



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:43 PM BST

PDB ID : 4O1P  
Title : Crystal Structure of RNase L in complex with 2-5A and AMP-PNP  
Authors : Huang, H.; Zeqiraj, E.; Ceccarelli, D.F.; Sicheri, F.  
Deposited on : 2013-12-16  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

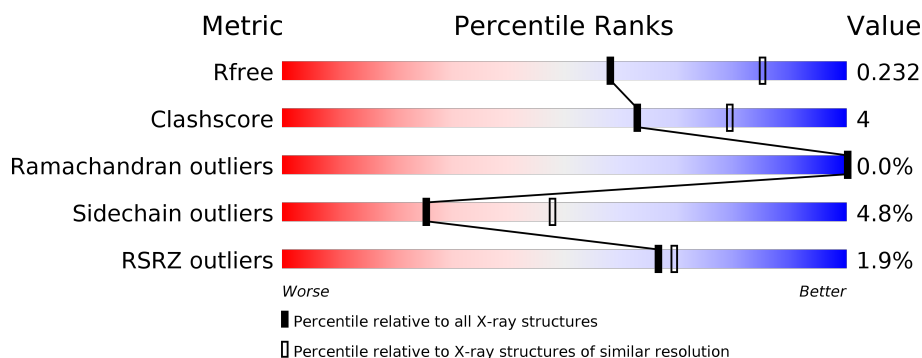
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>8%</span> <span>• 6%</span> </div> </div>
1	B	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>82%</span> <span>10%</span> <span>• 6%</span> </div> </div>
1	C	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>8%</span> <span>• 6%</span> </div> </div>
1	D	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>83%</span> <span>9%</span> <span>•• 7%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22829 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Ribonuclease L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5352	3358	945	1027	22			
1	B	671	Total	C	N	O	S	0	0	0
			5342	3351	944	1025	22			
1	C	673	Total	C	N	O	S	0	0	0
			5357	3361	946	1028	22			
1	D	668	Total	C	N	O	S	0	0	0
			5316	3337	940	1017	22			

There are 20 discrepancies between the modelled and reference sequences:

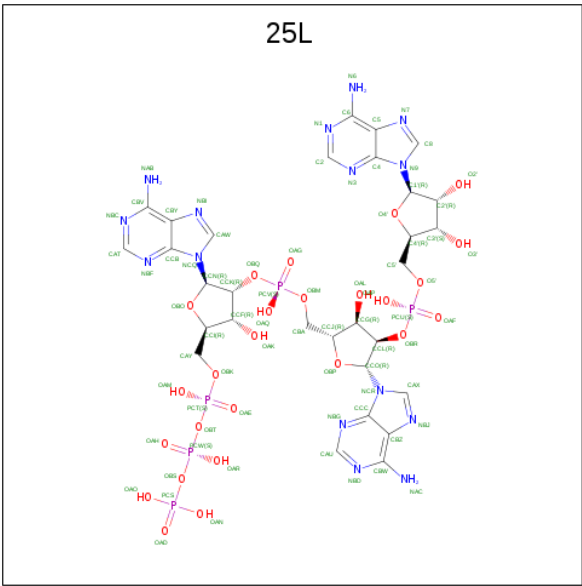
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	EXPRESSION TAG	UNP A5H025
A	17	ALA	-	EXPRESSION TAG	UNP A5H025
A	18	MET	-	EXPRESSION TAG	UNP A5H025
A	19	ASP	-	EXPRESSION TAG	UNP A5H025
A	20	PRO	-	EXPRESSION TAG	UNP A5H025
B	16	GLY	-	EXPRESSION TAG	UNP A5H025
B	17	ALA	-	EXPRESSION TAG	UNP A5H025
B	18	MET	-	EXPRESSION TAG	UNP A5H025
B	19	ASP	-	EXPRESSION TAG	UNP A5H025
B	20	PRO	-	EXPRESSION TAG	UNP A5H025
C	16	GLY	-	EXPRESSION TAG	UNP A5H025
C	17	ALA	-	EXPRESSION TAG	UNP A5H025
C	18	MET	-	EXPRESSION TAG	UNP A5H025
C	19	ASP	-	EXPRESSION TAG	UNP A5H025
C	20	PRO	-	EXPRESSION TAG	UNP A5H025
D	16	GLY	-	EXPRESSION TAG	UNP A5H025
D	17	ALA	-	EXPRESSION TAG	UNP A5H025
D	18	MET	-	EXPRESSION TAG	UNP A5H025
D	19	ASP	-	EXPRESSION TAG	UNP A5H025
D	20	PRO	-	EXPRESSION TAG	UNP A5H025

- # ANP

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

- Molecule 4 is [[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-4-[(2R,3R,4R,5R)-5-(6-aminopurin-9-yl)-4-[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-3-hydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-3-hydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl] phosphono hydrogen phosphate (three-letter code: 25L)

(formula: C<sub>30</sub>H<sub>40</sub>N<sub>15</sub>O<sub>25</sub>P<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
4	B	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
4	C	1	Total	C	N	O	P	0	0
			75	30	15	25	5		
4	D	1	Total	C	N	O	P	0	0
			75	30	15	25	5		

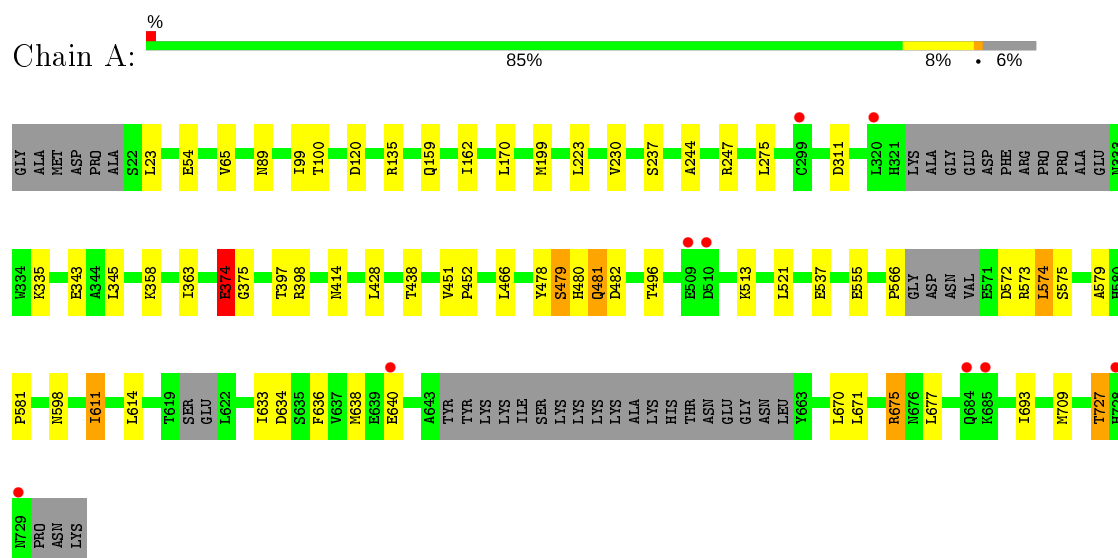
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	283	Total	O	0	0
			283	283		
5	C	255	Total	O	0	0
			255	255		
5	D	248	Total	O	0	0
			248	248		

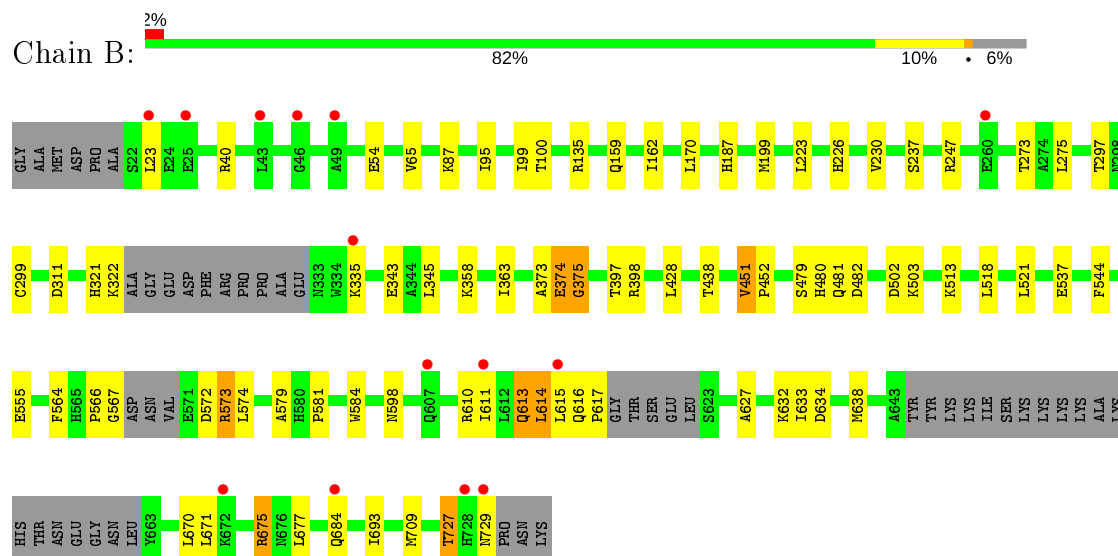
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

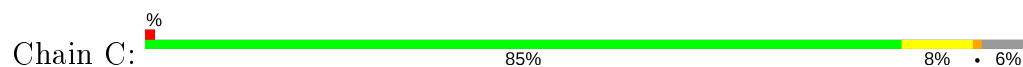
#### • Molecule 1: Ribonuclease L

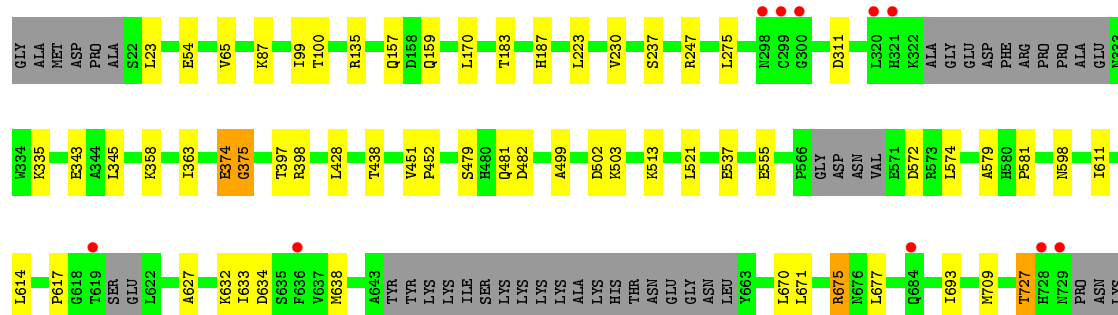


#### • Molecule 1: Ribonuclease L

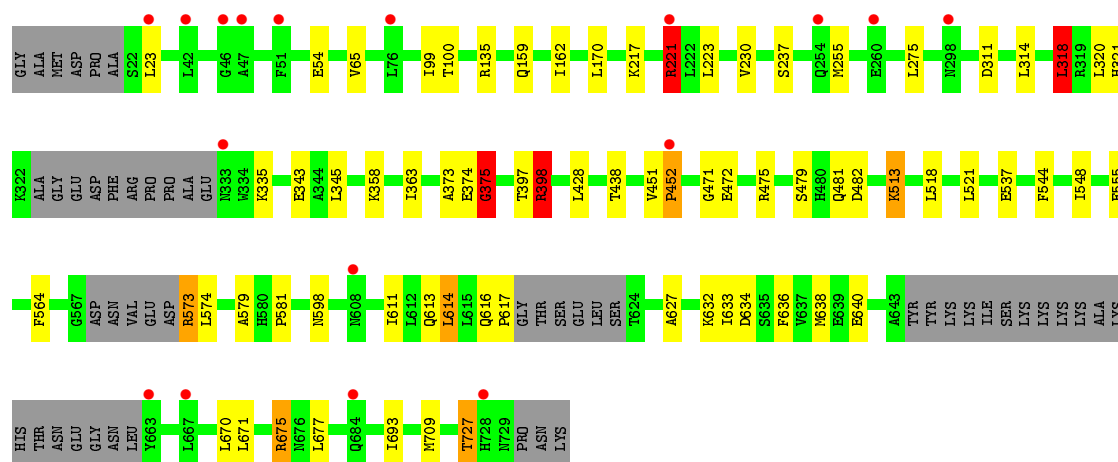
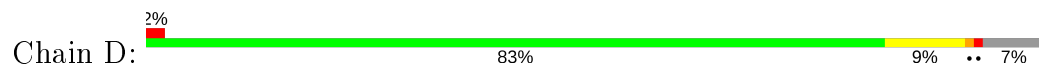


#### • Molecule 1: Ribonuclease L





### • Molecule 1: Ribonuclease L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.20 Å 267.39 Å 110.21 Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	59.20 – 2.50 59.20 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (59.20-2.50) 95.7 (59.20-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.196 , 0.231 0.198 , 0.232	Depositor DCC
$R_{free}$ test set	5618 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.256 for h,-k,-l	Xtriage
Reported twinning fraction	0.773 for H, K, L 0.227 for h,-k,-l	Depositor
Outliers	0 of 112073 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, 25L

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	0.60	14/5445 (0.3%)	0.62	5/7349 (0.1%)
1	B	0.57	10/5435 (0.2%)	0.64	4/7335 (0.1%)
1	C	0.53	9/5450 (0.2%)	0.62	4/7356 (0.1%)
1	D	0.56	7/5409 (0.1%)	0.64	6/7301 (0.1%)
All	All	0.57	40/21739 (0.2%)	0.63	19/29341 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	GLU	CD-OE2	-11.85	1.12	1.25
1	D	479	SER	CB-OG	-11.66	1.27	1.42
1	B	481	GLN	C-O	-11.54	1.01	1.23
1	A	479	SER	C-O	-11.13	1.02	1.23
1	C	481	GLN	C-O	-10.96	1.02	1.23
1	A	478	TYR	CE1-CZ	-10.49	1.25	1.38
1	B	479	SER	CB-OG	-10.46	1.28	1.42
1	B	374	GLU	CD-OE1	-10.32	1.14	1.25
1	D	481	GLN	C-O	-9.89	1.04	1.23
1	D	482	ASP	C-O	-9.65	1.05	1.23
1	A	374	GLU	CD-OE2	-9.48	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	375	GLY	C-O	-8.85	1.09	1.23
1	A	478	TYR	CZ-OH	-8.81	1.22	1.37
1	C	375	GLY	C-O	-8.74	1.09	1.23
1	A	481	GLN	C-O	-8.00	1.08	1.23
1	A	478	TYR	C-O	-7.78	1.08	1.23
1	A	480	HIS	C-O	-7.64	1.08	1.23
1	B	482	ASP	C-O	-7.51	1.09	1.23
1	B	479	SER	C-O	-7.32	1.09	1.23
1	A	478	TYR	CE2-CZ	-7.01	1.29	1.38
1	B	482	ASP	CG-OD1	-6.86	1.09	1.25
1	C	479	SER	C-O	-6.80	1.10	1.23
1	C	374	GLU	CD-OE2	-6.50	1.18	1.25
1	A	479	SER	CB-OG	-6.48	1.33	1.42
1	A	374	GLU	CD-OE1	-6.41	1.18	1.25
1	D	479	SER	C-O	-6.32	1.11	1.23
1	C	482	ASP	C-O	-6.23	1.11	1.23
1	C	374	GLU	C-O	-6.18	1.11	1.23
1	D	374	GLU	CD-OE1	-6.16	1.18	1.25
1	A	374	GLU	CB-CG	-6.00	1.40	1.52
1	B	375	GLY	C-O	-5.90	1.14	1.23
1	D	482	ASP	CG-OD1	-5.83	1.11	1.25
1	C	482	ASP	CG-OD1	-5.54	1.12	1.25
1	C	374	GLU	CD-OE1	-5.40	1.19	1.25
1	A	375	GLY	C-O	-5.39	1.15	1.23
1	B	373	ALA	C-O	-5.33	1.13	1.23
1	C	481	GLN	CD-NE2	-5.26	1.19	1.32
1	A	482	ASP	C-O	-5.25	1.13	1.23
1	B	374	GLU	CG-CD	-5.18	1.44	1.51
1	A	478	TYR	CD1-CE1	-5.15	1.31	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	482	ASP	CB-CG-OD1	10.03	127.33	118.30
1	B	482	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	375	GLY	N-CA-C	6.88	130.29	113.10
1	D	482	ASP	OD1-CG-OD2	-6.83	110.31	123.30
1	C	482	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	375	GLY	N-CA-C	6.43	129.17	113.10
1	D	221	ARG	C-N-CA	6.36	137.61	121.70
1	A	374	GLU	N-CA-C	6.34	128.13	111.00
1	D	318	LEU	CA-CB-CG	5.94	128.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	ASP	OD1-CG-OD2	-5.82	112.24	123.30
1	A	375	GLY	N-CA-C	5.78	127.55	113.10
1	C	157	GLN	CB-CA-C	5.73	121.86	110.40
1	B	480	HIS	N-CA-C	5.71	126.42	111.00
1	C	157	GLN	CA-CB-CG	5.37	125.20	113.40
1	D	375	GLY	N-CA-C	5.34	126.45	113.10
1	A	374	GLU	CA-C-N	5.28	126.76	116.20
1	A	479	SER	CB-CA-C	5.11	119.80	110.10
1	D	398	ARG	CB-CA-C	5.04	120.47	110.40
1	A	480	HIS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	375	GLY	Peptide
1	B	451	VAL	Mainchain
1	C	375	GLY	Peptide
1	D	375	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5352	0	5268	47	0
1	B	5342	0	5252	70	0
1	C	5357	0	5270	36	0
1	D	5316	0	5228	47	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	1	0
2	D	31	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	75	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	75	0	34	1	0
4	C	75	0	34	1	0
4	D	75	0	34	0	0
5	A	244	0	0	10	0
5	B	283	0	0	15	0
5	C	255	0	0	8	0
5	D	248	0	0	5	0
All	All	22829	0	21206	186	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 4.

All (186) 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:B:398:ARG:NH2	1:B:503:LYS:HE3	1.54	1.19
1:B:613:GLN:HG3	1:B:614:LEU:N	1.64	1.11
1:B:613:GLN:HG3	1:B:614:LEU:H	1.18	1.06
1:D:375:GLY:HA2	5:D:1006:HOH:O	1.59	1.02
1:B:452:PRO:HB3	5:B:1008:HOH:O	1.69	0.93
1:C:503:LYS:CG	5:C:1071:HOH:O	2.14	0.92
1:B:398:ARG:HH22	1:B:503:LYS:HE3	1.33	0.91
1:A:611:ILE:HG22	5:A:1075:HOH:O	1.72	0.90
1:C:503:LYS:HG2	5:C:1071:HOH:O	1.70	0.89
1:D:471:GLY:O	1:D:475:ARG:HG2	1.77	0.84
1:A:572:ASP:HB3	1:A:575:SER:OG	1.77	0.84
1:D:581:PRO:HB2	1:D:709:MET:HE3	1.63	0.80
1:D:613:GLN:O	1:D:616:GLN:HB2	1.80	0.80
1:A:374:GLU:O	1:B:162:ILE:HG23	1.82	0.79
1:B:581:PRO:HB2	1:B:709:MET:HE3	1.64	0.79
1:B:610:ARG:O	1:B:613:GLN:HG2	1.83	0.79
1:B:610:ARG:O	1:B:613:GLN:CG	2.30	0.79
1:D:544:PHE:HD1	1:D:564:PHE:CD2	2.02	0.78
1:B:95:ILE:HG13	5:B:1269:HOH:O	1.81	0.78
1:B:615:LEU:C	1:B:617:PRO:HD3	2.05	0.77
1:D:544:PHE:CD1	1:D:564:PHE:CD2	2.73	0.77
1:A:566:PRO:HA	1:A:573:ARG:NH2	1.99	0.77
1:A:374:GLU:O	1:B:162:ILE:CG2	2.32	0.77
1:B:613:GLN:CG	1:B:614:LEU:N	2.46	0.76
1:A:581:PRO:HB2	1:A:709:MET:HE3	1.65	0.76
1:B:398:ARG:CZ	1:B:503:LYS:HE3	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:PRO:HB2	1:C:709:MET:HE3	1.66	0.75
1:A:247:ARG:HD2	5:A:1202:HOH:O	1.89	0.72
1:B:226:HIS:CE1	1:C:183:THR:HG21	2.25	0.72
1:D:221:ARG:CG	1:D:255:MET:SD	2.79	0.71
1:B:544:PHE:CD2	1:B:564:PHE:CD2	2.79	0.70
1:C:499:ALA:O	5:C:1049:HOH:O	2.10	0.70
1:A:598:ASN:OD1	1:A:675:ARG:NH1	2.25	0.69
1:B:598:ASN:OD1	1:B:675:ARG:NH1	2.25	0.69
1:C:598:ASN:OD1	1:C:675:ARG:NH1	2.25	0.69
1:D:598:ASN:OD1	1:D:675:ARG:NH1	2.25	0.69
1:D:221:ARG:HG2	1:D:255:MET:SD	2.33	0.68
1:B:729:ASN:HA	5:B:1229:HOH:O	1.92	0.68
1:B:544:PHE:HD2	1:B:564:PHE:CD2	2.11	0.68
1:C:503:LYS:CE	5:C:1071:HOH:O	2.42	0.66
1:B:613:GLN:CD	1:B:614:LEU:HD13	2.15	0.66
1:C:374:GLU:O	1:D:162:ILE:HG23	1.95	0.66
1:D:513:LYS:HE2	5:D:1178:HOH:O	1.96	0.66
1:A:398:ARG:NH1	5:A:1130:HOH:O	2.29	0.66
1:D:544:PHE:CE1	1:D:564:PHE:HD2	2.12	0.65
1:C:398:ARG:HB3	1:C:502:ASP:HB2	1.77	0.65
1:D:398:ARG:NH2	5:D:1051:HOH:O	2.28	0.65
1:A:199:MET:HE2	5:A:1165:HOH:O	1.97	0.64
1:B:199:MET:CE	5:B:1042:HOH:O	2.46	0.64
1:D:375:GLY:CA	5:D:1006:HOH:O	2.28	0.64
1:D:472:GLU:HA	1:D:475:ARG:HG3	1.79	0.63
1:A:247:ARG:HB3	5:A:1202:HOH:O	1.98	0.63
1:C:503:LYS:HG2	1:C:503:LYS:O	1.98	0.63
1:A:452:PRO:HA	5:A:1015:HOH:O	1.99	0.62
1:A:374:GLU:O	1:A:374:GLU:HG3	1.99	0.62
1:B:544:PHE:CE2	1:B:564:PHE:HD2	2.17	0.62
1:A:479:SER:OG	1:A:481:GLN:NE2	2.32	0.61
1:B:297:THR:OG1	5:B:1139:HOH:O	2.16	0.61
1:B:633:ILE:HG21	1:B:638:MET:SD	2.41	0.61
1:D:452:PRO:HA	5:D:1192:HOH:O	2.00	0.61
1:D:633:ILE:HG21	1:D:638:MET:SD	2.41	0.61
1:A:566:PRO:HA	1:A:573:ARG:CZ	2.32	0.60
1:D:221:ARG:HG3	1:D:255:MET:SD	2.42	0.60
1:B:199:MET:HE2	5:B:1042:HOH:O	2.02	0.60
1:A:451:VAL:HB	1:A:452:PRO:HD2	1.84	0.59
1:A:633:ILE:HG21	1:A:638:MET:SD	2.42	0.59
1:D:451:VAL:HB	1:D:452:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:PHE:CZ	1:A:640:GLU:OE2	2.55	0.59
1:C:633:ILE:HG21	1:C:638:MET:SD	2.42	0.59
1:C:581:PRO:HB2	1:C:709:MET:CE	2.33	0.59
1:A:581:PRO:HB2	1:A:709:MET:CE	2.33	0.59
1:C:451:VAL:HB	1:C:452:PRO:HD2	1.84	0.59
1:C:581:PRO:HG2	1:C:709:MET:HE1	1.84	0.59
1:D:581:PRO:HB2	1:D:709:MET:CE	2.32	0.58
1:A:566:PRO:HB3	1:A:573:ARG:NE	2.19	0.58
1:B:398:ARG:NH2	1:B:503:LYS:HG3	2.19	0.58
1:A:574:LEU:H	1:A:574:LEU:CD2	2.16	0.58
1:B:581:PRO:HB2	1:B:709:MET:CE	2.33	0.57
1:B:684:GLN:HB2	5:B:1223:HOH:O	2.03	0.57
1:D:581:PRO:HG2	1:D:709:MET:HE1	1.86	0.57
1:D:471:GLY:O	1:D:475:ARG:CG	2.51	0.57
1:B:610:ARG:O	1:B:613:GLN:HG3	2.02	0.56
2:C:901:ANP:H8	2:C:901:ANP:H5'1	1.87	0.56
1:A:581:PRO:HG2	1:A:709:MET:HE1	1.87	0.56
1:B:321:HIS:O	1:B:322:LYS:CB	2.55	0.55
1:B:581:PRO:HG2	1:B:709:MET:HE1	1.88	0.55
1:C:503:LYS:HG3	5:C:1071:HOH:O	1.96	0.55
1:A:566:PRO:HB3	1:A:573:ARG:CD	2.37	0.55
1:B:610:ARG:HH11	1:B:613:GLN:HE21	1.54	0.55
1:C:503:LYS:HE2	5:C:1071:HOH:O	2.05	0.54
1:A:566:PRO:CB	1:A:573:ARG:NE	2.70	0.54
1:D:636:PHE:CZ	1:D:640:GLU:OE2	2.60	0.54
1:B:615:LEU:O	1:B:617:PRO:HD3	2.07	0.53
1:C:247:ARG:HD3	5:C:1045:HOH:O	2.08	0.53
1:B:398:ARG:NH2	1:B:503:LYS:CE	2.48	0.53
1:A:244:ALA:HA	5:A:1202:HOH:O	2.08	0.52
1:C:572:ASP:HB3	5:C:1202:HOH:O	2.08	0.52
1:B:610:ARG:NH1	1:B:613:GLN:NE2	2.58	0.52
1:D:314:LEU:O	1:D:318:LEU:HD22	2.10	0.52
1:A:574:LEU:H	1:A:574:LEU:HD22	1.74	0.51
1:A:566:PRO:CA	1:A:573:ARG:CZ	2.89	0.50
1:B:40:ARG:HD2	5:B:1234:HOH:O	2.11	0.50
1:D:614:LEU:C	1:D:616:GLN:H	2.15	0.50
1:B:451:VAL:O	1:B:452:PRO:C	2.49	0.50
1:B:572:ASP:OD1	1:B:572:ASP:N	2.45	0.50
1:B:247:ARG:HD3	5:B:1031:HOH:O	2.10	0.49
1:D:616:GLN:HB3	1:D:617:PRO:HD3	1.94	0.49
1:C:677:LEU:HD11	1:C:693:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:ANP:H5'1	2:A:901:ANP:H8	1.95	0.48
1:A:374:GLU:OE2	1:A:398:ARG:NH2	2.47	0.48
1:A:159:GLN:HE21	1:B:363:ILE:HG21	1.78	0.48
1:D:221:ARG:HG2	1:D:255:MET:CG	2.42	0.48
1:D:65:VAL:O	1:D:100:THR:HG21	2.12	0.48
1:A:677:LEU:HD11	1:A:693:ILE:HD13	1.96	0.48
1:B:677:LEU:HD11	1:B:693:ILE:HD13	1.96	0.48
1:A:100:THR:HG22	5:B:1224:HOH:O	2.14	0.48
1:C:572:ASP:OD1	1:C:572:ASP:N	2.47	0.48
1:D:677:LEU:HD11	1:D:693:ILE:HD13	1.95	0.48
1:B:566:PRO:N	1:B:567:GLY:HA3	2.29	0.47
1:D:544:PHE:HE1	1:D:564:PHE:HD2	1.61	0.47
1:A:65:VAL:O	1:A:100:THR:HG21	2.14	0.47
1:C:65:VAL:O	1:C:100:THR:HG21	2.15	0.47
1:B:99:ILE:O	1:B:135:ARG:NH1	2.48	0.47
1:B:65:VAL:O	1:B:100:THR:HG21	2.14	0.47
1:A:162:ILE:HG23	1:B:374:GLU:O	2.14	0.47
1:C:87:LYS:HE2	4:C:904:25L:OAP	2.15	0.46
1:D:373:ALA:HB3	1:D:398:ARG:NH1	2.29	0.46
1:C:159:GLN:HE21	1:D:363:ILE:HG21	1.80	0.46
1:A:566:PRO:CB	1:A:573:ARG:CZ	2.93	0.46
1:B:555:GLU:HG3	1:B:709:MET:CE	2.46	0.46
1:A:555:GLU:HG3	1:A:709:MET:CE	2.46	0.46
1:A:374:GLU:O	1:B:162:ILE:HG22	2.14	0.46
1:D:555:GLU:HG3	1:D:709:MET:CE	2.46	0.46
1:A:579:ALA:HB2	1:A:727:THR:HG21	1.97	0.46
1:C:374:GLU:O	1:D:162:ILE:CG2	2.63	0.46
1:B:226:HIS:CE1	1:C:183:THR:CG2	2.97	0.45
1:B:555:GLU:HG3	1:B:709:MET:HE2	1.98	0.45
1:C:555:GLU:HG3	1:C:709:MET:CE	2.46	0.45
1:D:518:LEU:HD21	1:D:573:ARG:HE	1.80	0.45
1:A:99:ILE:O	1:A:135:ARG:NH1	2.49	0.45
1:B:518:LEU:HD21	1:B:573:ARG:HE	1.81	0.45
1:B:187:HIS:CD2	1:C:187:HIS:CB	2.99	0.45
1:D:555:GLU:HG3	1:D:709:MET:HE2	1.99	0.45
1:B:398:ARG:HH21	1:B:503:LYS:HG3	1.81	0.45
1:D:99:ILE:O	1:D:135:ARG:NH1	2.50	0.45
1:A:199:MET:CE	5:A:1165:HOH:O	2.60	0.45
1:C:99:ILE:O	1:C:135:ARG:NH1	2.49	0.45
1:B:634:ASP:HB2	5:B:1041:HOH:O	2.16	0.45
1:C:579:ALA:HB2	1:C:727:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASN:ND2	5:A:1019:HOH:O	2.50	0.45
1:B:579:ALA:HB2	1:B:727:THR:HG21	1.98	0.44
1:B:566:PRO:N	1:B:567:GLY:CA	2.80	0.44
1:B:187:HIS:CD2	1:C:187:HIS:HB2	2.53	0.43
1:D:217:LYS:O	1:D:221:ARG:HB2	2.17	0.43
1:D:579:ALA:HB2	1:D:727:THR:HG21	1.99	0.43
1:A:159:GLN:NE2	1:B:363:ILE:HG21	2.34	0.43
1:A:555:GLU:HG3	1:A:709:MET:HE2	2.00	0.43
1:B:616:GLN:N	1:B:617:PRO:HD3	2.31	0.43
1:B:87:LYS:HE2	4:B:904:25L:OAP	2.18	0.43
1:B:398:ARG:HG2	1:B:502:ASP:O	2.19	0.43
1:B:729:ASN:C	5:B:1229:HOH:O	2.56	0.42
1:C:503:LYS:O	1:C:503:LYS:CG	2.66	0.42
1:C:363:ILE:HG21	1:D:159:GLN:HE21	1.84	0.42
1:D:373:ALA:HB3	1:D:398:ARG:CZ	2.49	0.42
1:A:374:GLU:HB3	1:A:398:ARG:HH21	1.85	0.42
1:A:466:LEU:HD23	5:A:1054:HOH:O	2.19	0.41
1:C:633:ILE:HG12	1:C:634:ASP:N	2.35	0.41
1:D:544:PHE:CZ	1:D:548:ILE:HG13	2.55	0.41
1:A:363:ILE:HG21	1:B:159:GLN:HE21	1.85	0.41
1:B:610:ARG:HH11	1:B:613:GLN:NE2	2.13	0.41
1:B:581:PRO:HA	1:B:584:TRP:CG	2.56	0.41
1:B:544:PHE:CE2	1:B:564:PHE:CD2	3.01	0.41
1:B:398:ARG:HB3	1:B:502:ASP:HB2	2.03	0.41
1:D:581:PRO:HG2	1:D:709:MET:CE	2.50	0.41
1:C:555:GLU:HG3	1:C:709:MET:HE2	2.02	0.41
1:B:299:CYS:HB2	5:B:1067:HOH:O	2.20	0.40
1:A:633:ILE:HG12	1:A:634:ASP:N	2.36	0.40
1:B:273:THR:HG21	5:B:1025:HOH:O	2.20	0.40
1:C:627:ALA:O	1:C:632:LYS:NZ	2.51	0.40
1:D:633:ILE:HG12	1:D:634:ASP:N	2.35	0.40
1:A:89:ASN:O	1:A:120:ASP:HB2	2.22	0.40
1:B:627:ALA:O	1:B:632:LYS:NZ	2.52	0.40
1:C:159:GLN:NE2	1:D:363:ILE:HG21	2.37	0.40
1:D:318:LEU:O	1:D:321:HIS:O	2.40	0.40
1:B:729:ASN:CA	5:B:1229:HOH:O	2.59	0.40
1:D:627:ALA:O	1:D:632:LYS:NZ	2.52	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	662/717 (92%)	651 (98%)	11 (2%)	0	100	100
1	B	661/717 (92%)	651 (98%)	10 (2%)	0	100	100
1	C	663/717 (92%)	651 (98%)	12 (2%)	0	100	100
1	D	658/717 (92%)	646 (98%)	11 (2%)	1 (0%)	47	68
All	All	2644/2868 (92%)	2599 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	452	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	578/617 (94%)	551 (95%)	27 (5%)	26	49
1	B	576/617 (93%)	549 (95%)	27 (5%)	26	49
1	C	578/617 (94%)	552 (96%)	26 (4%)	27	51
1	D	572/617 (93%)	542 (95%)	30 (5%)	23	44
All	All	2304/2468 (93%)	2194 (95%)	110 (5%)	25	48

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	54	GLU
1	A	170	LEU
1	A	223	LEU
1	A	230	VAL
1	A	237	SER
1	A	275	LEU
1	A	311	ASP
1	A	335	LYS
1	A	343	GLU
1	A	345	LEU
1	A	358	LYS
1	A	374	GLU
1	A	397	THR
1	A	428	LEU
1	A	438	THR
1	A	496	THR
1	A	513	LYS
1	A	521	LEU
1	A	537	GLU
1	A	574	LEU
1	A	611	ILE
1	A	614	LEU
1	A	670	LEU
1	A	671	LEU
1	A	675	ARG
1	A	727	THR
1	B	23	LEU
1	B	54	GLU
1	B	170	LEU
1	B	223	LEU
1	B	230	VAL
1	B	237	SER
1	B	275	LEU
1	B	311	ASP
1	B	335	LYS
1	B	343	GLU
1	B	345	LEU
1	B	358	LYS
1	B	397	THR
1	B	428	LEU
1	B	438	THR
1	B	513	LYS

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Mol	Chain	Res	Type
1	B	521	LEU
1	B	537	GLU
1	B	573	ARG
1	B	574	LEU
1	B	611	ILE
1	B	613	GLN
1	B	614	LEU
1	B	670	LEU
1	B	671	LEU
1	B	675	ARG
1	B	727	THR
1	C	23	LEU
1	C	54	GLU
1	C	170	LEU
1	C	223	LEU
1	C	230	VAL
1	C	237	SER
1	C	275	LEU
1	C	311	ASP
1	C	335	LYS
1	C	343	GLU
1	C	345	LEU
1	C	358	LYS
1	C	397	THR
1	C	428	LEU
1	C	438	THR
1	C	513	LYS
1	C	521	LEU
1	C	537	GLU
1	C	574	LEU
1	C	611	ILE
1	C	614	LEU
1	C	617	PRO
1	C	670	LEU
1	C	671	LEU
1	C	675	ARG
1	C	727	THR
1	D	23	LEU
1	D	54	GLU
1	D	170	LEU
1	D	221	ARG
1	D	223	LEU

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Mol	Chain	Res	Type
1	D	230	VAL
1	D	237	SER
1	D	275	LEU
1	D	311	ASP
1	D	318	LEU
1	D	320	LEU
1	D	335	LYS
1	D	343	GLU
1	D	345	LEU
1	D	358	LYS
1	D	397	THR
1	D	398	ARG
1	D	428	LEU
1	D	438	THR
1	D	513	LYS
1	D	521	LEU
1	D	537	GLU
1	D	573	ARG
1	D	574	LEU
1	D	611	ILE
1	D	614	LEU
1	D	670	LEU
1	D	671	LEU
1	D	675	ARG
1	D	727	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	414	ASN
1	A	481	GLN
1	B	159	GLN
1	B	226	HIS
1	B	561	HIS
1	B	613	GLN
1	C	159	GLN
1	C	226	HIS
1	C	414	ASN
1	C	446	HIS
1	D	561	HIS

### 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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	25L	A	904	-	68,83,83	2.59	11 (16%)	81,130,130	2.12	13 (16%)
4	25L	C	904	-	68,83,83	2.60	12 (17%)	81,130,130	2.07	14 (17%)
2	ANP	D	901	3	29,33,33	2.31	12 (41%)	31,52,52	3.00	10 (32%)
2	ANP	C	901	3	29,33,33	2.27	11 (37%)	31,52,52	2.83	10 (32%)
2	ANP	B	901	3	29,33,33	2.25	12 (41%)	31,52,52	2.65	11 (35%)
2	ANP	A	901	3	29,33,33	2.37	9 (31%)	31,52,52	2.79	9 (29%)
4	25L	D	904	-	68,83,83	2.64	11 (16%)	81,130,130	2.13	16 (19%)
4	25L	B	904	-	68,83,83	2.63	11 (16%)	81,130,130	2.06	12 (14%)

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	25L	A	904	-	-	6/40/100/100	0/9/9/9
4	25L	C	904	-	-	5/40/100/100	0/9/9/9
2	ANP	D	901	3	-	2/14/38/38	0/3/3/3
2	ANP	C	901	3	-	7/14/38/38	0/3/3/3
2	ANP	B	901	3	-	2/14/38/38	0/3/3/3
2	ANP	A	901	3	-	7/14/38/38	0/3/3/3
4	25L	D	904	-	-	1/40/100/100	0/9/9/9
4	25L	B	904	-	-	0/40/100/100	0/9/9/9

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	904	25L	CAT-NBF	9.74	1.47	1.32
4	B	904	25L	CAT-NBF	9.63	1.47	1.32
4	D	904	25L	C2-N3	9.51	1.47	1.32
4	D	904	25L	CAT-NBF	9.45	1.47	1.32
4	C	904	25L	C2-N3	9.21	1.47	1.32
4	A	904	25L	C2-N3	9.18	1.46	1.32
4	A	904	25L	CAT-NBF	9.18	1.46	1.32
4	B	904	25L	CAU-NBG	9.14	1.46	1.32
4	B	904	25L	C2-N3	9.09	1.46	1.32
4	D	904	25L	CAU-NBG	8.99	1.46	1.32
4	C	904	25L	CAU-NBG	8.97	1.46	1.32
4	A	904	25L	CAU-NBG	8.16	1.45	1.32
4	A	904	25L	C2-N1	7.81	1.48	1.33
4	D	904	25L	CAT-NBC	7.45	1.47	1.33
4	A	904	25L	CAT-NBC	7.30	1.47	1.33
4	C	904	25L	C2-N1	7.28	1.47	1.33
4	D	904	25L	CAU-NBD	7.26	1.47	1.33
4	B	904	25L	C2-N1	7.10	1.47	1.33
4	B	904	25L	CAU-NBD	7.03	1.47	1.33
4	D	904	25L	C2-N1	6.99	1.46	1.33
4	C	904	25L	CAU-NBD	6.87	1.46	1.33
4	B	904	25L	CAT-NBC	6.78	1.46	1.33
4	C	904	25L	CAT-NBC	6.57	1.46	1.33
4	A	904	25L	CAU-NBD	6.53	1.46	1.33
2	A	901	ANP	PB-O3A	5.42	1.65	1.59
2	C	901	ANP	C2-N3	5.34	1.40	1.32
2	B	901	ANP	PG-N3B	5.28	1.77	1.63
2	A	901	ANP	PG-N3B	4.90	1.76	1.63
2	D	901	ANP	PG-N3B	4.62	1.75	1.63
2	A	901	ANP	C2-N3	4.35	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	ANP	PG-N3B	4.30	1.74	1.63
2	D	901	ANP	C2-N3	4.18	1.38	1.32
2	A	901	ANP	C2-N1	4.13	1.41	1.33
2	C	901	ANP	C2-N1	4.12	1.41	1.33
2	B	901	ANP	C2-N3	4.07	1.38	1.32
2	D	901	ANP	PB-O3A	4.02	1.64	1.59
2	D	901	ANP	C2'-C1'	-3.94	1.47	1.53
2	C	901	ANP	PG-O3G	-3.65	1.46	1.56
2	B	901	ANP	PB-N3B	3.62	1.72	1.63
2	B	901	ANP	PG-O3G	-3.62	1.47	1.56
2	C	901	ANP	PB-O2B	-3.48	1.47	1.56
2	D	901	ANP	O4'-C1'	3.39	1.45	1.41
2	B	901	ANP	PB-O2B	-3.33	1.47	1.56
2	A	901	ANP	PG-O2G	-3.29	1.47	1.56
2	D	901	ANP	PG-O2G	-3.24	1.48	1.56
2	A	901	ANP	PB-O2B	-3.19	1.48	1.56
2	B	901	ANP	PG-O2G	-3.10	1.48	1.56
2	D	901	ANP	PG-O3G	-3.07	1.48	1.56
4	A	904	25L	OBO-CCN	3.05	1.45	1.41
2	B	901	ANP	C2-N1	3.03	1.39	1.33
2	C	901	ANP	PG-O2G	-2.96	1.48	1.56
2	D	901	ANP	PB-N3B	2.96	1.71	1.63
2	A	901	ANP	PG-O3G	-2.93	1.48	1.56
4	B	904	25L	O4'-C1'	2.91	1.45	1.41
2	D	901	ANP	PB-O2B	-2.84	1.49	1.56
2	D	901	ANP	C2-N1	2.81	1.39	1.33
4	A	904	25L	O4'-C1'	2.73	1.44	1.41
2	C	901	ANP	O4'-C1'	2.71	1.44	1.41
4	C	904	25L	C5-C4	2.65	1.47	1.40
4	B	904	25L	CBZ-CCC	2.60	1.47	1.40
2	A	901	ANP	C6-C5	-2.53	1.33	1.43
4	D	904	25L	CBY-CCB	2.52	1.47	1.40
2	B	901	ANP	C2'-C1'	-2.52	1.49	1.53
2	B	901	ANP	C5-C4	-2.49	1.34	1.40
4	A	904	25L	CBY-CCB	2.47	1.47	1.40
4	D	904	25L	CBZ-CCC	2.45	1.47	1.40
2	A	901	ANP	C2'-C1'	-2.43	1.50	1.53
4	B	904	25L	OBO-CCN	2.42	1.44	1.41
2	B	901	ANP	C6-C5	-2.41	1.34	1.43
2	C	901	ANP	C6-C5	-2.37	1.34	1.43
4	D	904	25L	C5-C4	2.36	1.47	1.40
4	B	904	25L	CBY-CCB	2.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	904	25L	OBO-CCN	2.35	1.44	1.41
2	C	901	ANP	C5-C4	-2.34	1.34	1.40
4	A	904	25L	CBZ-CCC	2.30	1.47	1.40
4	B	904	25L	C5-C4	2.29	1.47	1.40
4	A	904	25L	C5-C4	2.29	1.47	1.40
4	C	904	25L	CBZ-CCC	2.25	1.46	1.40
2	C	901	ANP	PB-O3A	2.24	1.61	1.59
4	C	904	25L	O4'-C1'	2.23	1.44	1.41
2	D	901	ANP	C5-C4	-2.19	1.35	1.40
2	B	901	ANP	PB-O1B	2.19	1.49	1.46
2	B	901	ANP	O5'-C5'	-2.18	1.36	1.44
4	C	904	25L	CBY-CCB	2.15	1.46	1.40
4	D	904	25L	OBP-CCO	2.09	1.44	1.41
4	C	904	25L	OBP-CCO	2.06	1.44	1.41
2	D	901	ANP	C6-C5	-2.05	1.35	1.43
4	D	904	25L	OBO-CCN	2.04	1.43	1.41
2	C	901	ANP	O5'-C5'	-2.02	1.37	1.44

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	ANP	O1G-PG-N3B	-12.16	93.86	111.77
2	C	901	ANP	O1G-PG-N3B	-10.37	96.50	111.77
2	A	901	ANP	O1G-PG-N3B	-9.74	97.43	111.77
4	A	904	25L	NBG-CAU-NBD	-9.35	114.07	128.68
4	C	904	25L	NBF-CAT-NBC	-9.31	114.12	128.68
4	D	904	25L	NBG-CAU-NBD	-9.30	114.14	128.68
4	D	904	25L	N3-C2-N1	-8.70	115.07	128.68
4	A	904	25L	NBF-CAT-NBC	-8.69	115.09	128.68
4	B	904	25L	NBG-CAU-NBD	-8.67	115.13	128.68
4	B	904	25L	N3-C2-N1	-8.64	115.17	128.68
4	D	904	25L	NBF-CAT-NBC	-8.56	115.30	128.68
4	A	904	25L	N3-C2-N1	-8.48	115.42	128.68
4	C	904	25L	N3-C2-N1	-8.45	115.47	128.68
4	B	904	25L	NBF-CAT-NBC	-8.09	116.04	128.68
4	C	904	25L	NBG-CAU-NBD	-8.06	116.08	128.68
2	B	901	ANP	O1G-PG-N3B	-8.01	99.97	111.77
2	C	901	ANP	N3-C2-N1	-6.70	118.21	128.68
2	B	901	ANP	N3-C2-N1	-6.65	118.28	128.68
2	D	901	ANP	N3-C2-N1	-5.63	119.88	128.68
2	A	901	ANP	N3-C2-N1	-5.36	120.30	128.68
2	A	901	ANP	O2B-PB-O1B	4.99	120.38	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ANP	C1'-N9-C4	-4.40	118.91	126.64
2	D	901	ANP	O1B-PB-N3B	-4.17	105.64	111.77
2	A	901	ANP	O3G-PG-O2G	4.15	118.69	107.64
4	D	904	25L	CAU-NBD-CBW	3.94	125.49	118.75
2	C	901	ANP	O3G-PG-O2G	3.92	118.09	107.64
2	B	901	ANP	O3G-PG-O2G	3.89	117.99	107.64
4	B	904	25L	CCB-CBY-NBI	-3.86	105.38	109.40
2	D	901	ANP	O3G-PG-O2G	3.82	117.82	107.64
2	C	901	ANP	C1'-N9-C4	-3.80	119.97	126.64
2	B	901	ANP	O4'-C4'-C5'	-3.78	96.93	109.37
4	C	904	25L	CCC-CBZ-NBJ	-3.72	105.52	109.40
2	C	901	ANP	O2B-PB-O1B	3.59	117.44	109.92
2	D	901	ANP	O2B-PB-O1B	3.55	117.37	109.92
4	A	904	25L	CAU-NBD-CBW	3.49	124.72	118.75
4	B	904	25L	C4-C5-N7	-3.44	105.81	109.40
2	A	901	ANP	C1'-N9-C4	-3.41	120.64	126.64
2	C	901	ANP	O4'-C1'-C2'	-3.41	101.94	106.93
4	A	904	25L	C3'-C2'-C1'	3.36	106.04	100.98
4	A	904	25L	CAT-NBC-CBV	3.34	124.47	118.75
4	C	904	25L	CAT-NBC-CBV	3.27	124.34	118.75
2	B	901	ANP	O2B-PB-O1B	3.23	116.68	109.92
2	A	901	ANP	O4'-C1'-C2'	-3.20	102.25	106.93
4	B	904	25L	CCC-CBZ-NBJ	-3.20	106.07	109.40
4	D	904	25L	CAT-NBC-CBV	3.17	124.17	118.75
2	A	901	ANP	PA-O3A-PB	-3.07	121.81	132.62
2	B	901	ANP	PA-O3A-PB	-3.06	121.83	132.62
4	C	904	25L	C2-N1-C6	3.04	123.95	118.75
4	D	904	25L	C2-N1-C6	3.01	123.90	118.75
4	A	904	25L	CCB-CBY-NBI	-2.96	106.32	109.40
4	B	904	25L	CAU-NBD-CBW	2.94	123.78	118.75
2	D	901	ANP	O5'-PA-O1A	-2.94	97.59	109.07
4	D	904	25L	CCC-CBZ-NBJ	-2.88	106.40	109.40
4	D	904	25L	CCB-CBY-NBI	-2.80	106.48	109.40
4	B	904	25L	CCN-NCQ-CCB	-2.78	121.76	126.64
4	A	904	25L	C4-C5-N7	-2.77	106.52	109.40
4	B	904	25L	PCW-OBT-PCT	-2.76	123.35	132.83
4	C	904	25L	CCB-CBY-NBI	-2.74	106.54	109.40
4	B	904	25L	C2-N1-C6	2.69	123.35	118.75
4	C	904	25L	PCW-OBT-PCT	-2.69	123.60	132.83
4	B	904	25L	CAT-NBC-CBV	2.68	123.34	118.75
2	A	901	ANP	O5'-PA-O1A	-2.68	98.61	109.07
2	C	901	ANP	O4'-C4'-C5'	-2.64	100.68	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	904	25L	CCN-NCQ-CCB	-2.62	122.04	126.64
4	D	904	25L	C4-C5-N7	-2.55	106.75	109.40
4	A	904	25L	C2-N1-C6	2.53	123.08	118.75
2	D	901	ANP	O3G-PG-O1G	2.50	119.73	113.45
4	D	904	25L	OAP-PCU-OAF	2.49	124.56	112.24
4	A	904	25L	CCC-CBZ-NBJ	-2.49	106.80	109.40
2	D	901	ANP	C1'-N9-C4	-2.44	122.35	126.64
2	D	901	ANP	C4-C5-N7	-2.43	106.87	109.40
2	C	901	ANP	PA-O3A-PB	-2.39	124.20	132.62
4	A	904	25L	PCW-OBT-PCT	-2.37	124.69	132.83
4	D	904	25L	OBR-CCL-CCO	-2.37	101.59	110.10
4	B	904	25L	OAM-PCT-OAE	2.31	123.66	112.24
4	D	904	25L	CCG-CCL-CCO	2.28	107.17	102.89
4	C	904	25L	CCN-NCQ-CCB	-2.26	122.67	126.64
4	C	904	25L	OAQ-PCV-OAG	2.20	123.14	112.24
4	C	904	25L	C3'-C2'-C1'	2.20	104.29	100.98
2	A	901	ANP	C3'-C2'-C1'	2.19	104.28	100.98
4	C	904	25L	CAU-NBD-CBW	2.19	122.50	118.75
4	C	904	25L	C4-C5-N7	-2.18	107.13	109.40
2	D	901	ANP	C3'-C2'-C1'	2.17	104.25	100.98
2	B	901	ANP	C4-C5-N7	-2.16	107.14	109.40
4	A	904	25L	OAO-PCS-OAN	2.15	115.84	107.64
2	B	901	ANP	O3G-PG-O1G	2.13	118.81	113.45
4	D	904	25L	PCW-OBT-PCT	-2.12	125.56	132.83
2	C	901	ANP	O2G-PG-O1G	2.11	118.75	113.45
2	B	901	ANP	O2G-PG-O1G	2.10	118.74	113.45
4	C	904	25L	OAO-PCS-OAN	2.07	115.57	107.64
2	C	901	ANP	O5'-PA-O1A	2.07	117.16	109.07
2	B	901	ANP	O1B-PB-N3B	2.07	114.81	111.77
4	D	904	25L	C3'-C2'-C1'	2.04	104.05	100.98
4	A	904	25L	OAP-PCU-OAF	2.03	122.30	112.24
4	D	904	25L	OAO-PCS-OAN	2.03	115.39	107.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	904	25L	PCW-OBS-PCS-OAN
4	C	904	25L	PCW-OBS-PCS-OAO
2	D	901	ANP	PG-N3B-PB-O1B
2	C	901	ANP	PB-N3B-PG-O1G
2	C	901	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	901	ANP	C5'-O5'-PA-O1A
2	B	901	ANP	PG-N3B-PB-O1B
2	A	901	ANP	PB-N3B-PG-O1G
2	A	901	ANP	PG-N3B-PB-O1B
2	A	901	ANP	PG-N3B-PB-O3A
2	A	901	ANP	C5'-O5'-PA-O2A
2	D	901	ANP	O4'-C4'-C5'-O5'
2	B	901	ANP	O4'-C4'-C5'-O5'
4	C	904	25L	C5'-O5'-PCU-OB
4	A	904	25L	C5'-O5'-PCU-OB
2	C	901	ANP	C5'-O5'-PA-O3A
2	A	901	ANP	C5'-O5'-PA-O3A
4	A	904	25L	CAY-OBK-PCT-OB
2	C	901	ANP	C5'-O5'-PA-O2A
4	A	904	25L	C5'-O5'-PCU-OAF
4	A	904	25L	C5'-O5'-PCU-OAP
2	A	901	ANP	O4'-C4'-C5'-O5'
4	A	904	25L	CCL-OBK-PCU-O5'
4	C	904	25L	PCW-OBS-PCS-OAD
2	C	901	ANP	PB-O3A-PA-O2A
4	D	904	25L	PCS-OBS-PCW-OAH
4	C	904	25L	C5'-O5'-PCU-OAF
2	A	901	ANP	C5'-O5'-PA-O1A
2	C	901	ANP	O4'-C4'-C5'-O5'
4	A	904	25L	CCO-CCL-OBK-PCU

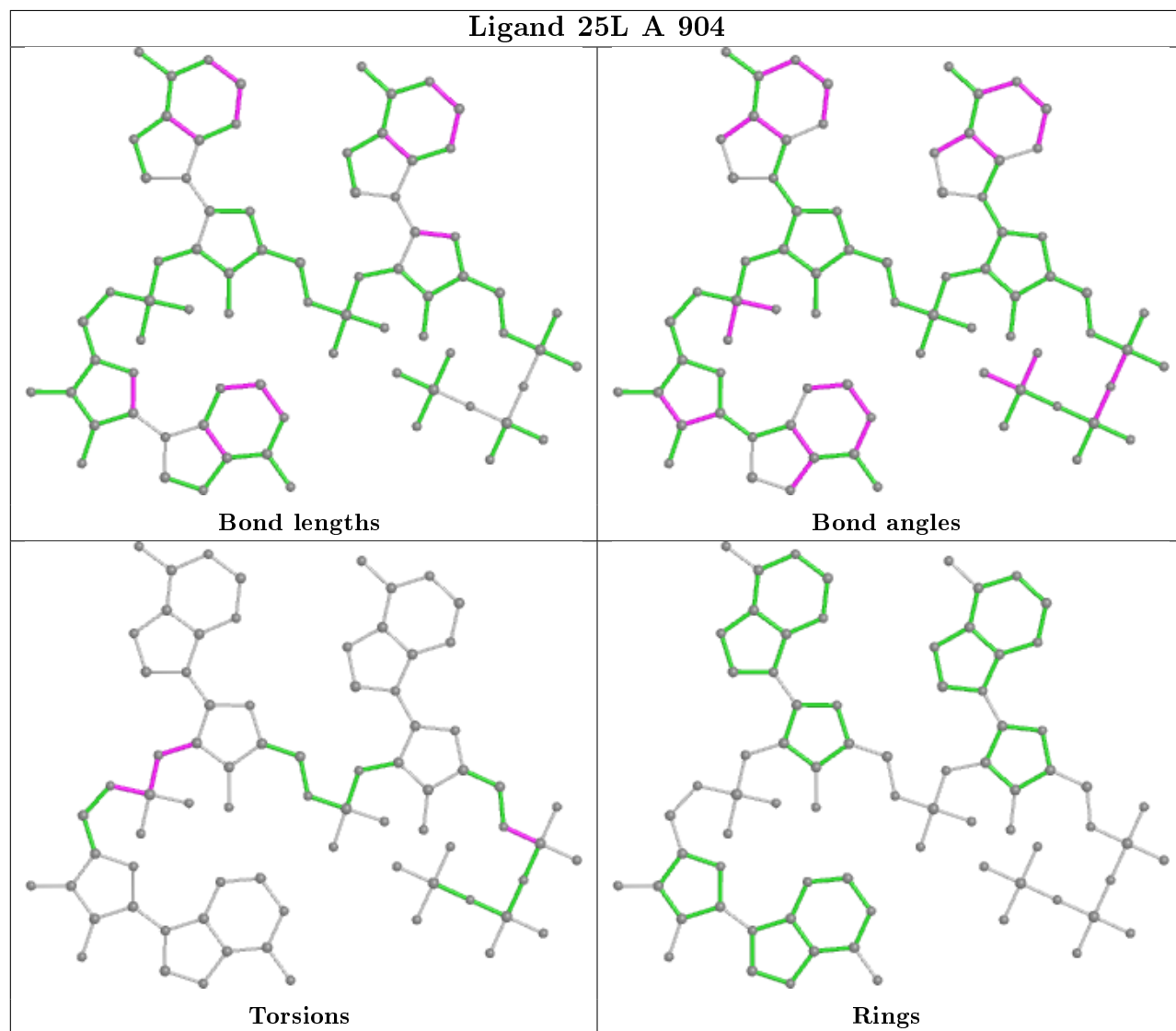
There are no ring outliers.

4 monomers are involved in 4 short contacts:

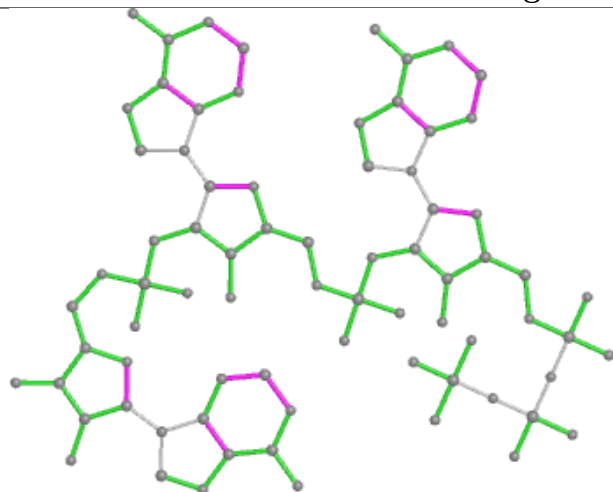
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	904	25L	1	0
2	C	901	ANP	1	0
2	A	901	ANP	1	0
4	B	904	25L	1	0

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 than 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

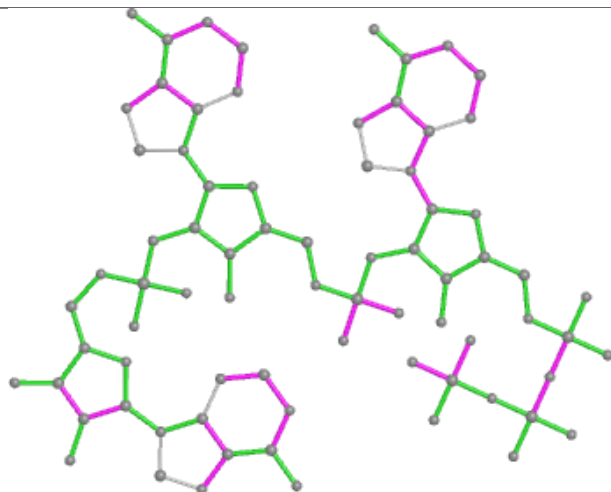
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



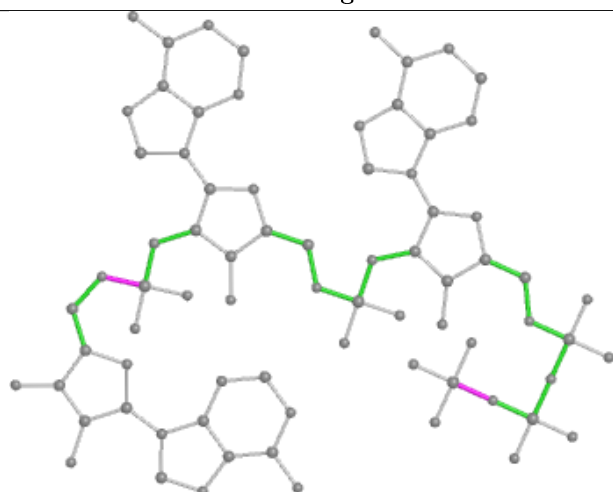
## Ligand 25L C 904



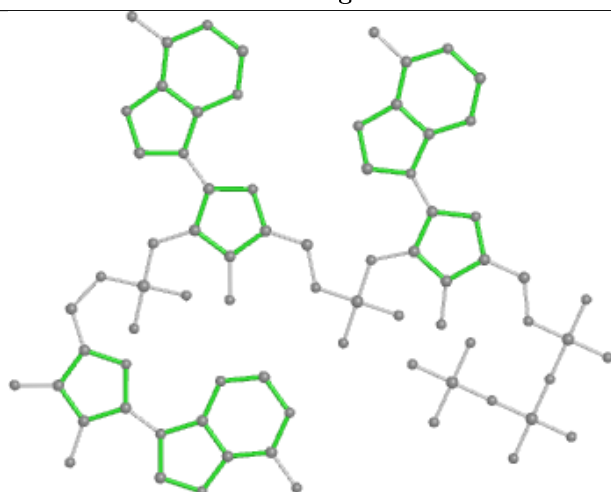
Bond lengths



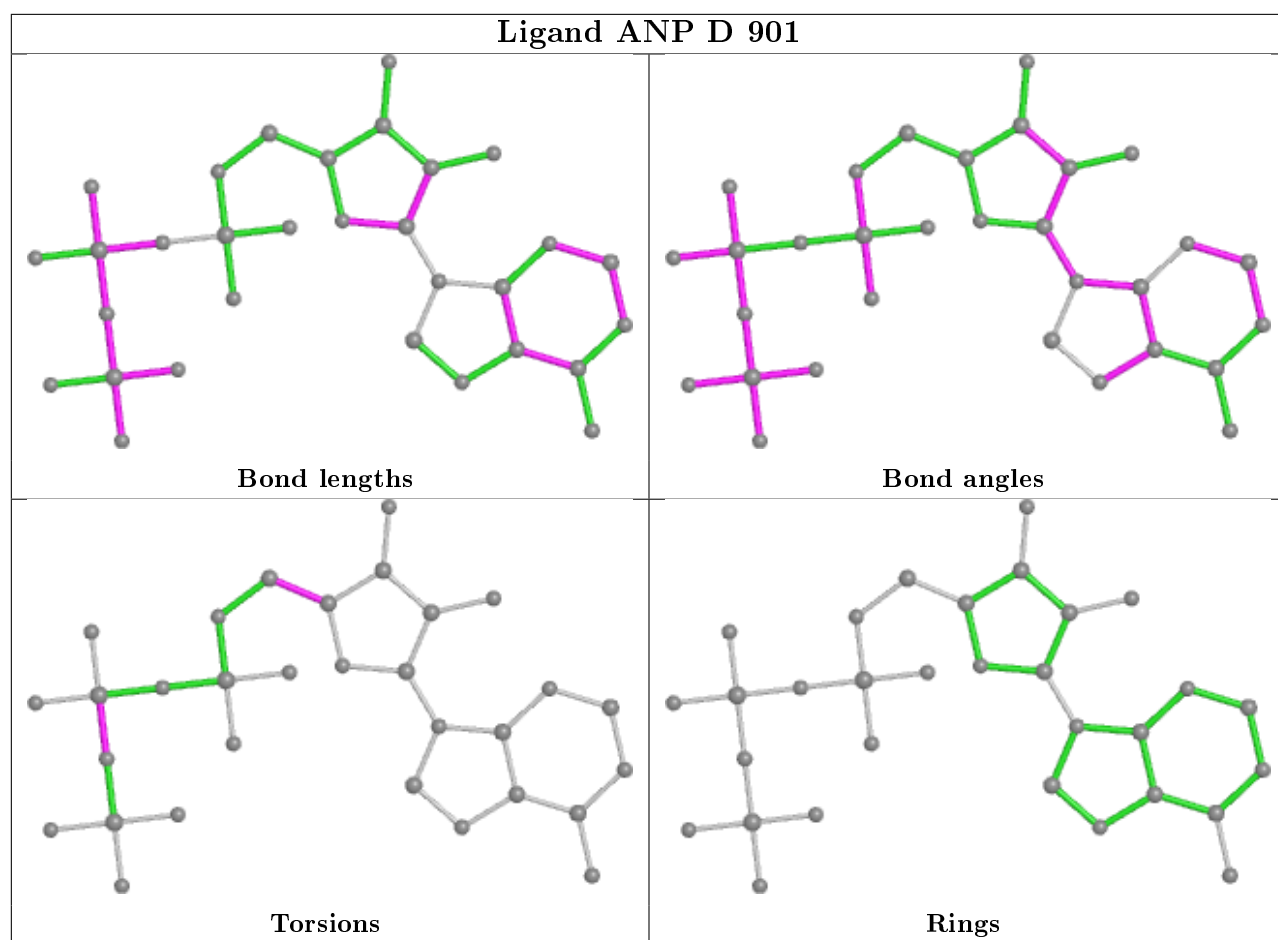
Bond angles

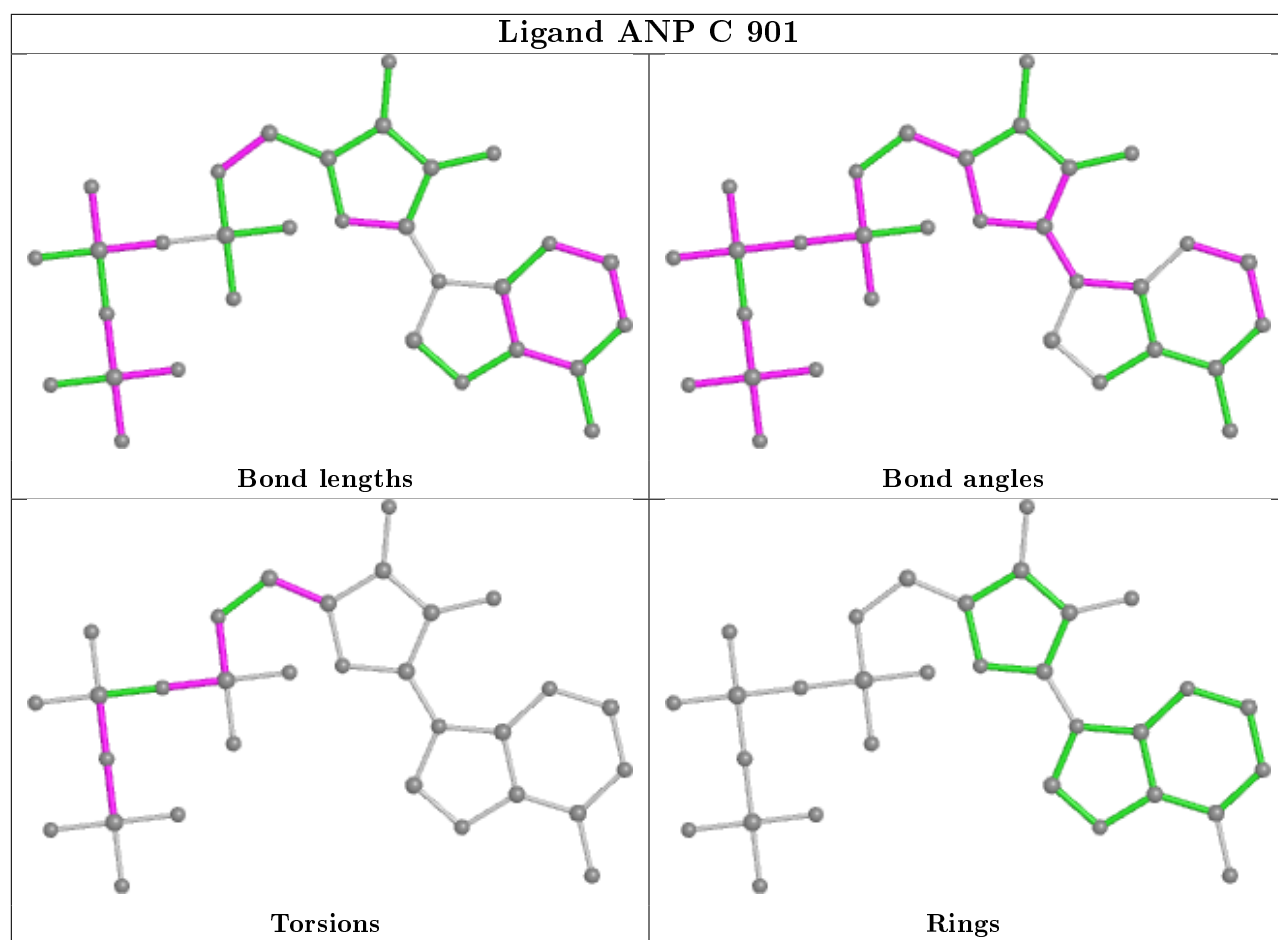


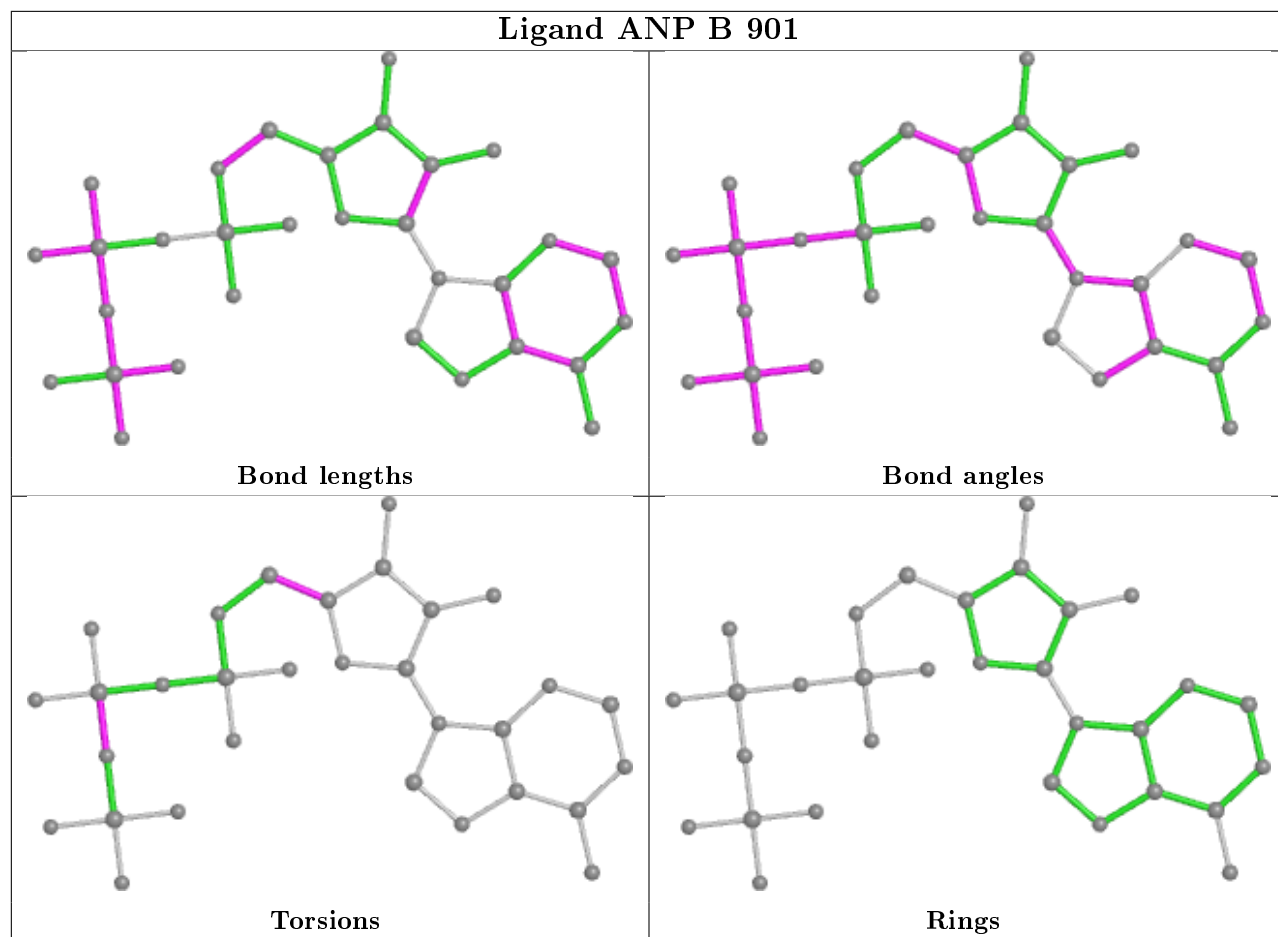
Torsions



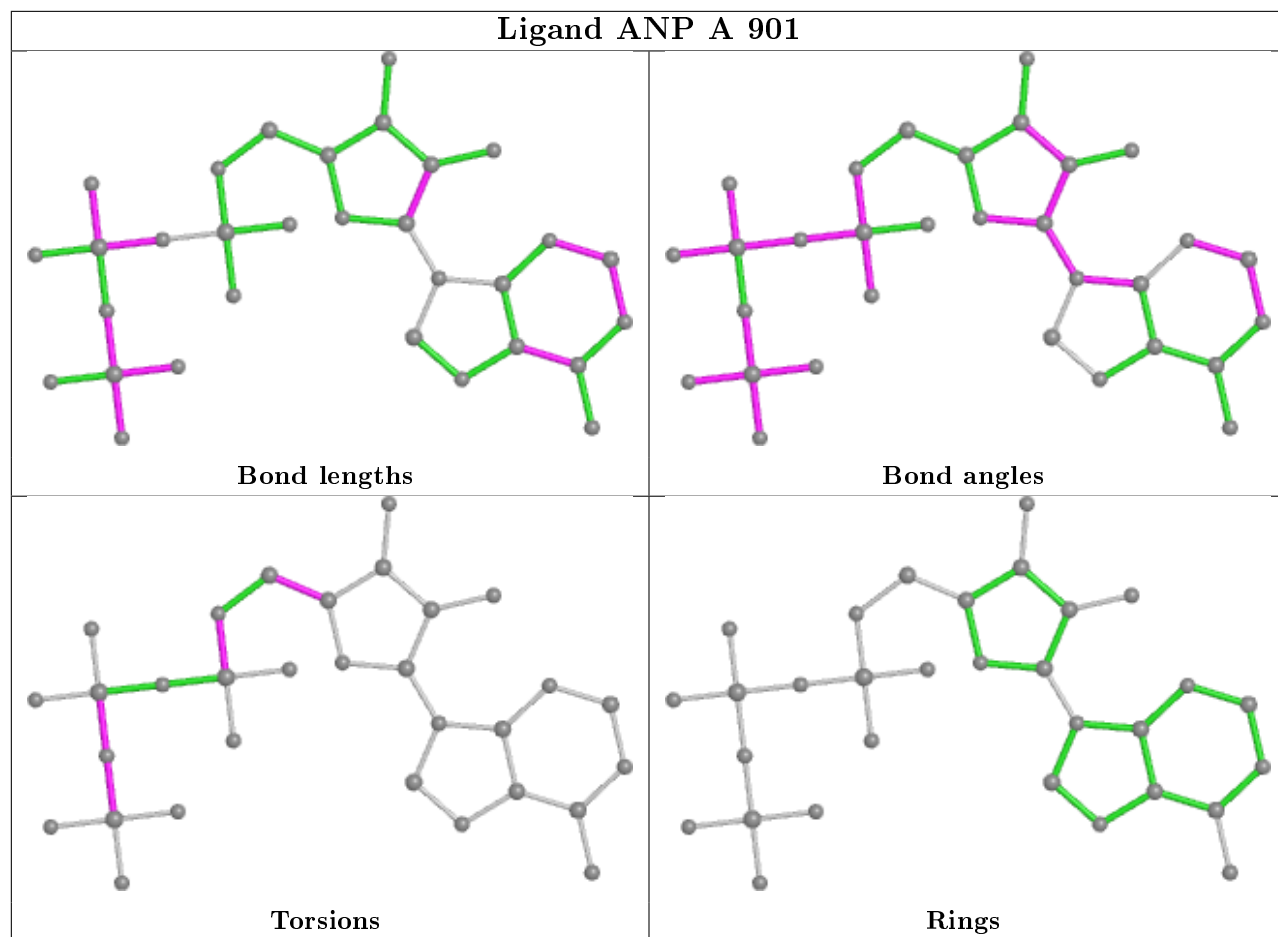
Rings



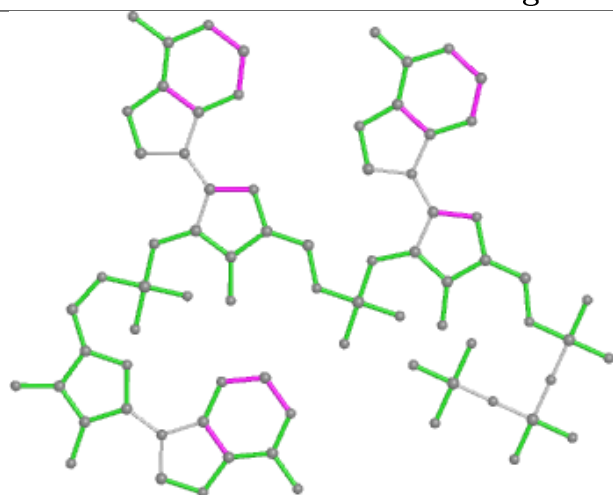




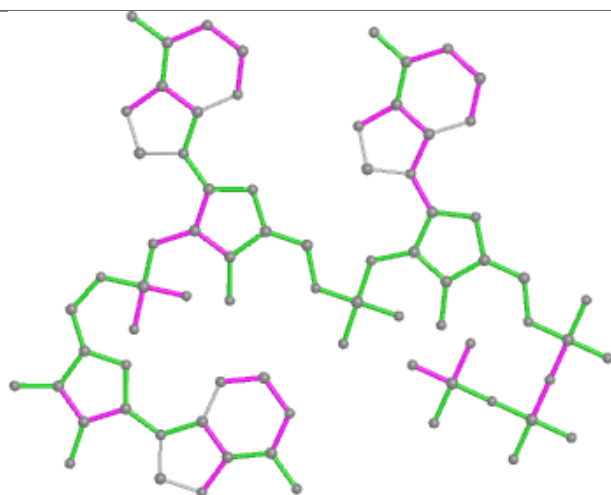




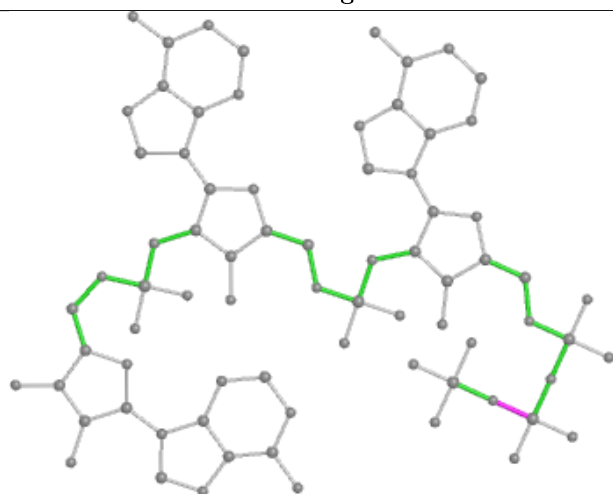
## Ligand 25L D 904



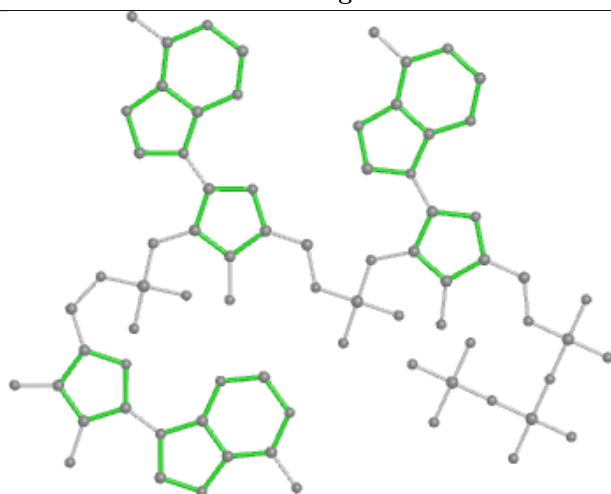
Bond lengths



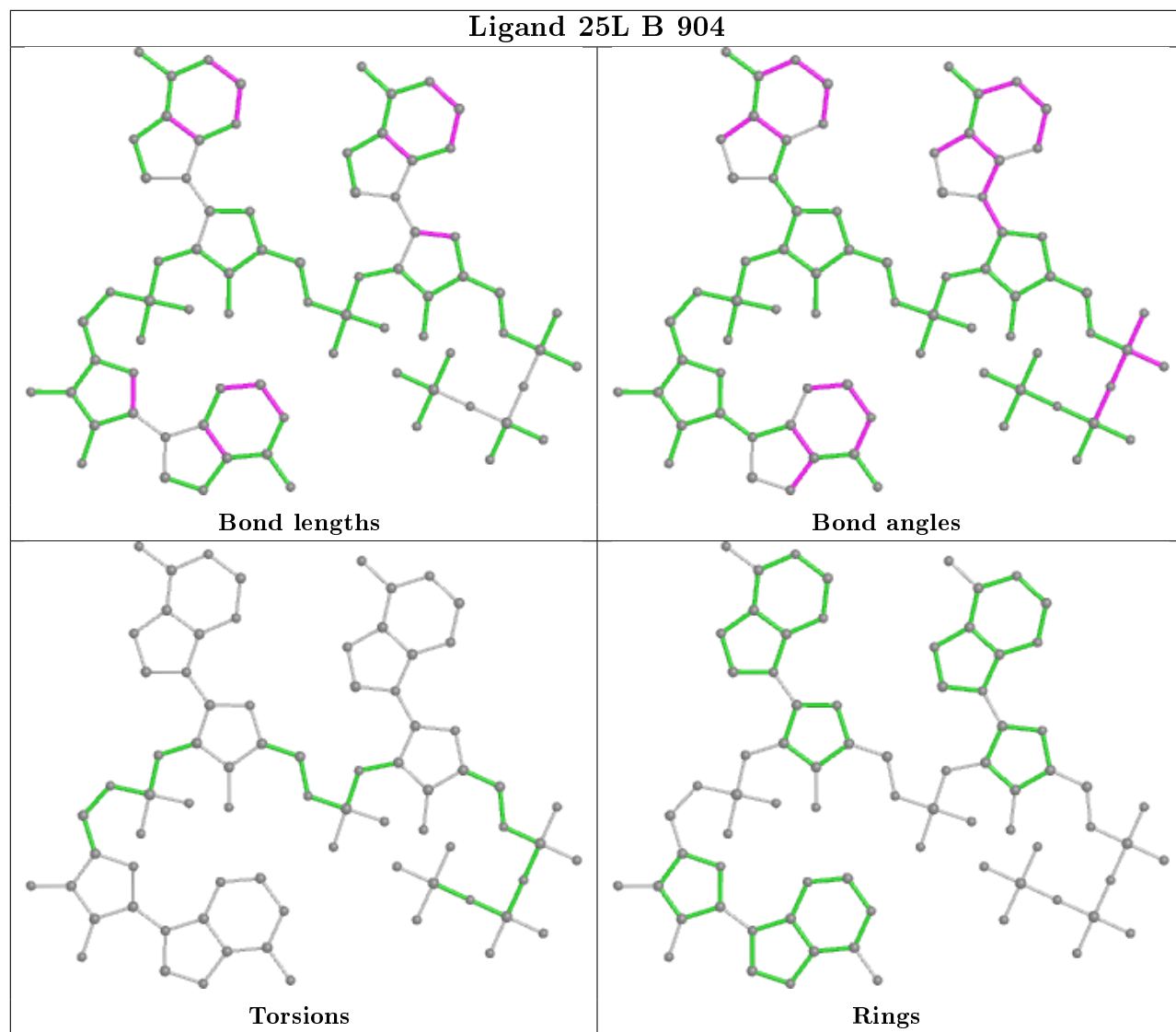
Bond angles



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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	672/717 (93%)	-0.17	9 (1%) 77 79	25, 51, 88, 108	0
1	B	671/717 (93%)	-0.05	14 (2%) 63 66	27, 47, 88, 118	0
1	C	673/717 (93%)	-0.18	10 (1%) 73 75	24, 46, 90, 111	0
1	D	668/717 (93%)	-0.00	17 (2%) 57 61	26, 51, 92, 119	0
All	All	2684/2868 (93%)	-0.10	50 (1%) 66 69	24, 49, 90, 119	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	728	HIS	4.7
1	C	684	GLN	4.7
1	A	684	GLN	4.5
1	C	299	CYS	4.3
1	B	607	GLN	3.9
1	B	684	GLN	3.5
1	B	23	LEU	3.4
1	D	608	ASN	3.2
1	B	25	GLU	3.2
1	A	685	LYS	3.2
1	B	611	ILE	3.2
1	B	43	LEU	3.1
1	B	335	LYS	3.1
1	B	728	HIS	2.9
1	C	728	HIS	2.9
1	D	333	ASN	2.9
1	B	615	LEU	2.8
1	B	729	ASN	2.8
1	D	42	LEU	2.8
1	D	51	PHE	2.6
1	C	729	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	76	LEU	2.6
1	D	663	TYR	2.6
1	D	254	GLN	2.6
1	A	640	GLU	2.6
1	A	320	LEU	2.5
1	D	684	GLN	2.5
1	C	321	HIS	2.5
1	A	728	HIS	2.4
1	A	729	ASN	2.4
1	A	509	GLU	2.4
1	C	636	PHE	2.4
1	B	672	LYS	2.4
1	D	260	GLU	2.4
1	B	46	GLY	2.3
1	C	320	LEU	2.3
1	B	260	GLU	2.3
1	C	619	THR	2.3
1	D	46	GLY	2.2
1	B	49	ALA	2.2
1	D	23	LEU	2.2
1	D	452	PRO	2.2
1	A	299	CYS	2.2
1	C	298	ASN	2.1
1	C	300	GLY	2.1
1	D	221	ARG	2.1
1	D	47	ALA	2.0
1	D	298	ASN	2.0
1	A	510	ASP	2.0
1	D	667	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

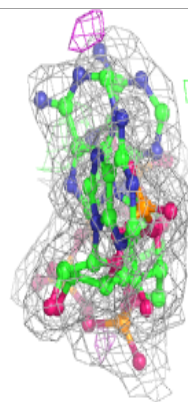
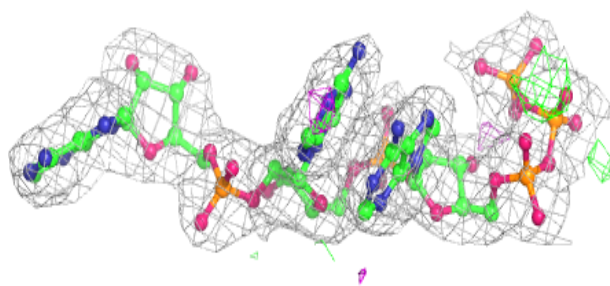
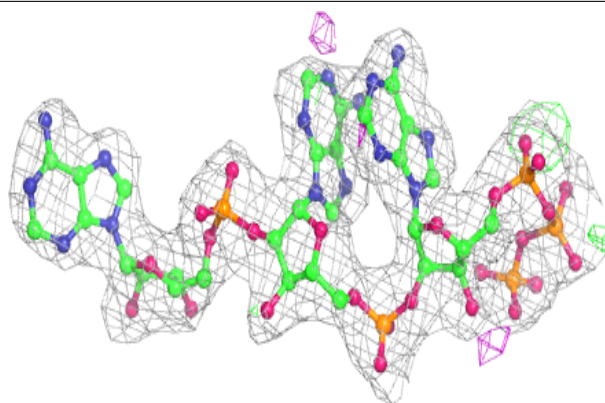
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	902	1/1	0.89	0.19	53,53,53,53	0
3	MG	A	902	1/1	0.91	0.23	27,27,27,27	0
3	MG	B	903	1/1	0.93	0.11	31,31,31,31	0
3	MG	D	903	1/1	0.93	0.14	55,55,55,55	0
3	MG	C	902	1/1	0.93	0.20	29,29,29,29	0
3	MG	C	903	1/1	0.95	0.21	24,24,24,24	0
3	MG	B	902	1/1	0.96	0.27	25,25,25,25	0
4	25L	D	904	75/75	0.96	0.11	35,43,51,53	0
4	25L	A	904	75/75	0.96	0.12	34,43,52,59	0
3	MG	A	903	1/1	0.96	0.20	25,25,25,25	0
2	ANP	D	901	31/31	0.97	0.12	31,36,57,63	0
2	ANP	B	901	31/31	0.97	0.11	28,35,60,66	0
4	25L	B	904	75/75	0.97	0.11	28,35,52,54	0
2	ANP	A	901	31/31	0.97	0.11	29,32,47,51	0
4	25L	C	904	75/75	0.98	0.11	30,35,53,54	0
2	ANP	C	901	31/31	0.98	0.10	26,30,53,54	0

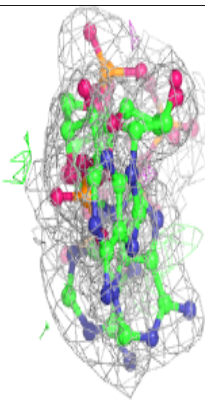
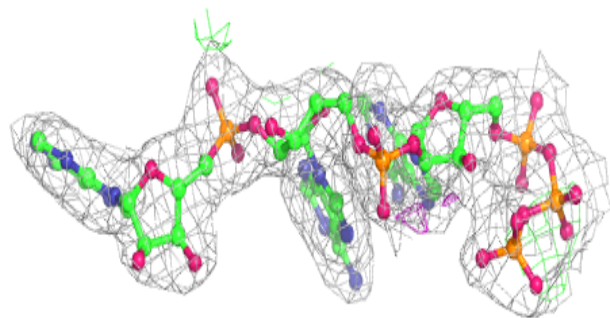
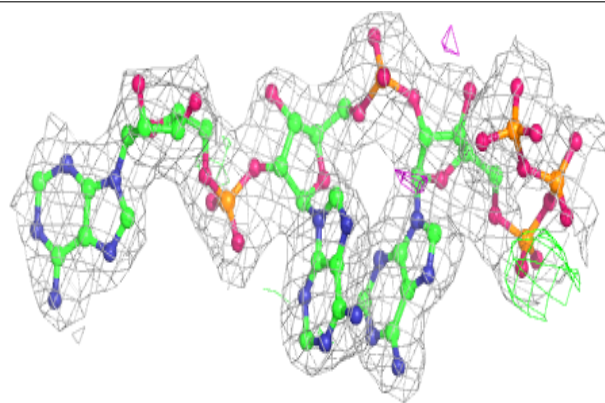
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 25L D 904:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

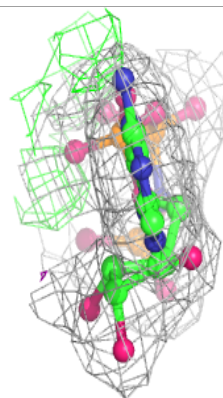
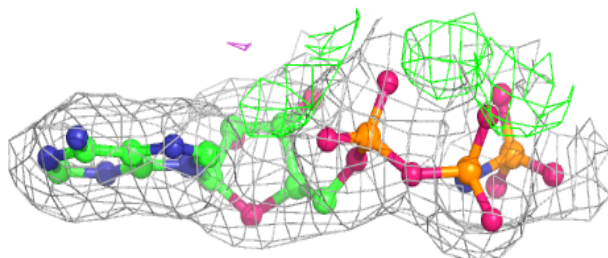
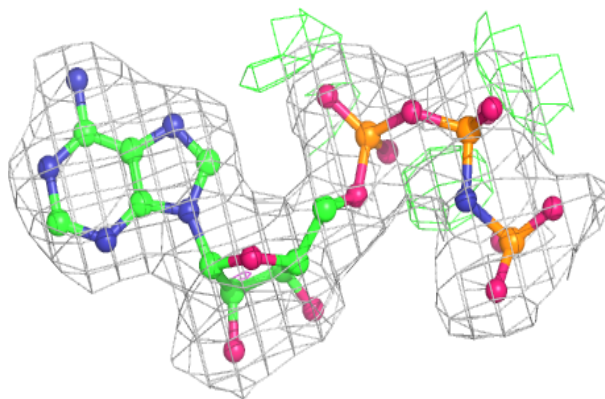
**Electron density around 25L A 904:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

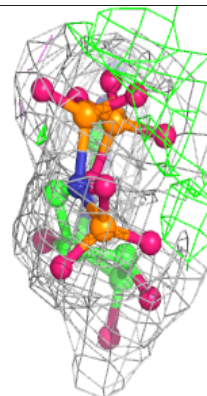
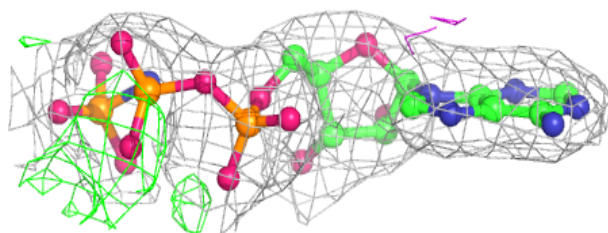
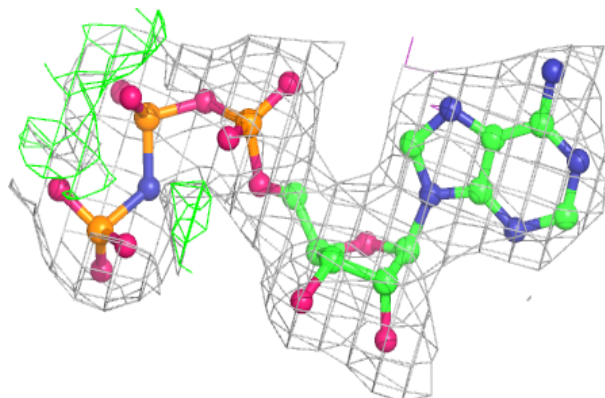


**Electron density around ANP D 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP B 901:**

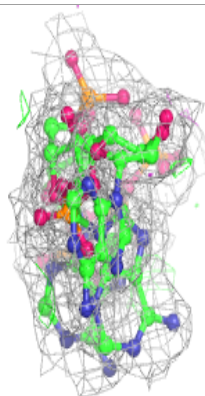
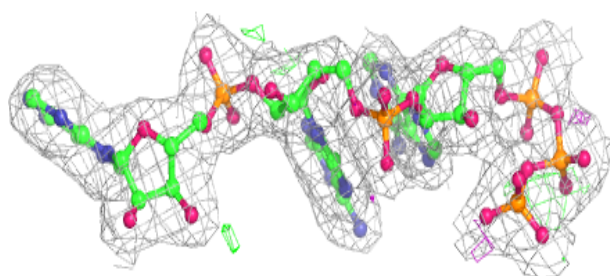
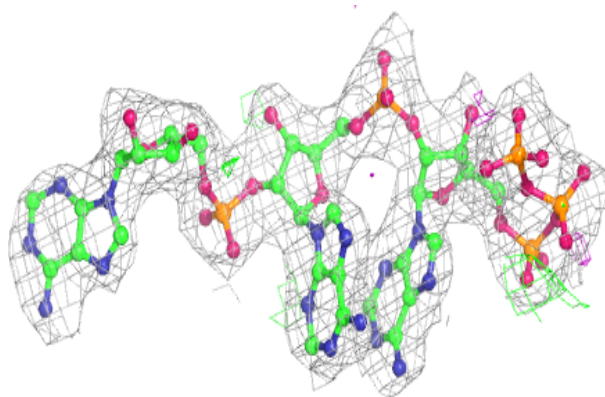
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



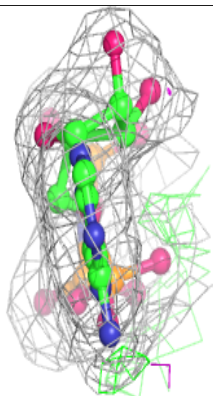
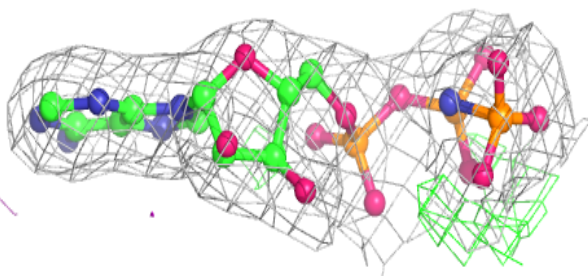
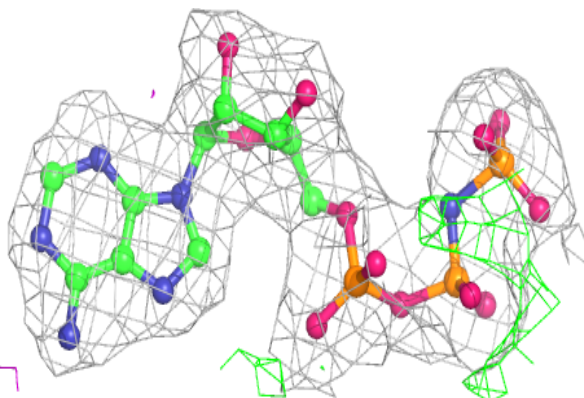


**Electron density around 25L B 904:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

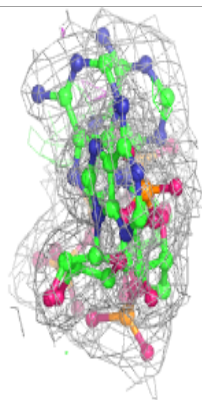
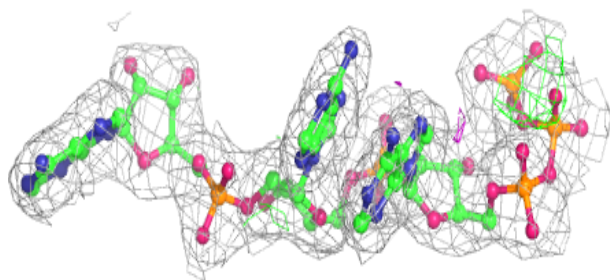
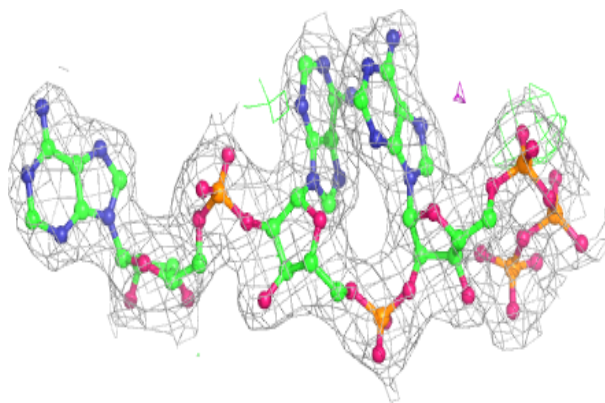
**Electron density around ANP A 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

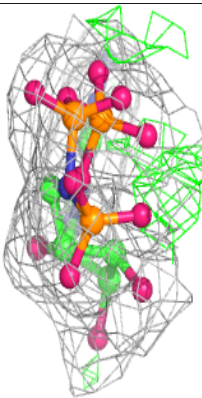
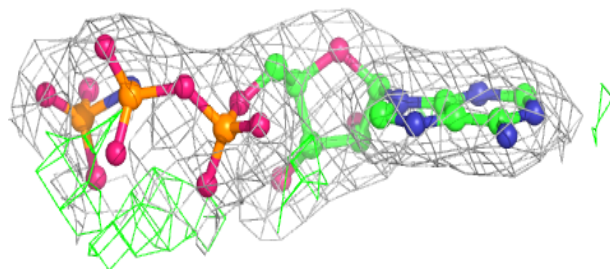
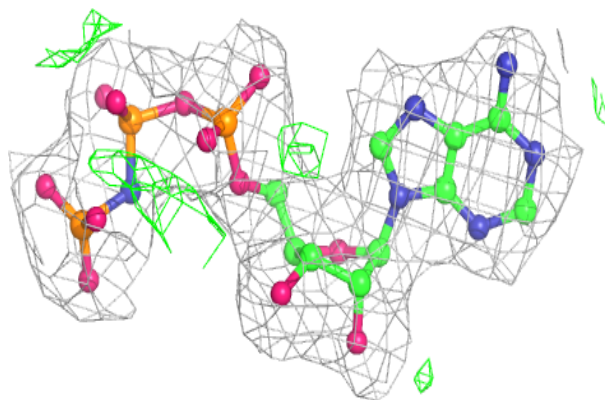


**Electron density around 25L C 904:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP C 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.