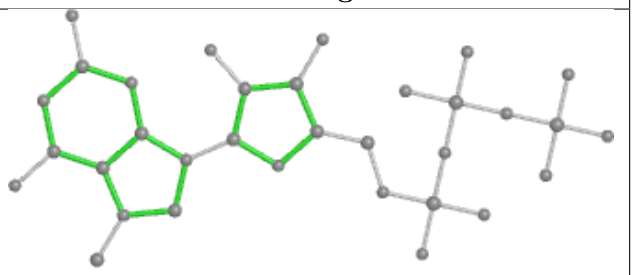
Bond lengths



Bond angles

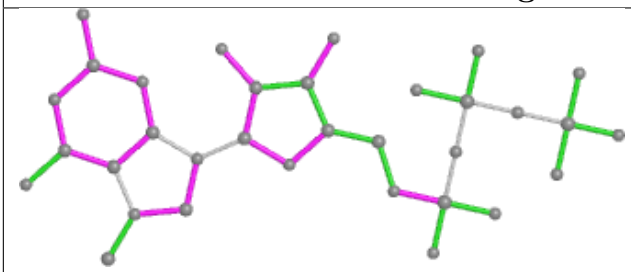


Torsions

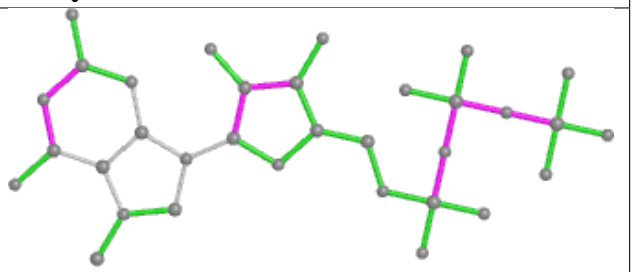


Rings

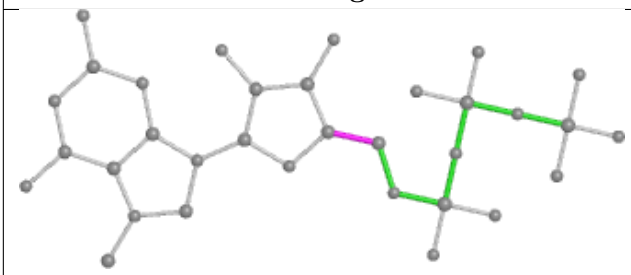
Ligand MGP Q 604



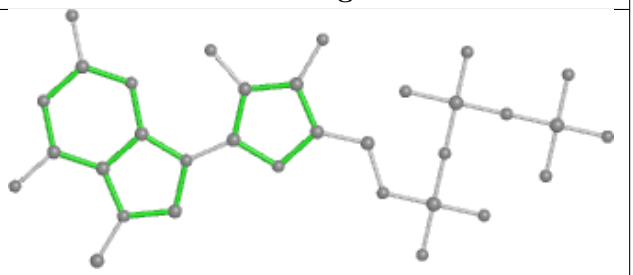
Bond lengths



Bond angles

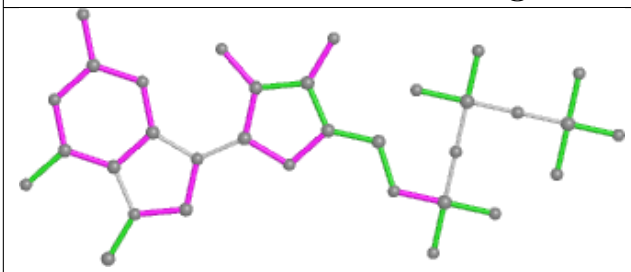


Torsions

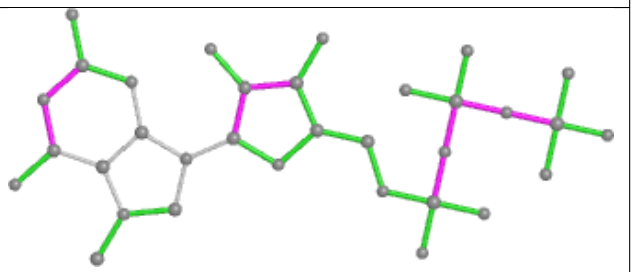


Rings

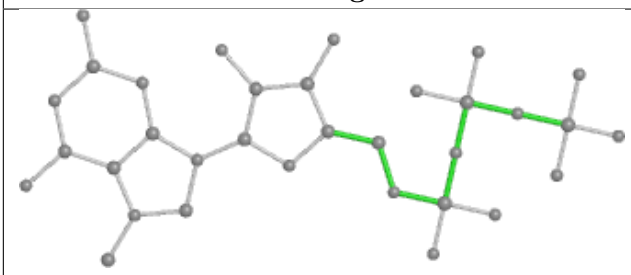
Ligand MGP A 1003



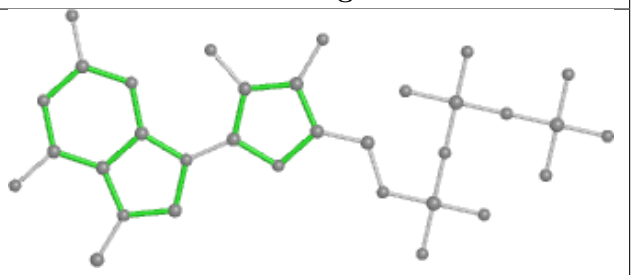
Bond lengths



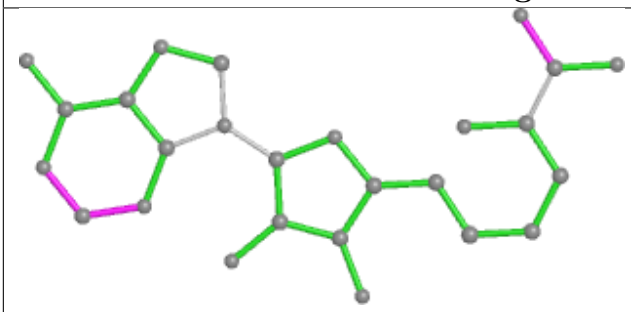
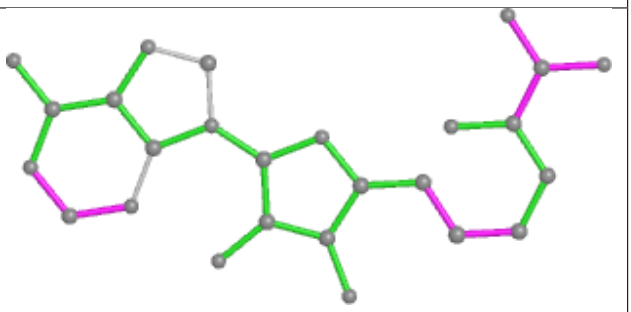
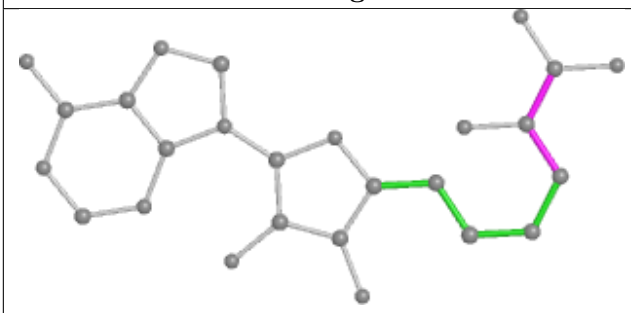
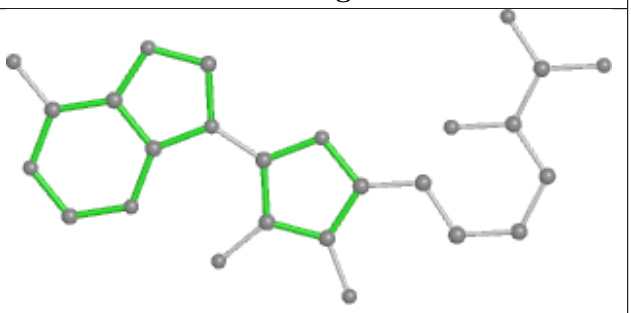
Bond angles

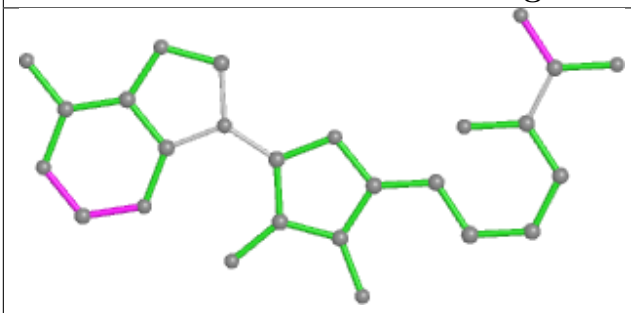
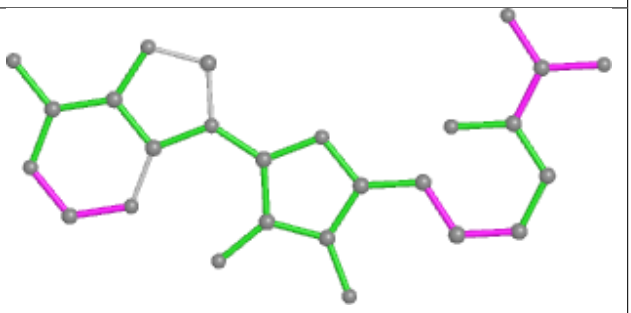
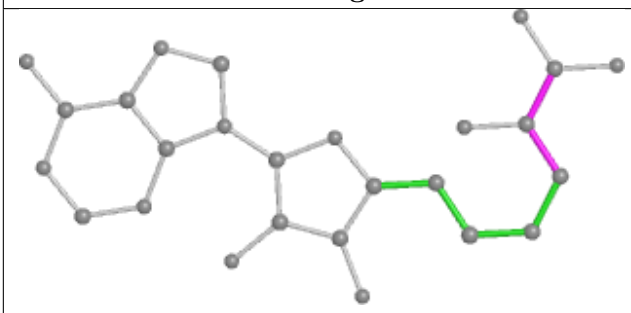
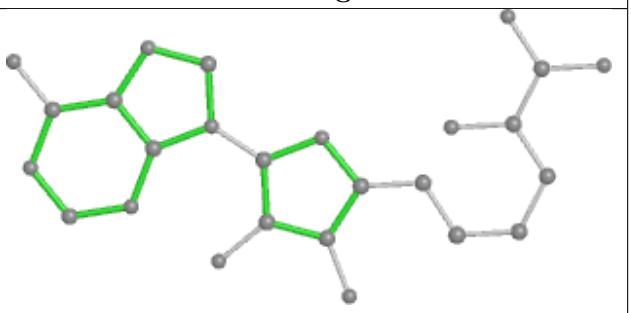


Torsions

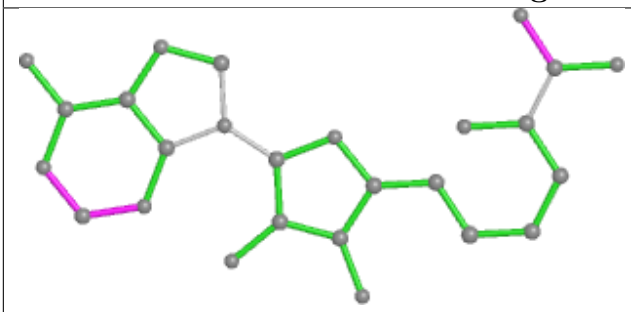


Rings

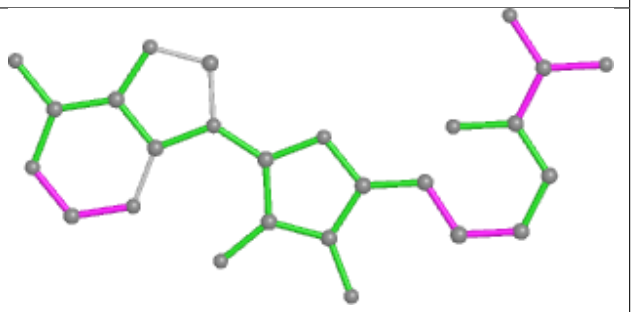
Ligand SAH A 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH C 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

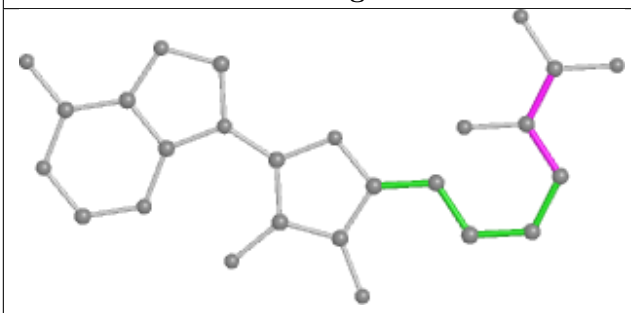
Ligand SAH I 603



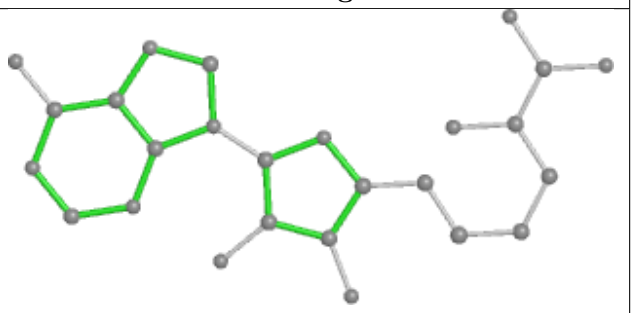
Bond lengths



Bond angles

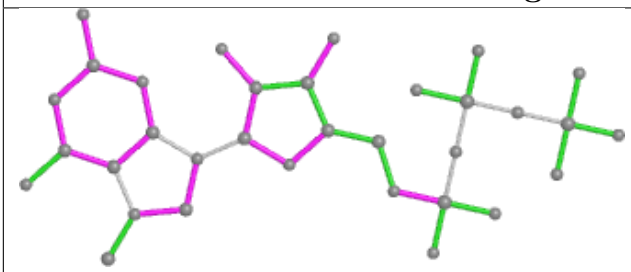


Torsions

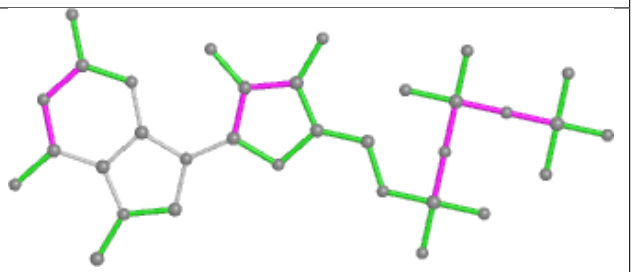


Rings

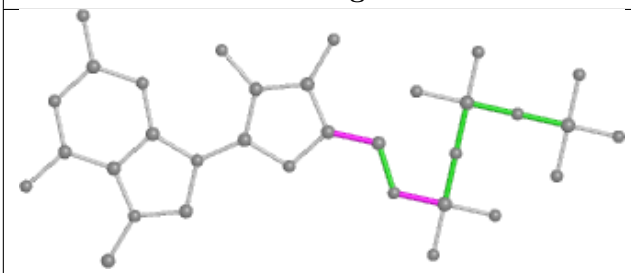
Ligand MGP I 604



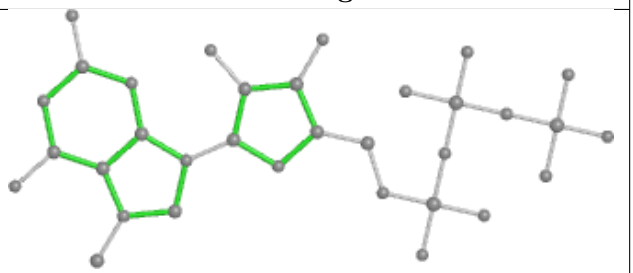
Bond lengths



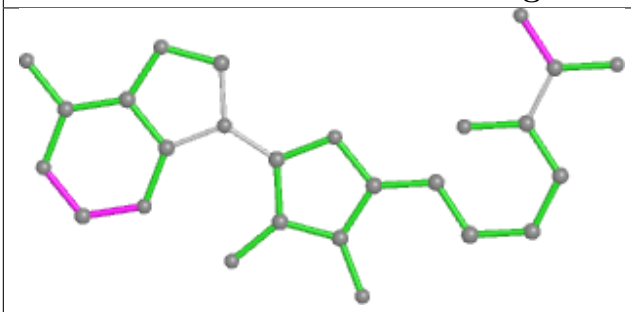
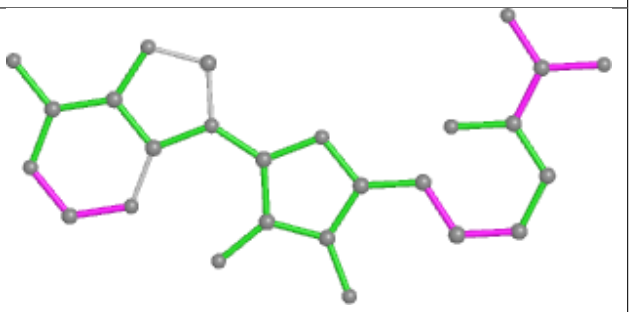
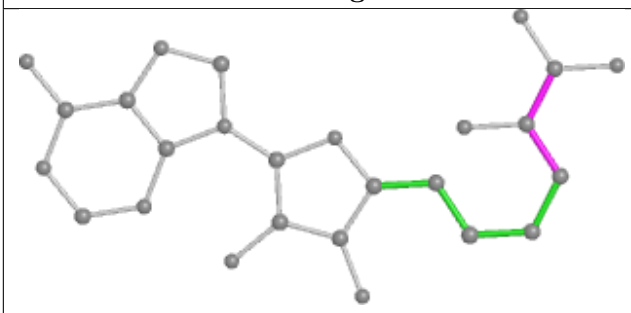
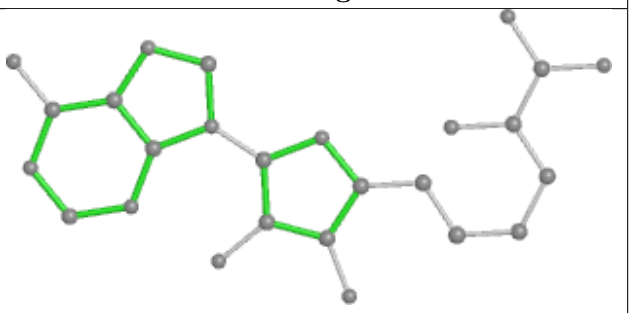
Bond angles

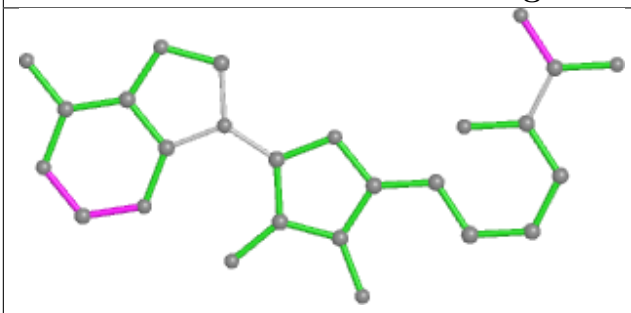
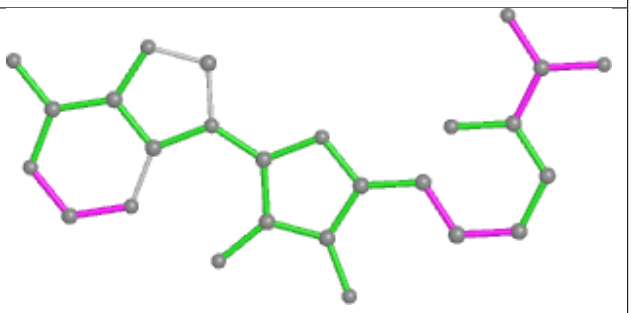
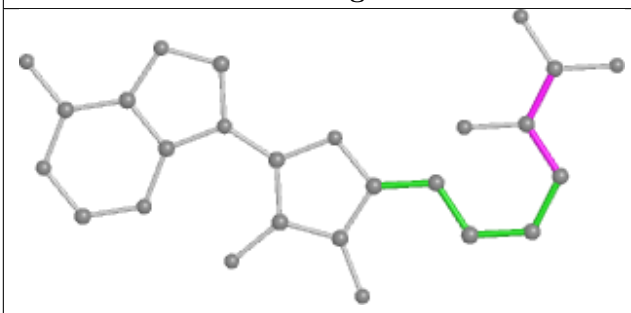
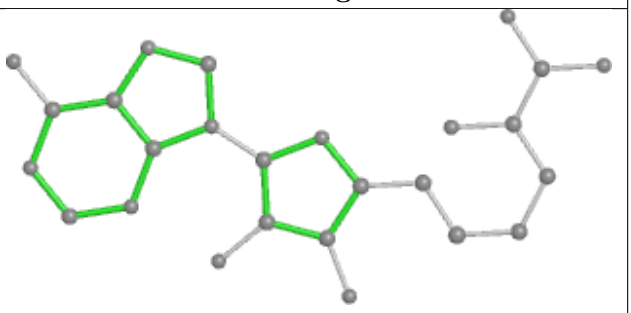


Torsions

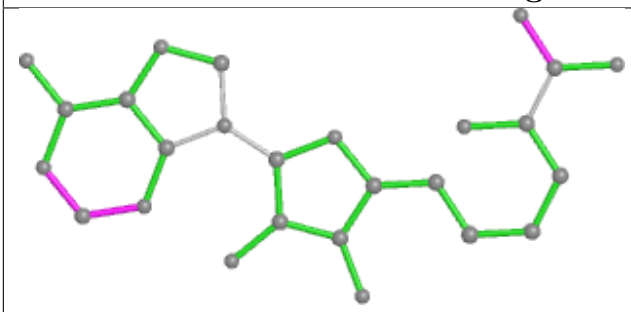


Rings

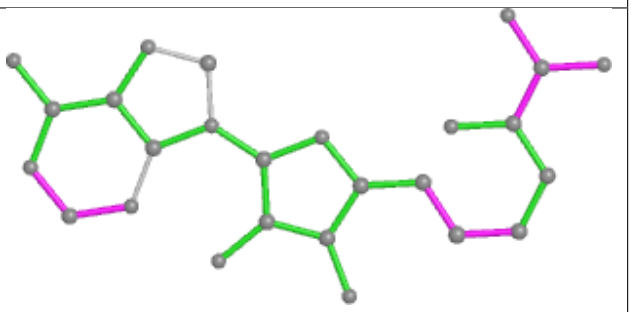
Ligand SAH K 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH O 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

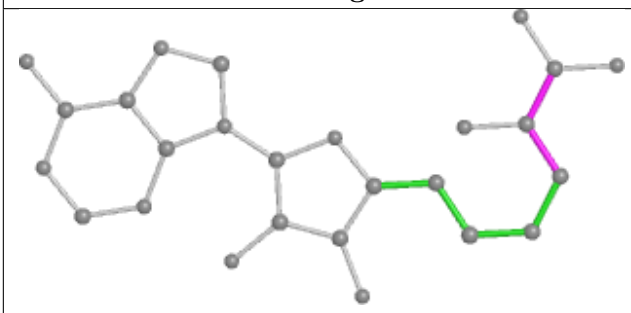
Ligand SAH E 603



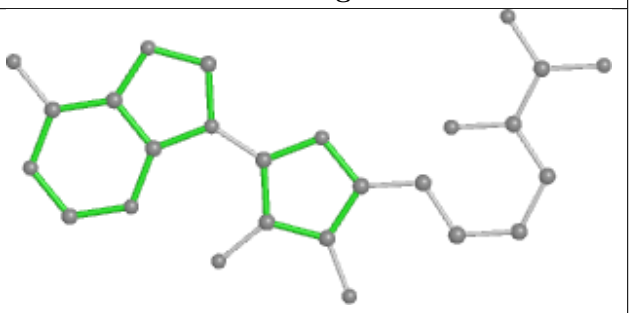
Bond lengths



Bond angles

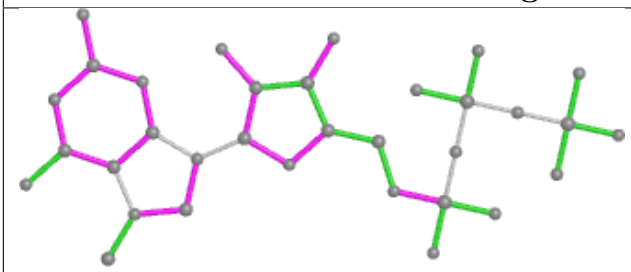


Torsions

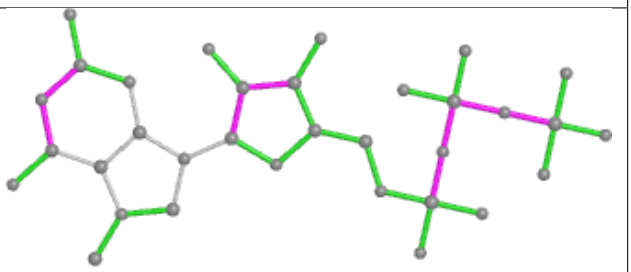


Rings

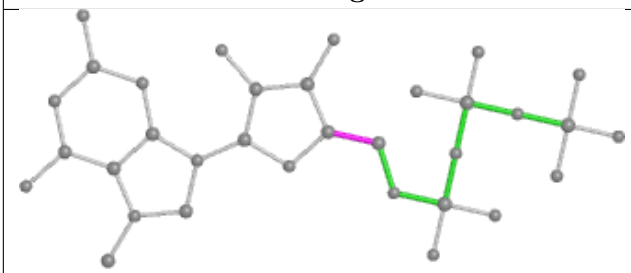
Ligand MGP S 604



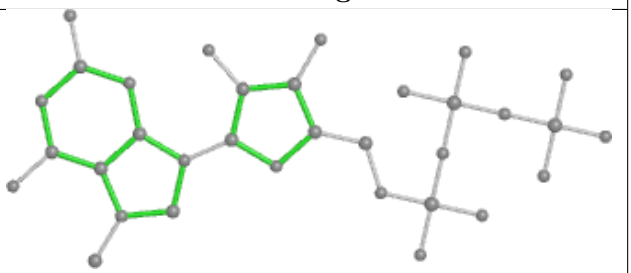
Bond lengths



Bond angles

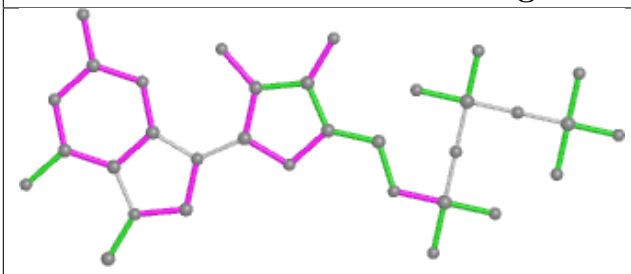


Torsions

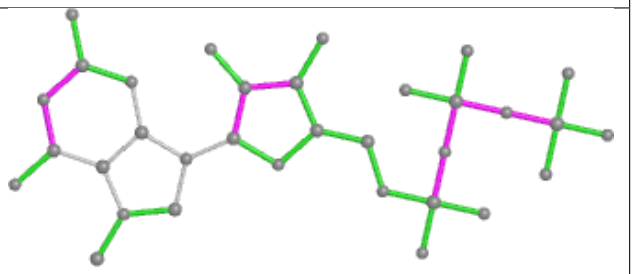


Rings

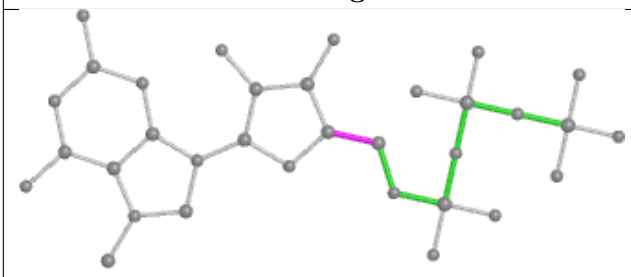
Ligand MGP O 604



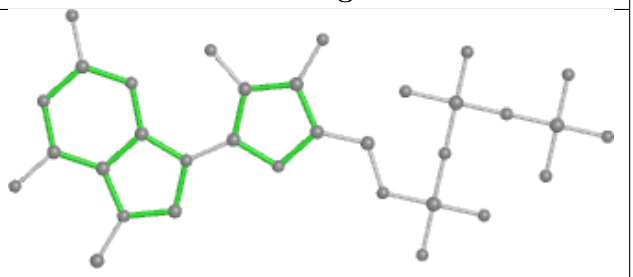
Bond lengths



Bond angles

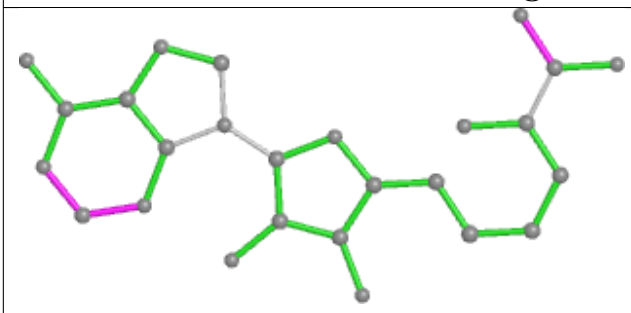


Torsions

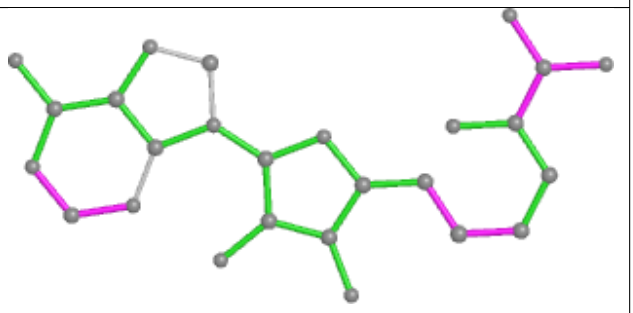


Rings

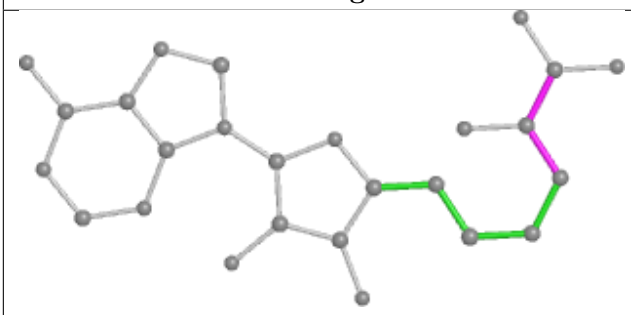
Ligand SAH V 603



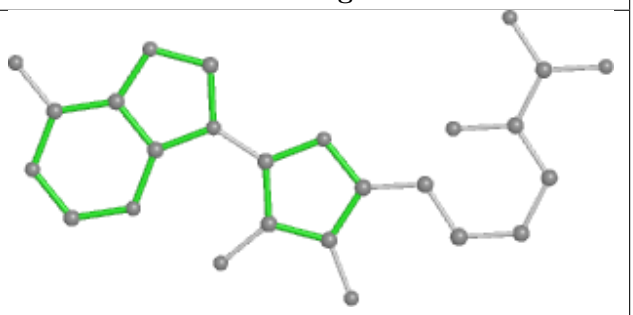
Bond lengths



Bond angles

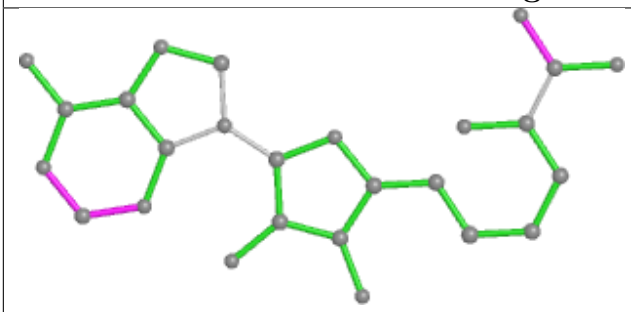


Torsions

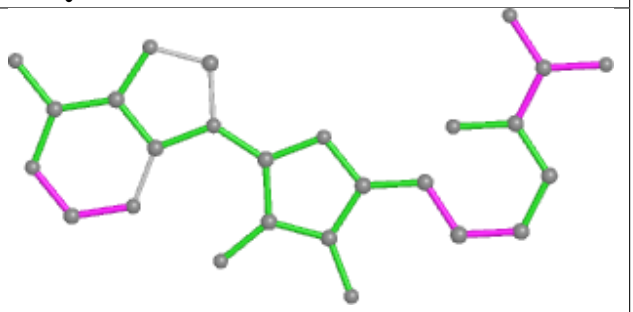


Rings

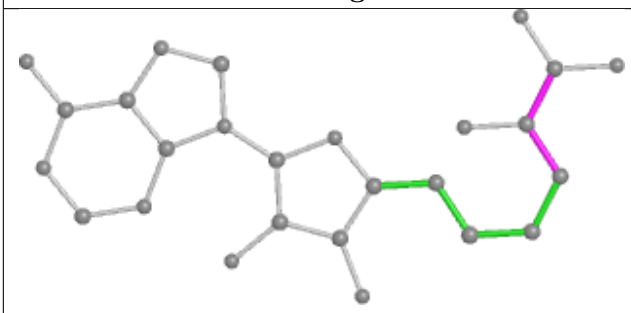
Ligand SAH Q 603



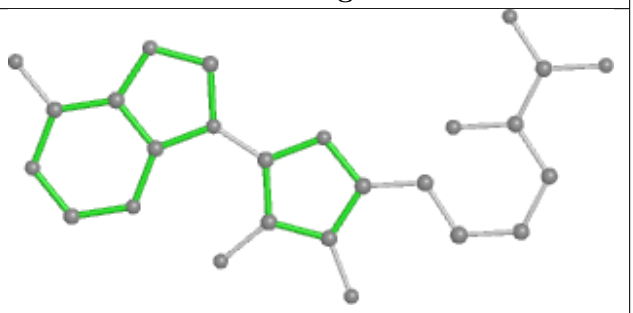
Bond lengths



Bond angles

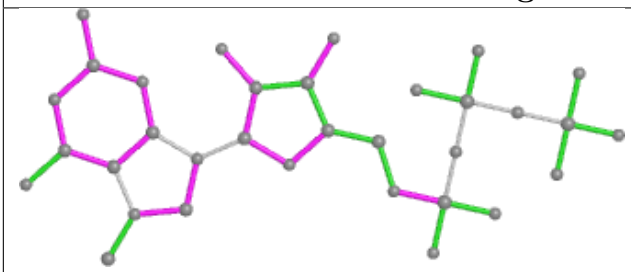


Torsions

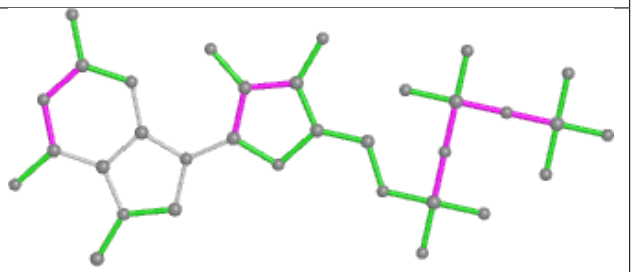


Rings

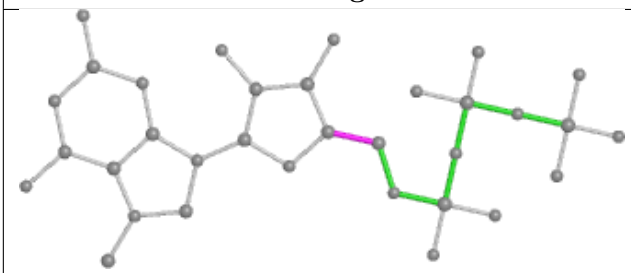
Ligand MGP K 604



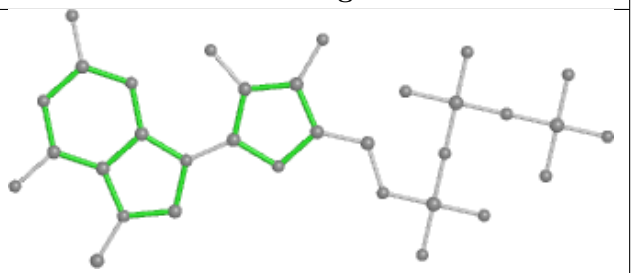
Bond lengths



Bond angles

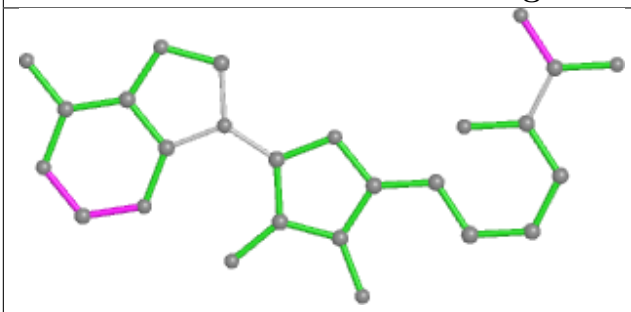


Torsions

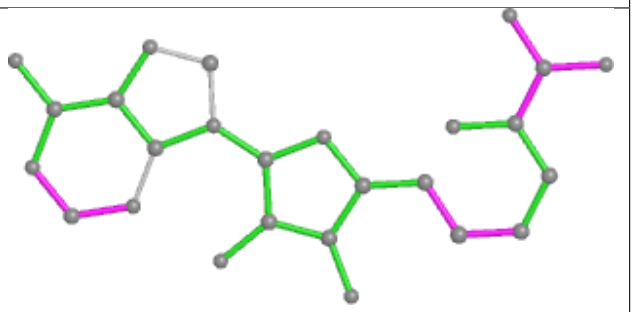


Rings

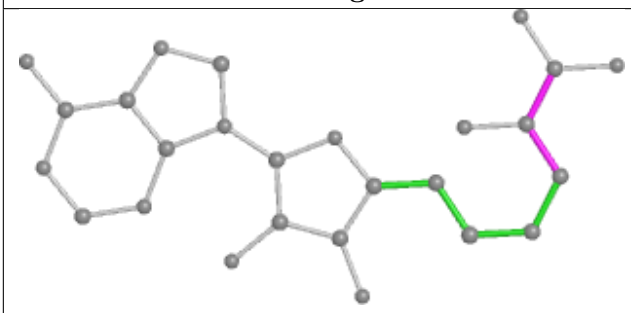
Ligand SAH G 603



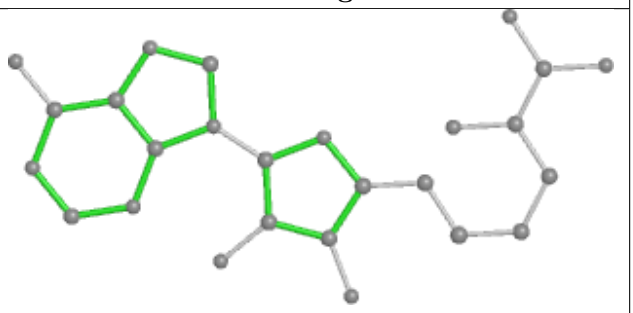
Bond lengths



Bond angles



Torsions



Rings

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.

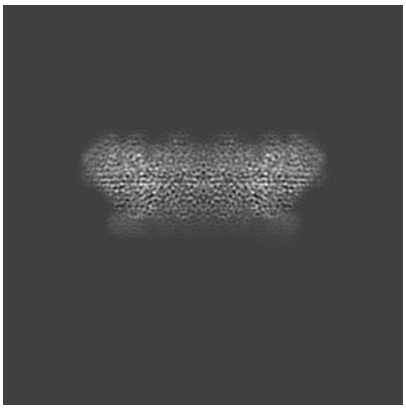
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15554. These allow visual inspection of the internal detail of the map and identification of artifacts.

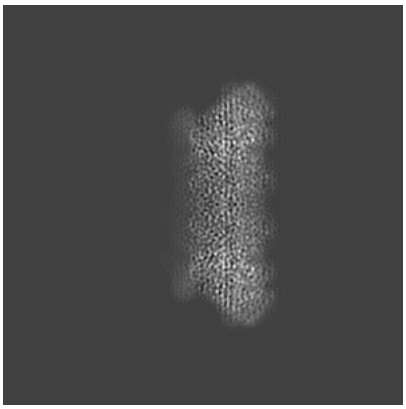
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

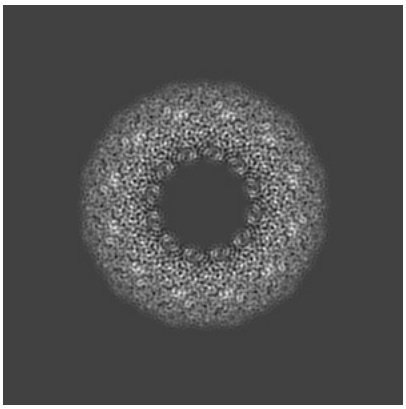
6.1.1 Primary map



X

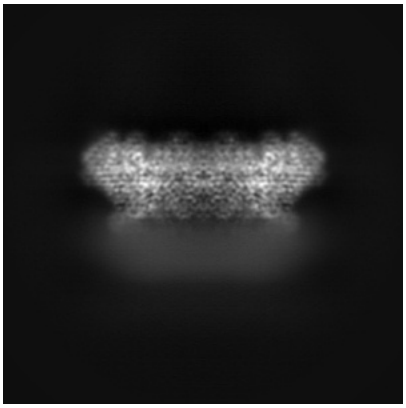


Y

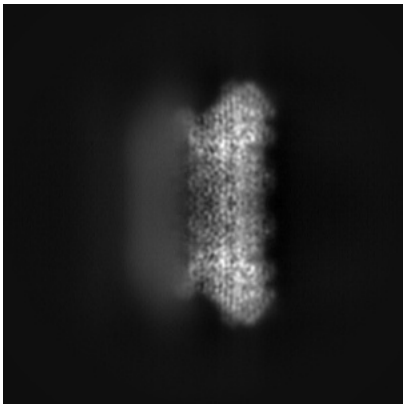


Z

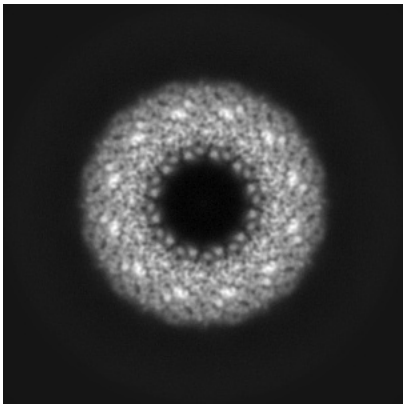
6.1.2 Raw map



X



Y

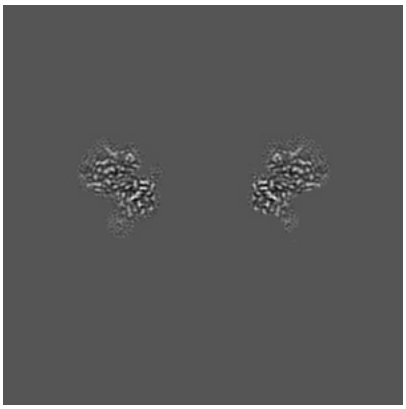


Z

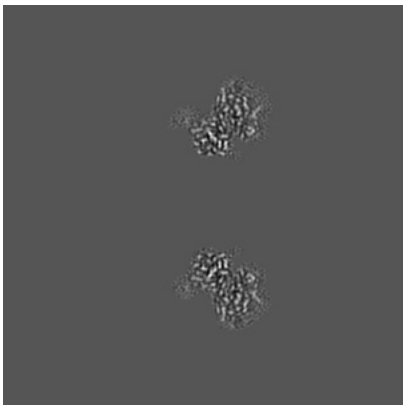
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

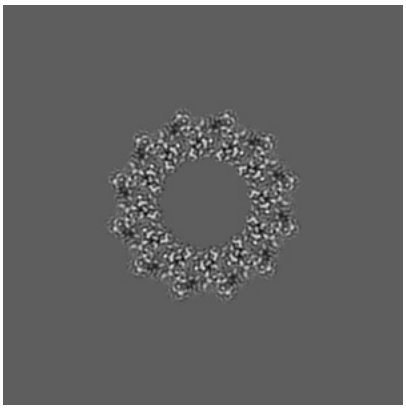
6.2.1 Primary map



X Index: 180

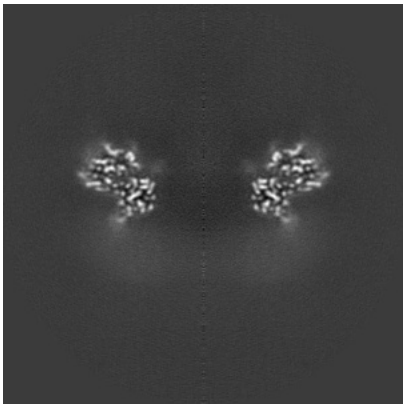


Y Index: 180

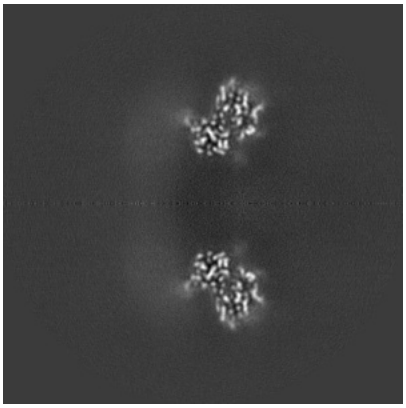


Z Index: 180

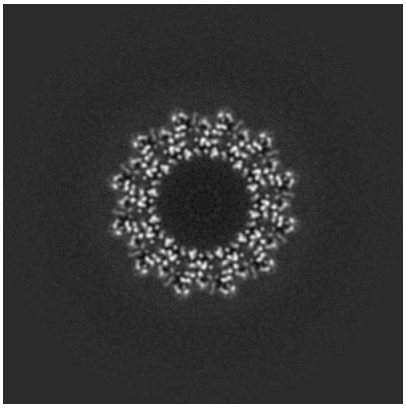
6.2.2 Raw map



X Index: 180



Y Index: 180

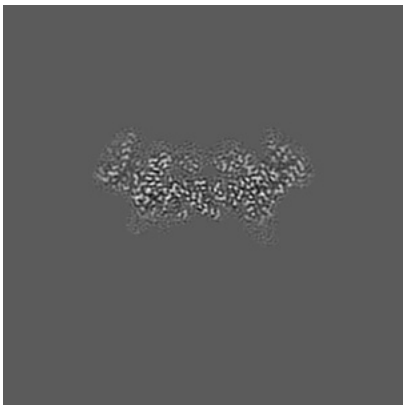


Z Index: 180

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

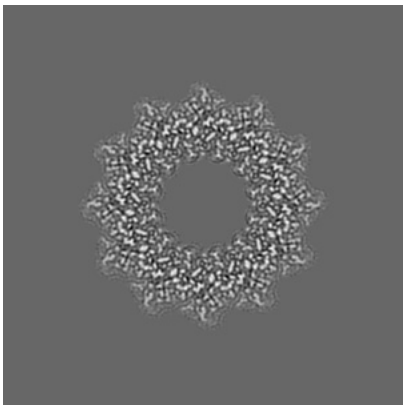
6.3 Largest variance slices (i)

6.3.1 Primary map



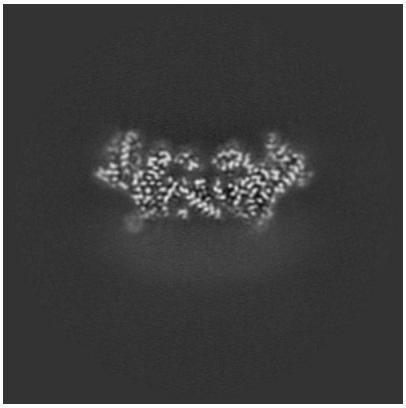
X Index: 125

Y Index: 125

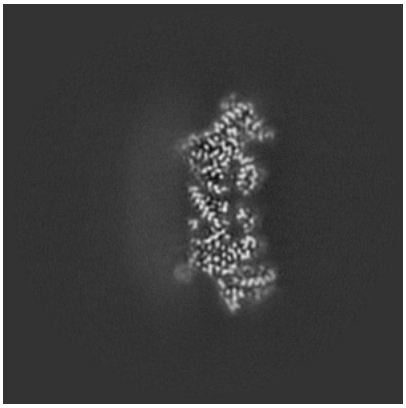


Z Index: 198

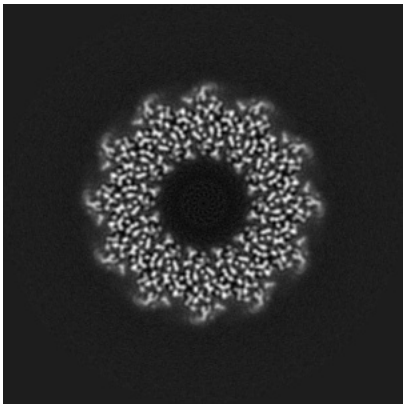
6.3.2 Raw map



X Index: 236



Y Index: 124

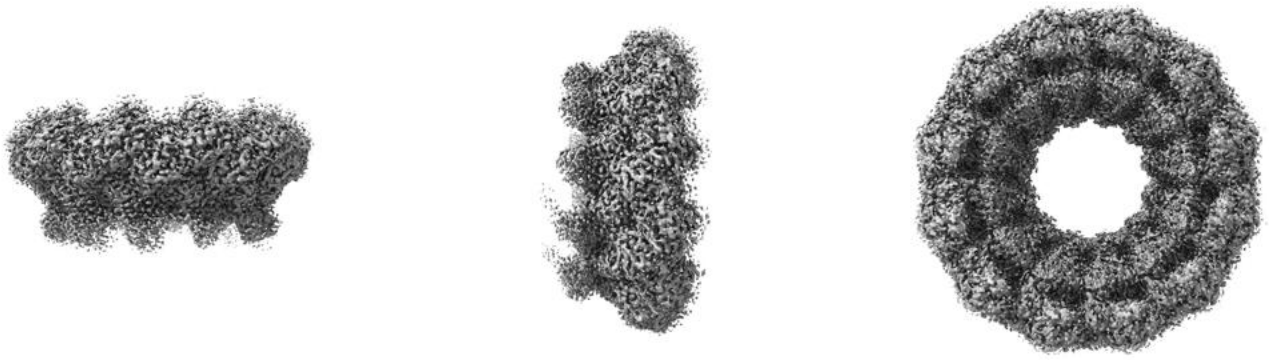


Z Index: 198

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

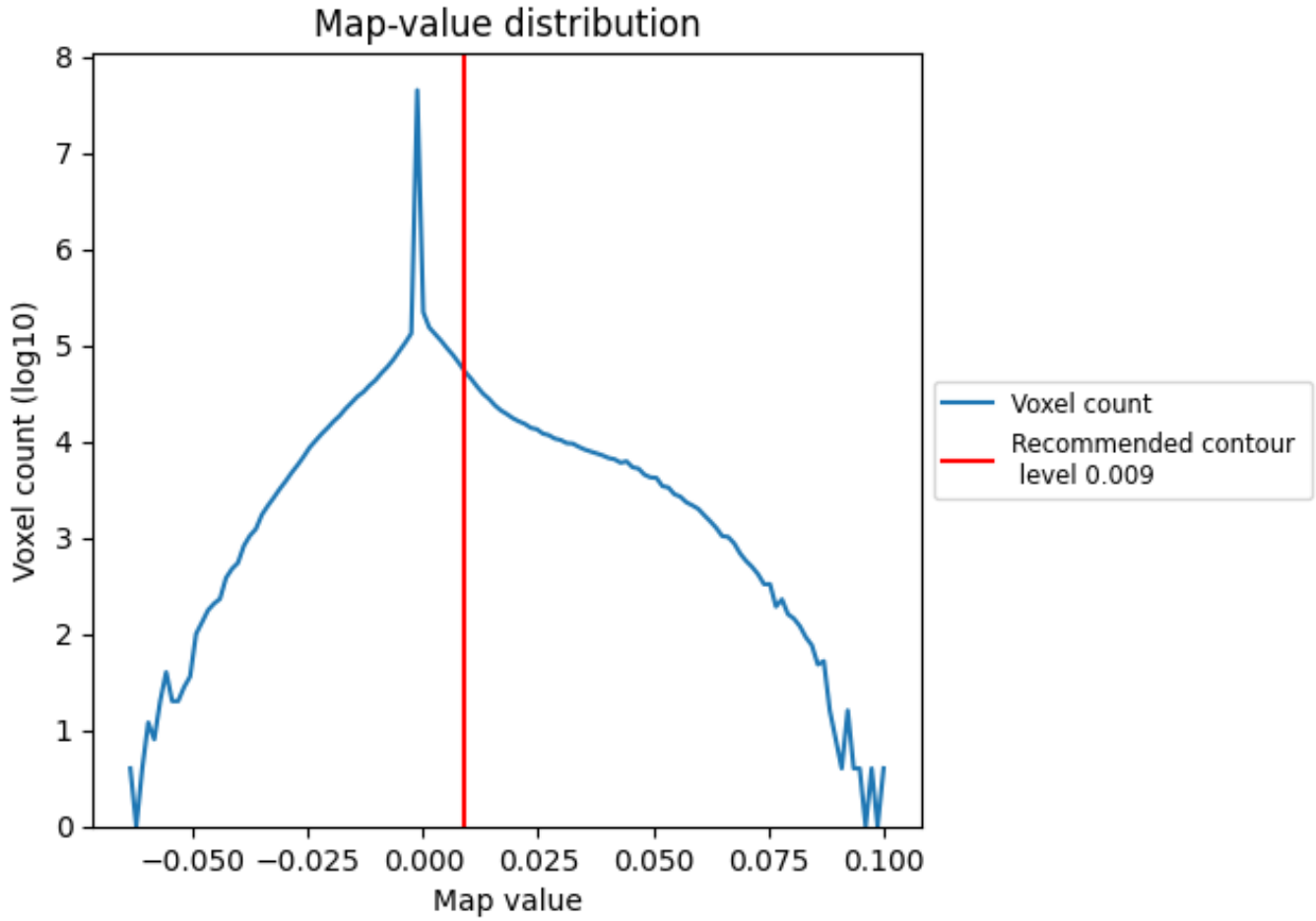
6.5 Mask visualisation (i)

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

7 Map analysis

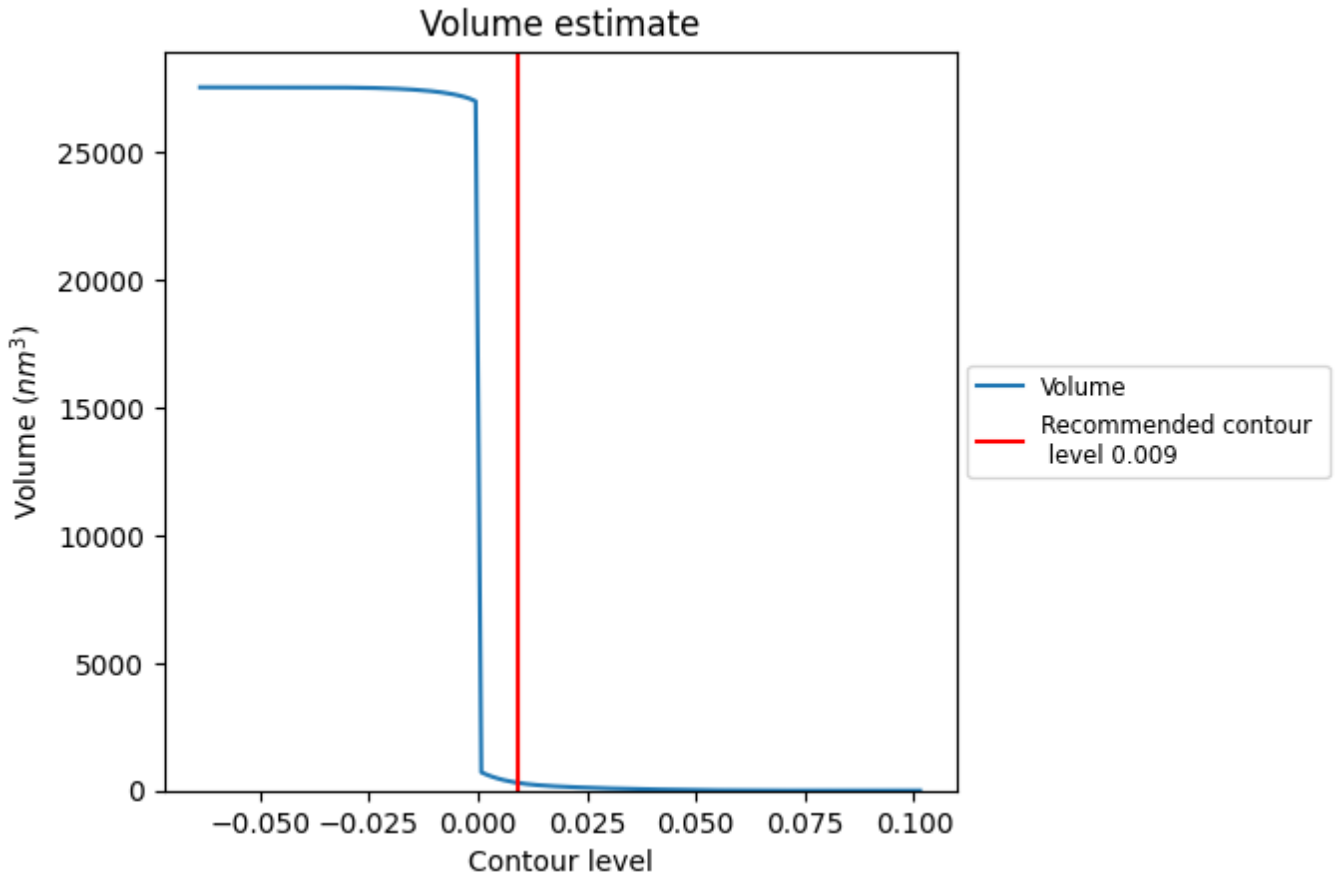
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

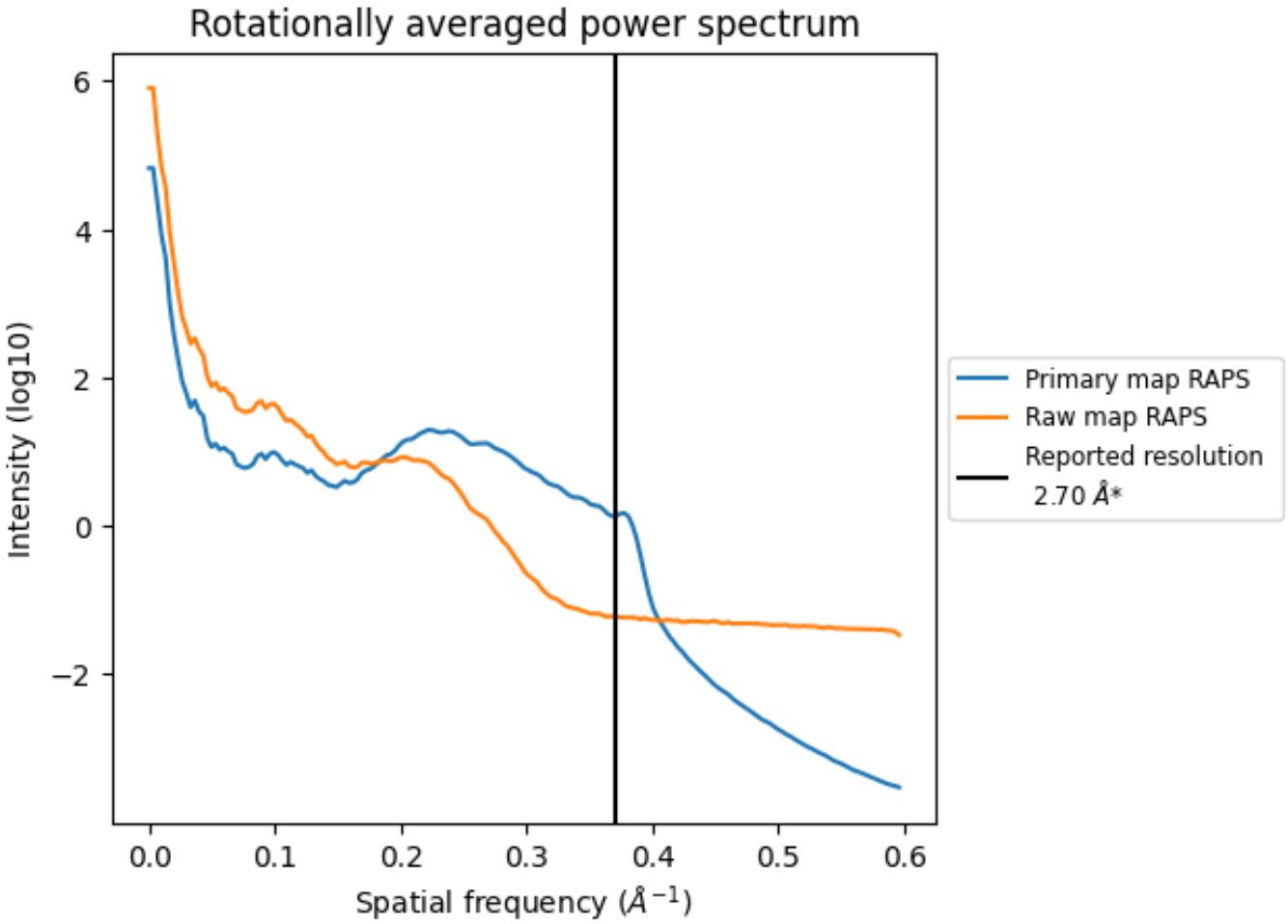
7.2 Volume estimate



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 279 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)

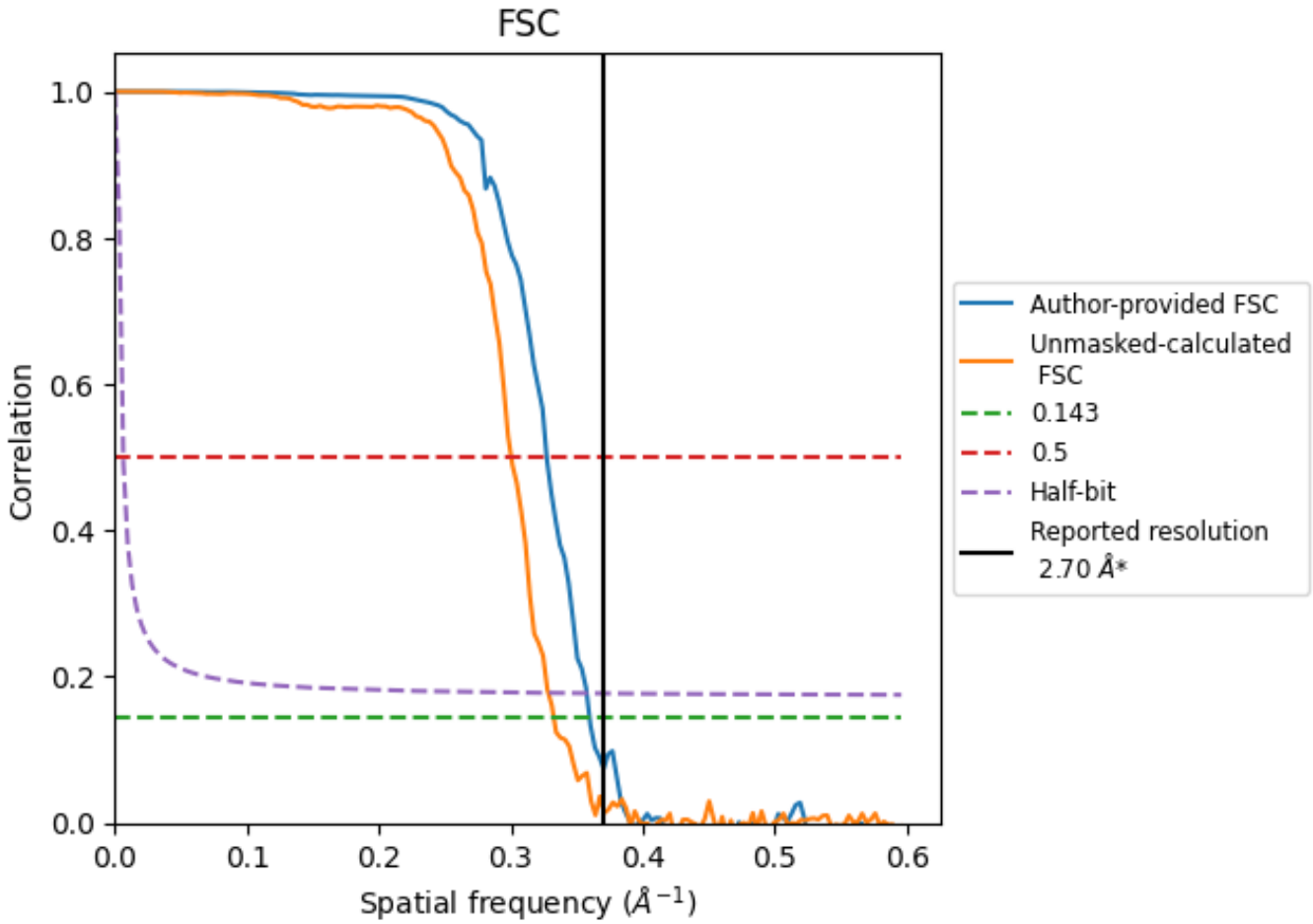


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

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)

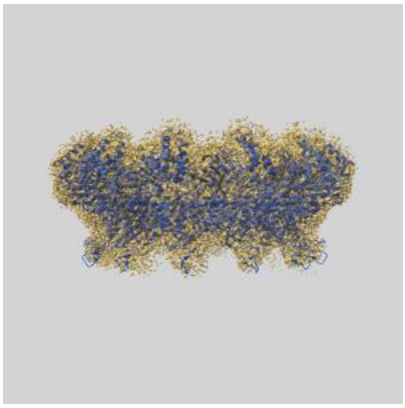
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.78	3.06	2.80
Unmasked-calculated*	3.01	3.33	3.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.01 differs from the reported value 2.7 by more than 10 %

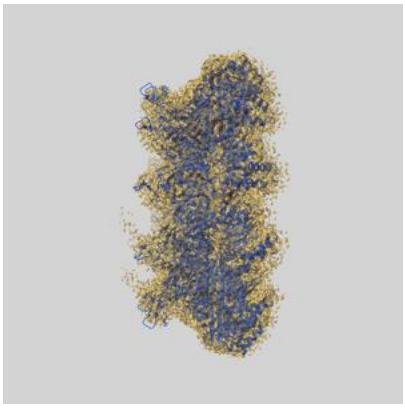
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15554 and PDB model 8AOW. Per-residue inclusion information can be found in section 3 on page 12.

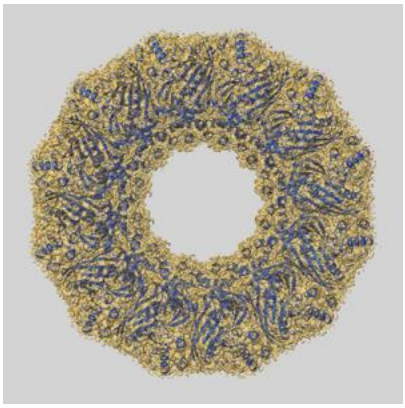
9.1 Map-model overlay



X



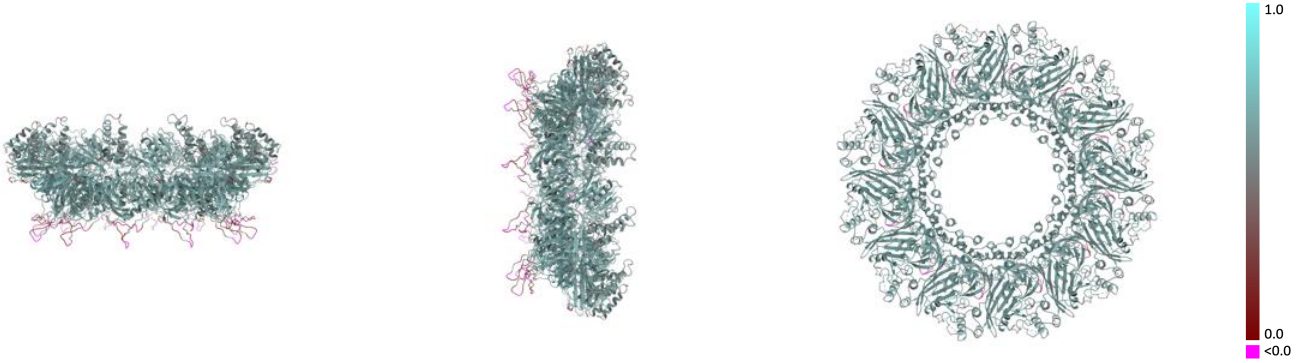
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

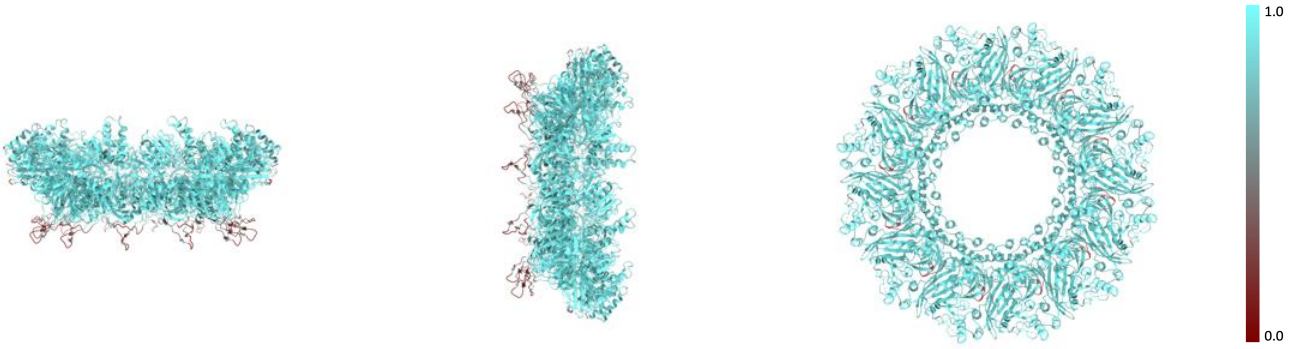
9.2 Q-score mapped to coordinate model (i)



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.

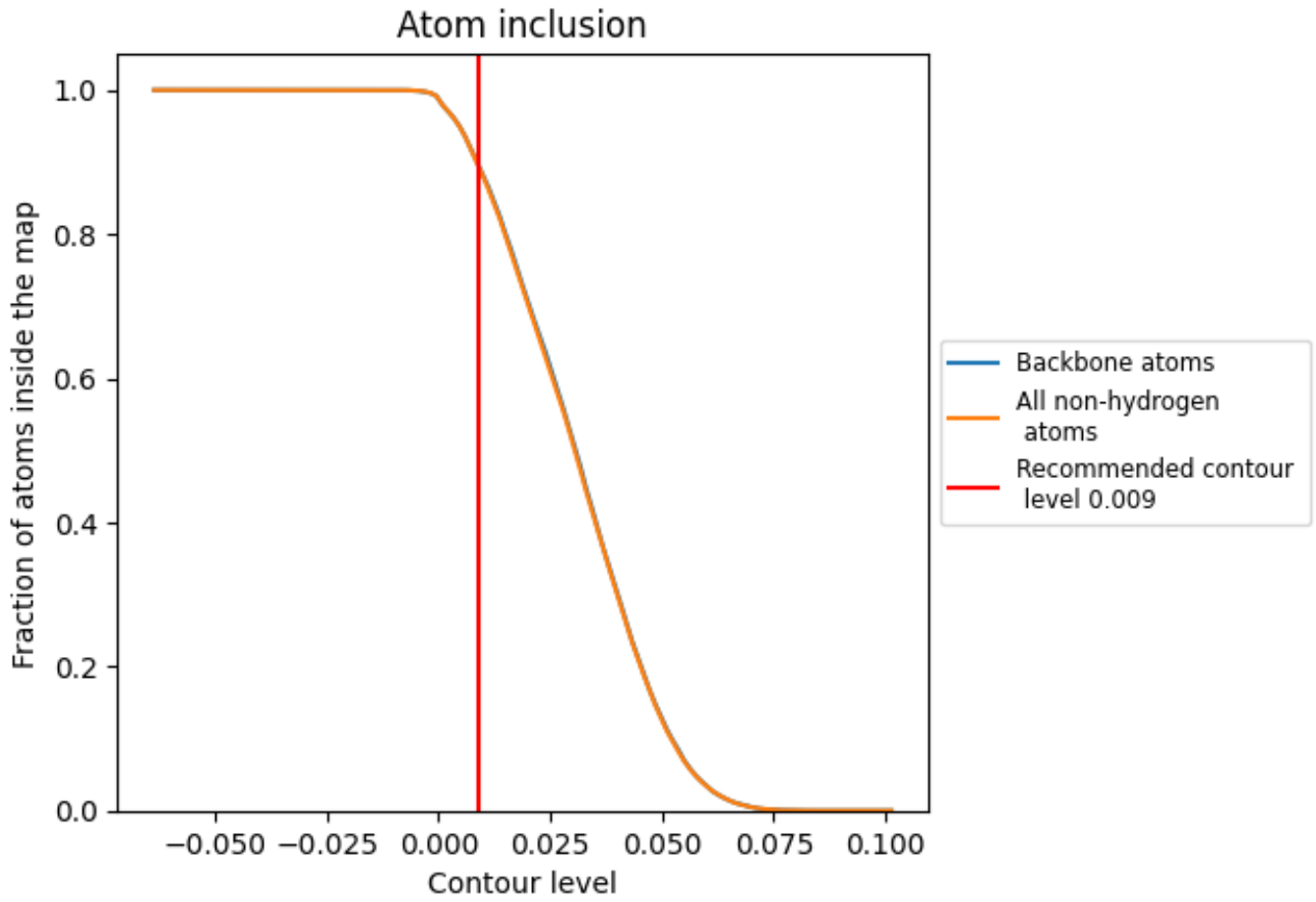
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.5840
A	0.8841	0.5740
C	0.8892	0.5760
E	0.8946	0.5810
G	0.9023	0.5880
I	0.9003	0.5940
K	0.9049	0.5960
M	0.9046	0.5940
O	0.9029	0.5890
Q	0.8992	0.5840
S	0.8949	0.5800
V	0.8864	0.5760
X	0.8838	0.5750