Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 05:56 AM EST

PDB ID	:	3NGT
Title	:	Structure of Leishmania NDKb complexed with AMP.
Authors	:	Trindade, D.M.; Sousa, T.A.C.B.; Tonoli, C.C.C.; Santos, C.R.; Arni, R.K.; Ward, R.J.; Oliveira, A.H.C.; Murakami, M.T.
Deposited on	:	2010-06-13
Resolution	:	2.57 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

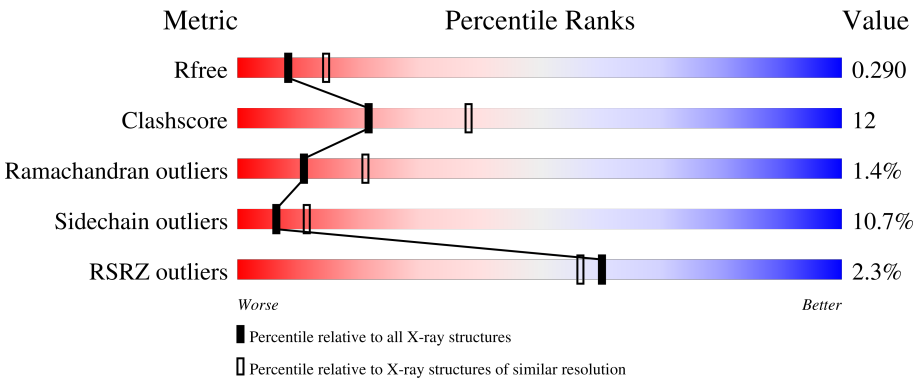
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	151	3%, 70%, 23%, 5%
1	B	151	%, 73%, 19%, 5%
1	C	151	%, 62%, 30%, 5%
1	D	151	%, 71%, 26%
1	E	151	%, 75%, 21%

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Mol	Chain	Length	Quality of chain
1	F	151	%; 70%; 26%
1	G	151	4%; 61%; 32%; 5%
1	H	151	5%; 70%; 18%; 8%
1	I	151	3%; 64%; 28%; 6%
1	J	151	%; 68%; 25%
1	K	151	%; 70%; 27%
1	L	151	7%; 49%; 28%; 5%; 17%
1	M	151	73%; 23%
1	N	151	2%; 73%; 21%; 6%

2 Entry composition (i)

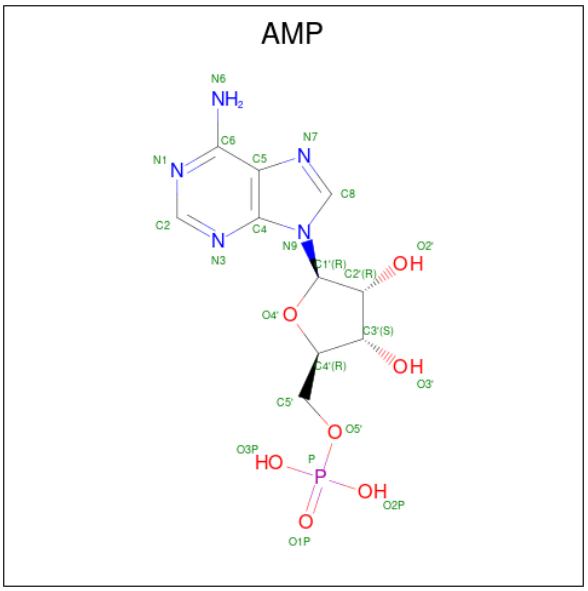
There are 3 unique types of molecules in this entry. The entry contains 16728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1171	744	203	219	5	27	1	0
			Total	C	N	O	S			
1	B	148	1159	739	200	214	6	24	2	0
			Total	C	N	O	S			
1	C	148	1156	737	200	214	5	26	1	0
			Total	C	N	O	S			
1	D	150	1165	741	202	218	4	15	0	0
			Total	C	N	O	S			
1	E	150	1168	743	202	218	5	33	1	0
			Total	C	N	O	S			
1	F	150	1168	743	202	218	5	31	1	0
			Total	C	N	O	S			
1	G	149	1159	738	201	216	4	44	0	0
			Total	C	N	O	S			
1	H	147	1148	731	199	214	4	51	1	0
			Total	C	N	O	S			
1	I	150	1168	743	202	218	5	42	1	0
			Total	C	N	O	S			
1	J	148	1149	733	200	212	4	15	0	0
			Total	C	N	O	S			
1	K	149	1165	741	202	217	5	15	1	0
			Total	C	N	O	S			
1	L	125	960	608	170	179	3	35	0	0
			Total	C	N	O	S			
1	M	149	1165	741	202	217	5	21	1	0
			Total	C	N	O	S			
1	N	150	1171	744	203	219	5	20	1	0

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	23	10	5	7	1	0	0
2	B	1	23	10	5	7	1	0	0
2	C	1	23	10	5	7	1	0	0
2	D	1	23	10	5	7	1	0	0
2	E	1	23	10	5	7	1	0	0
2	F	1	23	10	5	7	1	0	0
2	G	1	23	10	5	7	1	0	0
2	H	1	23	10	5	7	1	0	0
2	I	1	23	10	5	7	1	0	0
2	J	1	23	10	5	7	1	0	0
2	K	1	23	10	5	7	1	0	0
2	M	1	23	10	5	7	1	0	0
2	N	1	23	10	5	7	1	0	0

- Molecule 3 is water.

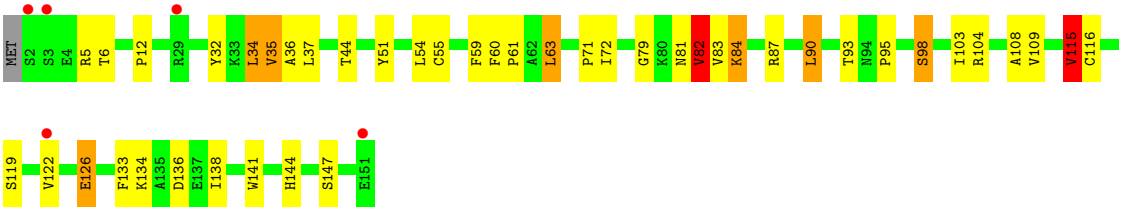
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	28	28	28	0	0
			Total	O		
3	B	39	39	39	0	0
			Total	O		
3	C	30	30	30	0	0
			Total	O		
3	D	26	26	26	0	0
			Total	O		
3	E	23	23	23	0	0
			Total	O		
3	F	30	30	30	0	0
			Total	O		
3	G	22	22	22	0	0
			Total	O		
3	H	18	18	18	0	0
			Total	O		
3	I	16	16	16	0	0
			Total	O		
3	J	22	22	22	0	0
			Total	O		
3	K	25	25	25	0	0
			Total	O		
3	L	10	10	10	0	0
			Total	O		
3	M	30	30	30	0	0
			Total	O		
3	N	38	38	38	0	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 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.

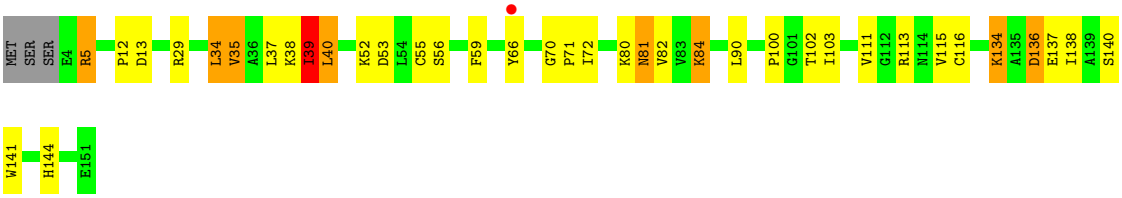
• Molecule 1: Nucleoside diphosphate kinase

Chain A:



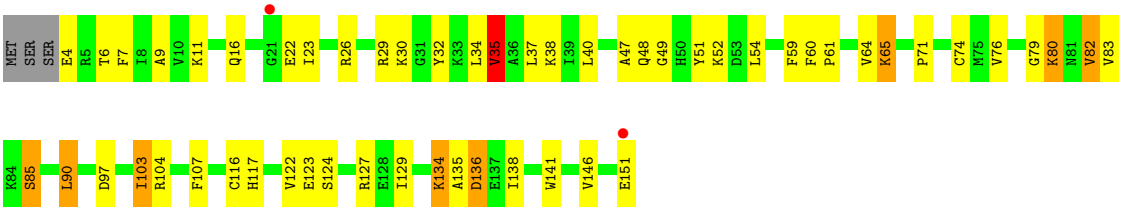
• Molecule 1: Nucleoside diphosphate kinase

Chain B:



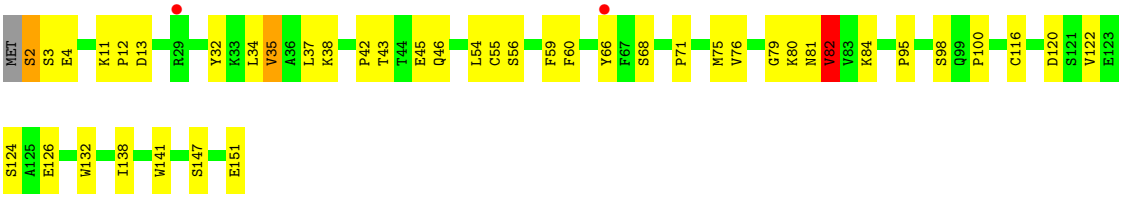
• Molecule 1: Nucleoside diphosphate kinase

Chain C:

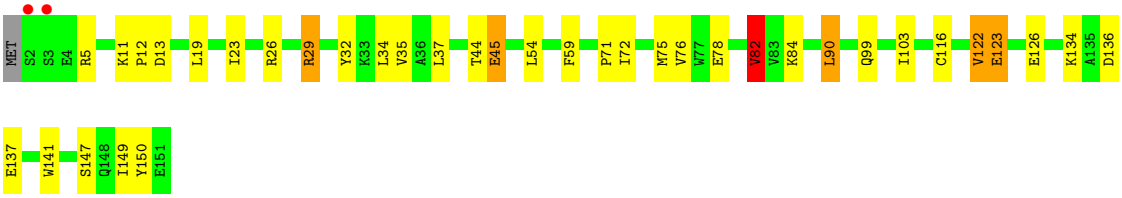


• Molecule 1: Nucleoside diphosphate kinase

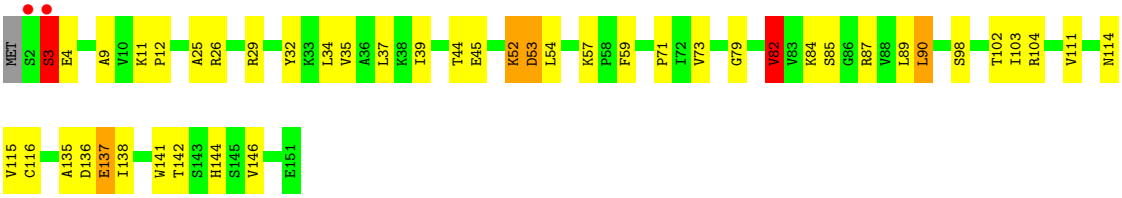
Chain D:



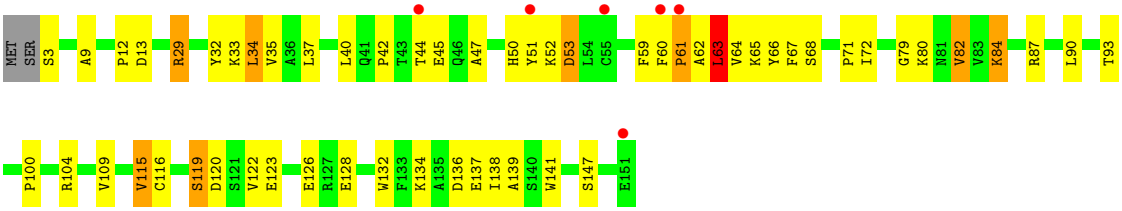
• Molecule 1: Nucleoside diphosphate kinase



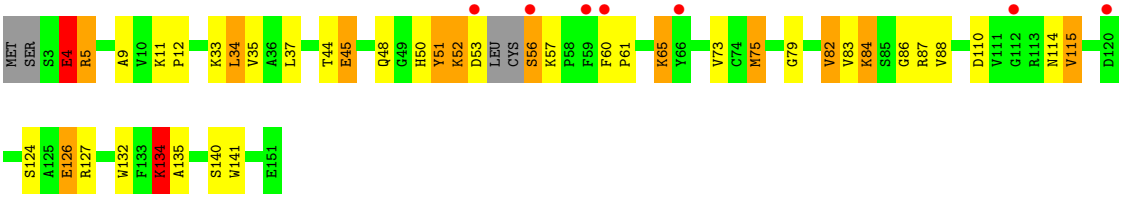
• Molecule 1: Nucleoside diphosphate kinase



• Molecule 1: Nucleoside diphosphate kinase

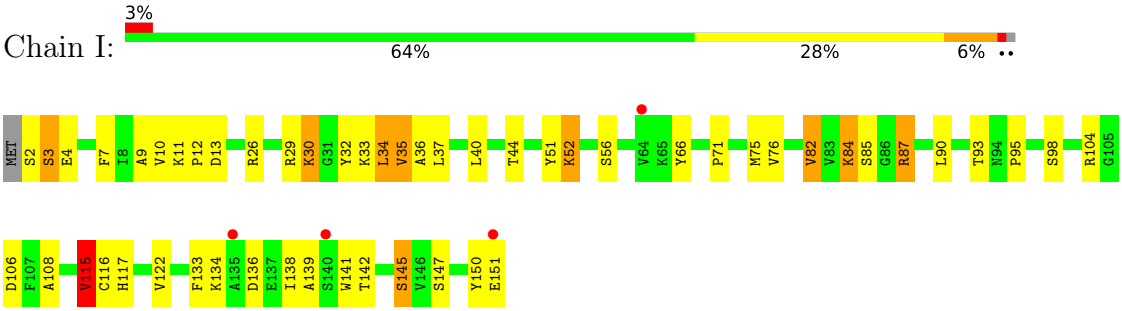


• Molecule 1: Nucleoside diphosphate kinase



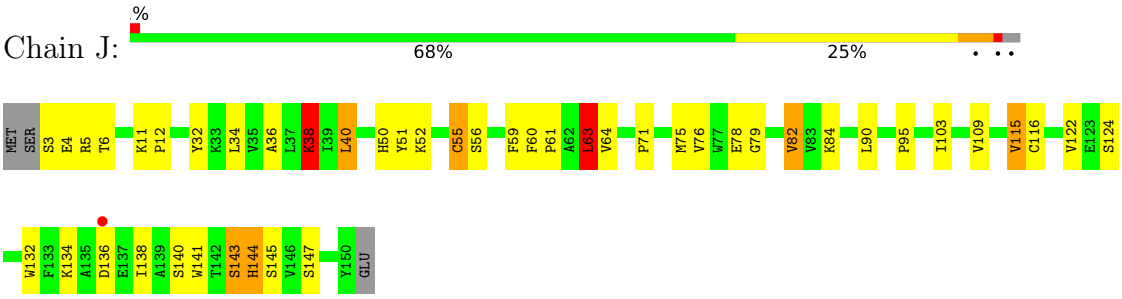
• Molecule 1: Nucleoside diphosphate kinase

Chain I:



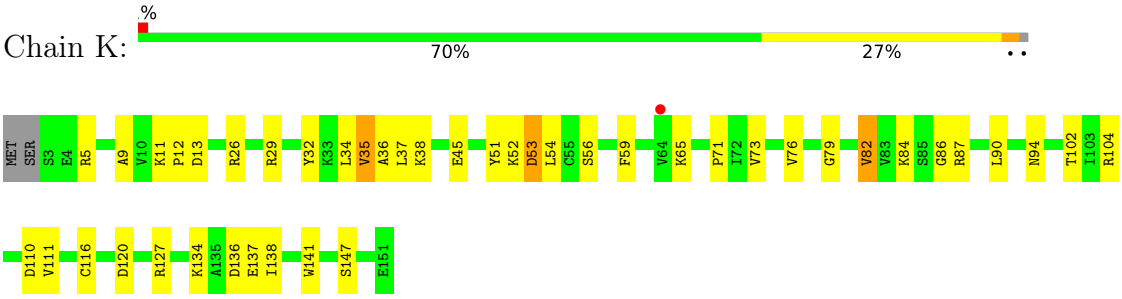
- Molecule 1: Nucleoside diphosphate kinase

Chain J:



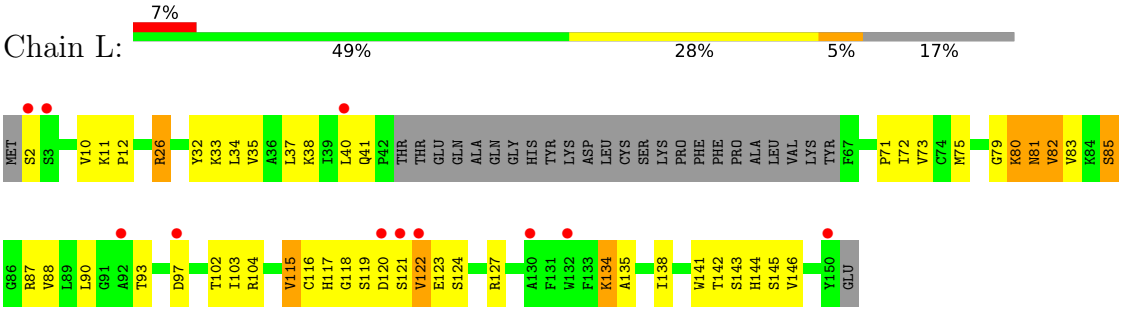
- Molecule 1: Nucleoside diphosphate kinase

Chain K:



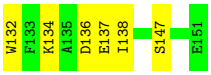
- Molecule 1: Nucleoside diphosphate kinase

Chain L:



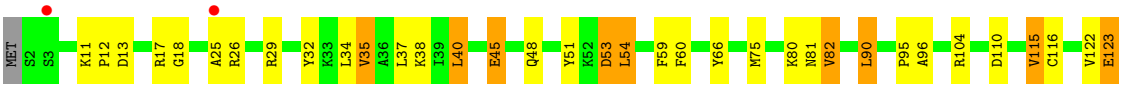
- Molecule 1: Nucleoside diphosphate kinase

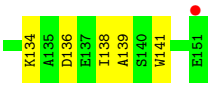
Chain M:



• Molecule 1: Nucleoside diphosphate kinase

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	233.95Å 233.95Å 265.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	161.00 – 2.57 37.26 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.4 (161.00-2.57) 97.4 (37.26-2.57)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.314 0.227 , 0.290	Depositor DCC
R_{free} test set	4338 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16728	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4726e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: AMP

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	0.92	4/1198 (0.3%)	1.04	5/1619 (0.3%)
1	B	1.10	4/1192 (0.3%)	0.98	5/1611 (0.3%)
1	C	0.97	3/1186 (0.3%)	0.92	3/1603 (0.2%)
1	D	0.95	1/1192 (0.1%)	0.90	7/1611 (0.4%)
1	E	1.12	4/1198 (0.3%)	0.86	4/1619 (0.2%)
1	F	1.02	5/1198 (0.4%)	1.08	10/1619 (0.6%)
1	G	1.16	8/1186 (0.7%)	0.91	4/1603 (0.2%)
1	H	0.93	4/1177 (0.3%)	1.04	7/1589 (0.4%)
1	I	0.98	6/1198 (0.5%)	0.90	2/1619 (0.1%)
1	J	0.86	1/1176 (0.1%)	0.86	2/1591 (0.1%)
1	K	1.05	3/1192 (0.3%)	0.90	3/1611 (0.2%)
1	L	0.73	1/979 (0.1%)	0.84	3/1322 (0.2%)
1	M	0.95	1/1192 (0.1%)	0.94	3/1611 (0.2%)
1	N	0.99	4/1198 (0.3%)	0.85	1/1619 (0.1%)
All	All	0.99	49/16462 (0.3%)	0.93	59/22247 (0.3%)

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	G	0	1
1	H	1	1
1	K	1	0
All	All	2	2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	126	GLU	CB-CG	20.25	1.90	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	45	GLU	CB-CG	-19.65	1.14	1.52
1	K	45	GLU	CA-CB	-18.73	1.12	1.53
1	E	99	GLN	CG-CD	-18.49	1.08	1.51
1	I	3	SER	CA-CB	-18.00	1.25	1.52
1	G	53	ASP	CB-CG	16.38	1.86	1.51
1	H	48	GLN	CG-CD	-15.31	1.15	1.51
1	B	134	LYS	CB-CG	-15.12	1.11	1.52
1	B	136	ASP	CB-CG	-14.98	1.20	1.51
1	E	45	GLU	CB-CG	-14.74	1.24	1.52
1	M	52	LYS	CB-CG	-14.13	1.14	1.52
1	K	65	LYS	CD-CE	13.57	1.85	1.51
1	N	53	ASP	CA-CB	-12.47	1.26	1.53
1	B	53	ASP	CA-CB	-12.34	1.26	1.53
1	F	137	GLU	CA-CB	11.45	1.79	1.53
1	F	3	SER	CA-CB	11.40	1.70	1.52
1	J	134	LYS	CB-CG	-11.37	1.21	1.52
1	A	136	ASP	CB-CG	-11.24	1.28	1.51
1	G	65	LYS	CB-CG	-11.06	1.22	1.52
1	N	123	GLU	CB-CG	-10.30	1.32	1.52
1	C	134	LYS	CB-CG	-10.08	1.25	1.52
1	G	134	LYS	CB-CG	-10.02	1.25	1.52
1	E	126	GLU	CG-CD	9.15	1.65	1.51
1	H	126	GLU	CA-CB	-9.12	1.33	1.53
1	F	53	ASP	CA-CB	8.84	1.73	1.53
1	A	126	GLU	CB-CG	-8.69	1.35	1.52
1	N	45	GLU	CB-CG	8.07	1.67	1.52
1	G	33	LYS	CB-CG	-7.81	1.31	1.52
1	I	2	SER	CA-CB	-7.70	1.41	1.52
1	I	87	ARG	CB-CG	-7.69	1.31	1.52
1	F	57	LYS	CB-CG	7.61	1.73	1.52
1	N	134	LYS	CB-CG	-7.39	1.32	1.52
1	A	134	LYS	CB-CG	-7.29	1.32	1.52
1	I	151	GLU	CB-CG	7.02	1.65	1.52
1	K	53	ASP	CA-CB	6.99	1.69	1.53
1	C	65	LYS	CB-CG	-6.95	1.33	1.52
1	H	127	ARG	CD-NE	-6.62	1.35	1.46
1	L	81	ASN	CA-CB	-6.50	1.36	1.53
1	B	84	LYS	CB-CG	-6.45	1.35	1.52
1	C	97	ASP	CB-CG	-6.05	1.39	1.51
1	H	65	LYS	CG-CD	-5.85	1.32	1.52
1	A	84	LYS	CB-CG	-5.79	1.36	1.52
1	I	142	THR	CB-OG1	-5.53	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	84	LYS	CG-CD	-5.38	1.34	1.52
1	G	84	LYS	CB-CG	5.37	1.67	1.52
1	G	80	LYS	CB-CG	-5.33	1.38	1.52
1	I	84	LYS	CB-CG	-5.31	1.38	1.52
1	E	84	LYS	CG-CD	5.25	1.70	1.52
1	G	45	GLU	CB-CG	-5.01	1.42	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	ASP	CB-CG-OD1	-15.46	104.38	118.30
1	H	127	ARG	CD-NE-CZ	15.32	145.06	123.60
1	A	136	ASP	CB-CG-OD2	15.27	132.04	118.30
1	I	2	SER	N-CA-CB	13.15	130.22	110.50
1	K	45	GLU	N-CA-CB	11.87	131.97	110.60
1	M	136	ASP	CB-CG-OD1	11.22	128.40	118.30
1	F	53	ASP	N-CA-CB	-10.83	91.11	110.60
1	H	126	GLU	CB-CA-C	10.53	131.46	110.40
1	M	136	ASP	CB-CG-OD2	-10.36	108.97	118.30
1	B	136	ASP	CA-CB-CG	10.28	136.01	113.40
1	E	99	GLN	CB-CG-CD	9.79	137.06	111.60
1	F	3	SER	CB-CA-C	-9.77	91.54	110.10
1	G	126	GLU	CA-CB-CG	-9.58	92.32	113.40
1	B	53	ASP	CB-CA-C	9.53	129.45	110.40
1	F	52	LYS	CB-CA-C	9.02	128.45	110.40
1	K	53	ASP	CB-CA-C	-8.29	93.81	110.40
1	H	48	GLN	CB-CG-CD	7.99	132.38	111.60
1	H	126	GLU	CA-CB-CG	7.88	130.75	113.40
1	D	45	GLU	CA-CB-CG	7.75	130.45	113.40
1	L	134	LYS	CB-CA-C	-7.09	96.22	110.40
1	K	65	LYS	CG-CD-CE	-6.99	90.94	111.90
1	J	63	LEU	CA-CB-CG	6.87	131.10	115.30
1	N	53	ASP	N-CA-CB	6.86	122.94	110.60
1	I	147	SER	N-CA-CB	-6.80	100.29	110.50
1	C	97	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	136	ASP	CA-CB-CG	6.64	128.01	113.40
1	L	80	LYS	CB-CA-C	-6.61	97.17	110.40
1	F	52	LYS	CA-CB-CG	6.46	127.61	113.40
1	F	3	SER	N-CA-CB	6.43	120.14	110.50
1	G	65	LYS	CA-CB-CG	6.41	127.49	113.40
1	F	45	GLU	CA-CB-CG	6.39	127.46	113.40
1	B	39	ILE	CB-CA-C	-6.34	98.92	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	H	45	GLU	CA-CB-CG	6.07	126.75	113.40
1	F	137	GLU	N-CA-CB	6.01	121.42	110.60
1	D	45	GLU	CB-CG-CD	5.98	130.34	114.20
1	L	26	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	E	99	GLN	CG-CD-OE1	5.84	133.28	121.60
1	A	82	VAL	CB-CA-C	-5.84	100.31	111.40
1	D	116	CYS	CA-CB-SG	-5.80	103.56	114.00
1	B	5	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	82	VAL	CB-CA-C	-5.72	100.54	111.40
1	D	82	VAL	CB-CA-C	-5.64	100.67	111.40
1	H	48	GLN	CG-CD-OE1	-5.59	110.42	121.60
1	D	126	GLU	CB-CG-CD	5.50	129.05	114.20
1	D	54	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	84	LYS	CA-CB-CG	5.42	125.33	113.40
1	E	99	GLN	CG-CD-NE2	-5.41	103.71	116.70
1	D	84	LYS	CB-CG-CD	5.38	125.58	111.60
1	F	137	GLU	CB-CA-C	-5.37	99.66	110.40
1	C	123	GLU	CA-CB-CG	5.30	125.06	113.40
1	G	53	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	53	ASP	CA-CB-CG	-5.29	101.76	113.40
1	E	82	VAL	CB-CA-C	-5.25	101.42	111.40
1	H	126	GLU	N-CA-CB	5.22	120.00	110.60
1	F	111	VAL	C-N-CA	-5.20	111.39	122.30
1	G	53	ASP	CA-CB-CG	-5.16	102.04	113.40
1	M	82	VAL	CB-CA-C	-5.08	101.74	111.40
1	J	38	LYS	CA-CB-CG	5.02	124.44	113.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	126	GLU	CA
1	K	45	GLU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	61	PRO	Peptide
1	H	56	SER	Peptide

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	1171	0	1156	39	0
1	B	1159	0	1152	21	0
1	C	1156	0	1147	37	0
1	D	1165	0	1152	26	0
1	E	1168	0	1157	23	0
1	F	1168	0	1157	24	0
1	G	1159	0	1147	37	0
1	H	1148	0	1135	29	0
1	I	1168	0	1157	34	0
1	J	1149	0	1141	33	0
1	K	1165	0	1151	32	0
1	L	960	0	955	27	0
1	M	1165	0	1151	25	0
1	N	1171	0	1156	26	0
2	A	23	0	12	3	0
2	B	23	0	12	2	0
2	C	23	0	12	4	0
2	D	23	0	12	1	0
2	E	23	0	12	3	0
2	F	23	0	12	1	0
2	G	23	0	12	2	0
2	H	23	0	12	0	0
2	I	23	0	12	2	0
2	J	23	0	12	2	0
2	K	23	0	12	2	0
2	M	23	0	12	4	0
2	N	23	0	12	2	0
3	A	28	0	0	4	0
3	B	39	0	0	1	0
3	C	30	0	0	4	0
3	D	26	0	0	1	0
3	E	23	0	0	3	0
3	F	30	0	0	1	0
3	G	22	0	0	3	0
3	H	18	0	0	1	0
3	I	16	0	0	1	0
3	J	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	25	0	0	3	0
3	L	10	0	0	1	0
3	M	30	0	0	0	0
3	N	38	0	0	2	0
All	All	16728	0	16070	375	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 12.

All (375) 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:M:90:LEU:HD12	1:M:103:ILE:HD12	1.33	1.08
1:D:2:SER:N	1:D:3:SER:HA	1.65	1.07
1:L:90:LEU:HG	1:L:116:CYS:SG	1.96	1.04
1:J:55:CYS:SG	1:J:55:CYS:O	2.19	1.01
1:C:38:LYS:HD2	3:C:355:HOH:O	1.56	1.01
1:K:29:ARG:HD2	3:K:159:HOH:O	1.62	0.97
1:G:109:VAL:HG22	3:G:277:HOH:O	1.66	0.94
1:B:59:PHE:CZ	2:B:152:AMP:H2'	2.02	0.94
1:K:94:ASN:HD22	1:K:111:VAL:HB	1.31	0.92
1:I:145:SER:HB3	1:J:144:HIS:NE2	1.86	0.91
1:K:94:ASN:ND2	1:K:111:VAL:HB	1.85	0.90
1:M:59:PHE:CZ	2:M:152:AMP:H2'	2.07	0.89
1:I:11:LYS:HD2	3:I:157:HOH:O	1.72	0.89
1:H:53:ASP:HB2	1:H:56:SER:N	1.88	0.88
1:E:59:PHE:CZ	2:E:152:AMP:H2'	2.09	0.88
1:F:90:LEU:HD12	1:F:103:ILE:HD13	1.56	0.88
1:N:38:LYS:HE3	1:N:40:LEU:HD13	1.59	0.85
1:B:35:VAL:HG13	1:B:138:ILE:HG23	1.60	0.84
1:D:35:VAL:HG13	1:D:138:ILE:HG23	1.60	0.83
1:L:26:ARG:HD3	3:L:342:HOH:O	1.77	0.83
1:H:5:ARG:CG	1:H:5:ARG:HH11	1.92	0.82
1:J:59:PHE:CZ	2:J:152:AMP:H2'	2.17	0.80
1:C:40:LEU:HD13	3:C:355:HOH:O	1.82	0.79
1:D:2:SER:N	1:D:3:SER:CA	2.47	0.78
1:A:93:THR:HG21	2:A:152:AMP:H4'	1.66	0.78
1:F:90:LEU:HG	1:F:116[A]:CYS:SG	2.23	0.78
1:M:90:LEU:HD12	1:M:103:ILE:CD1	2.12	0.77
1:J:40:LEU:HD23	1:J:40:LEU:O	1.83	0.77
1:A:90:LEU:HD12	1:A:103:ILE:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:LYS:NZ	1:D:132:TRP:O	2.18	0.76
1:A:59:PHE:CZ	2:A:152:AMP:H2'	2.21	0.76
1:F:35:VAL:HG13	1:F:138:ILE:HG23	1.67	0.75
1:H:5:ARG:HH11	1:H:5:ARG:HG2	1.50	0.74
1:B:90:LEU:HD12	1:B:103:ILE:HD12	1.70	0.72
1:N:35:VAL:HG22	1:N:139:ALA:O	1.90	0.72
1:H:4:GLU:HG2	1:H:83:VAL:HG23	1.71	0.71
1:D:42:PRO:HG2	1:D:68:SER:HA	1.73	0.71
1:E:122:VAL:O	1:E:123:GLU:CB	2.37	0.70
1:G:32:TYR:CD1	1:G:82:VAL:HG13	2.25	0.70
1:N:37:LEU:CD1	1:N:75:MET:HG2	2.21	0.69
1:J:50:HIS:CD2	1:J:132:TRP:HE1	2.09	0.69
1:N:104:ARG:NH2	1:N:116[B]:CYS:O	2.25	0.69
1:J:79:GLY:O	1:J:82:VAL:HG22	1.92	0.69
1:E:90:LEU:HD12	1:E:103:ILE:HD12	1.75	0.68
1:G:87:ARG:HD2	1:G:120:ASP:HA	1.75	0.68
1:D:80:LYS:O	1:D:81:ASN:HB2	1.93	0.68
1:E:90:LEU:HG	1:E:116[A]:CYS:SG	2.33	0.68
1:G:93:THR:HG21	2:G:152:AMP:H4'	1.74	0.68
1:C:48:GLN:HG3	1:C:64:VAL:HG11	1.76	0.67
1:C:35:VAL:HG13	1:C:138:ILE:HG23	1.76	0.67
1:N:54:LEU:HD11	2:N:152:AMP:H5'2	1.77	0.67
1:C:59:PHE:CZ	2:C:152:AMP:H2'	2.30	0.67
1:G:32:TYR:CE1	1:G:82:VAL:HG13	2.29	0.67
1:H:4:GLU:HB3	1:H:82:VAL:CG2	2.25	0.67
1:A:60:PHE:HB3	1:A:61:PRO:HD3	1.76	0.67
1:M:50:HIS:CD2	1:M:132:TRP:HE1	2.13	0.67
1:C:54:LEU:HD11	2:C:152:AMP:H5'1	1.76	0.66
1:H:50:HIS:CD2	1:H:132:TRP:HE1	2.13	0.66
1:F:32:TYR:CD1	1:F:82:VAL:HG13	2.29	0.66
1:M:32:TYR:CD1	1:M:82:VAL:HG13	2.30	0.66
1:K:79:GLY:O	1:K:82:VAL:HG22	1.96	0.64
1:D:43:THR:OG1	1:D:46:GLN:HG3	1.98	0.64
1:C:79:GLY:O	1:C:82:VAL:HG22	1.97	0.64
1:H:4:GLU:HB3	1:H:82:VAL:HG23	1.80	0.64
1:H:50:HIS:O	1:H:51:TYR:HB2	1.96	0.64
1:G:29:ARG:HD2	1:I:106:ASP:O	1.98	0.63
1:G:34:LEU:HD21	1:G:37:LEU:HD13	1.78	0.63
1:D:37:LEU:HD12	1:D:75:MET:HG2	1.81	0.63
1:I:32:TYR:CD1	1:I:82:VAL:HG13	2.34	0.63
1:F:32:TYR:CE1	1:F:82:VAL:HG13	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:LEU:HG	1:I:116[A]:CYS:SG	2.40	0.62
1:K:5:ARG:HD3	3:K:156:HOH:O	2.00	0.62
1:B:134:LYS:N	1:B:137:GLU:OE1	2.28	0.62
1:M:50:HIS:HD2	1:M:132:TRP:HE1	1.44	0.62
1:C:9:ALA:O	1:C:116[B]:CYS:SG	2.56	0.62
1:A:79:GLY:O	1:A:82:VAL:HG22	2.00	0.61
1:D:11:LYS:HB3	1:D:12:PRO:HD2	1.81	0.61
1:D:32:TYR:CD1	1:D:82:VAL:HG13	2.35	0.61
1:K:104:ARG:NH2	1:K:116[B]:CYS:O	2.32	0.61
1:A:90:LEU:CD1	1:A:103:ILE:HD12	2.31	0.60
1:F:79:GLY:O	1:F:82:VAL:HG22	2.00	0.60
1:M:59:PHE:CE2	2:M:152:AMP:H2'	2.37	0.60
1:N:25:ALA:O	1:N:29:ARG:HG2	2.00	0.60
1:E:5:ARG:HD3	1:E:78:GLU:OE2	2.02	0.60
1:J:4:GLU:HG3	1:J:82:VAL:CG2	2.32	0.60
1:J:50:HIS:HD2	1:J:132:TRP:HE1	1.48	0.60
1:H:37:LEU:CD1	1:H:75:MET:HG2	2.31	0.59
1:G:61:PRO:N	1:G:62:ALA:HB3	2.16	0.59
1:K:35:VAL:HG13	1:K:138:ILE:HG23	1.84	0.59
1:G:60:PHE:HB3	1:G:61:PRO:HD3	1.84	0.59
1:K:11:LYS:HB3	1:K:12:PRO:CD	2.32	0.59
1:N:37:LEU:HD12	1:N:75:MET:HG2	1.83	0.59
1:G:90:LEU:O	1:G:104:ARG:HG3	2.02	0.59
1:G:59:PHE:O	1:G:63:LEU:HB2	2.03	0.59
1:D:141:TRP:CG	1:E:71:PRO:HG2	2.39	0.58
1:J:71:PRO:HG2	1:K:141:TRP:CD1	2.38	0.58
1:C:90:LEU:HG	1:C:116[A]:CYS:SG	2.44	0.58
1:C:141:TRP:CG	1:F:71:PRO:HG3	2.38	0.58
1:G:13:ASP:HB3	1:G:66:TYR:OH	2.04	0.58
1:I:117:HIS:ND1	2:I:152:AMP:O1P	2.30	0.58
1:D:11:LYS:HB3	1:D:12:PRO:CD	2.34	0.58
1:N:32:TYR:CD1	1:N:82:VAL:HG13	2.39	0.58
1:K:32:TYR:CD1	1:K:82:VAL:HG13	2.39	0.58
1:G:50:HIS:CD2	1:G:132:TRP:HE1	2.23	0.57
1:G:42:PRO:HG2	1:G:68:SER:HA	1.87	0.57
1:H:53:ASP:O	1:H:56:SER:HB3	2.03	0.57
1:L:90:LEU:HG	1:L:116:CYS:HG	1.70	0.57
1:A:141:TRP:CD1	1:B:71:PRO:HG3	2.39	0.57
1:J:63:LEU:HD12	1:J:64:VAL:N	2.20	0.57
1:J:4:GLU:HG3	1:J:82:VAL:HG23	1.87	0.56
1:M:90:LEU:CD1	1:M:103:ILE:HD12	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:LEU:CG	1:L:116:CYS:SG	2.83	0.56
1:L:121:SER:HB2	1:L:124:SER:H	1.71	0.56
1:M:79:GLY:O	1:M:82:VAL:HG22	2.05	0.56
1:N:59:PHE:CZ	2:N:152:AMP:H2'	2.41	0.56
1:E:37:LEU:HD12	1:E:75:MET:HG2	1.87	0.56
1:I:13:ASP:HB3	1:I:66:TYR:OH	2.05	0.56
1:N:13:ASP:HB3	1:N:66:TYR:OH	2.06	0.56
1:C:32:TYR:CD1	1:C:82:VAL:HG13	2.41	0.55
1:F:25:ALA:O	1:F:29:ARG:HG3	2.06	0.55
1:H:79:GLY:O	1:H:82:VAL:HG22	2.05	0.55
1:D:56:SER:OG	1:N:48:GLN:NE2	2.38	0.55
1:N:29:ARG:HD2	3:N:161:HOH:O	2.05	0.55
1:I:33:LYS:HG3	1:I:141:TRP:CZ2	2.41	0.55
1:A:32:TYR:CD1	1:A:82:VAL:HG13	2.41	0.55
1:D:13:ASP:HB3	1:D:66:TYR:OH	2.07	0.55
1:K:59:PHE:CZ	2:K:152:AMP:H2'	2.42	0.55
1:J:90:LEU:HD23	1:J:103:ILE:HD12	1.89	0.55
1:C:30:LYS:O	1:C:30:LYS:HG3	2.05	0.55
1:F:135:ALA:HA	1:F:138:ILE:HD12	1.89	0.55
1:A:12:PRO:HD3	1:A:72:ILE:HG22	1.89	0.54
1:I:108:ALA:HB2	1:I:115:VAL:CG1	2.37	0.54
1:K:36:ALA:HB3	1:K:76:VAL:HG23	1.88	0.54
1:I:71:PRO:HG3	1:L:141:TRP:CG	2.43	0.54
1:A:108:ALA:HB2	1:A:115:VAL:CG1	2.37	0.54
1:E:12:PRO:HD3	1:E:72:ILE:HG22	1.89	0.54
1:K:54:LEU:HD13	1:K:59:PHE:HE1	1.72	0.54
1:D:4:GLU:OE1	3:D:356:HOH:O	2.18	0.54
1:H:34:LEU:HD21	1:H:37:LEU:HD13	1.90	0.54
1:N:26:ARG:HD3	3:N:157:HOH:O	2.07	0.54
1:J:60:PHE:HB3	1:J:61:PRO:HD3	1.89	0.54
1:A:37:LEU:HG	1:B:37:LEU:HG	1.90	0.54
1:E:54:LEU:CD1	2:E:152:AMP:H5'1	2.39	0.53
1:D:37:LEU:CD1	1:D:75:MET:HG2	2.38	0.53
1:A:35:VAL:CG1	1:A:138:ILE:HG23	2.39	0.53
1:E:90:LEU:HD12	1:E:103:ILE:CD1	2.38	0.53
1:N:80:LYS:O	1:N:81:ASN:HB2	2.08	0.53
1:G:137:GLU:HG2	3:G:257:HOH:O	2.09	0.53
1:H:37:LEU:HD12	1:H:75:MET:HG2	1.90	0.53
1:L:104:ARG:NH2	1:L:116:CYS:O	2.42	0.52
1:E:54:LEU:HD11	2:E:152:AMP:H5'1	1.90	0.52
1:G:61:PRO:CD	1:G:62:ALA:HB3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:50:HIS:O	1:H:51:TYR:HD2	1.92	0.52
1:A:63:LEU:HD13	3:A:188:HOH:O	2.08	0.52
1:J:59:PHE:CE2	2:J:152:AMP:H2'	2.44	0.52
1:K:51:TYR:O	1:K:52:LYS:C	2.48	0.52
1:L:35:VAL:CG1	1:L:138:ILE:HG23	2.39	0.52
1:N:13:ASP:OD1	1:N:13:ASP:N	2.41	0.52
1:M:34:LEU:HD11	1:M:37:LEU:HD22	1.91	0.52
1:I:141:TRP:CG	1:L:71:PRO:HG2	2.46	0.51
1:M:81:ASN:O	1:M:85:SER:HB3	2.10	0.51
1:G:79:GLY:O	1:G:82:VAL:HG22	2.10	0.51
1:L:79:GLY:O	1:L:82:VAL:HG22	2.10	0.51
1:G:35:VAL:HG13	1:G:138:ILE:HG23	1.92	0.51
1:G:100:PRO:HG2	1:K:102:THR:HG22	1.92	0.51
1:A:109:VAL:HG11	1:E:150:TYR:HE1	1.74	0.51
1:D:59:PHE:CZ	2:D:152:AMP:H2'	2.46	0.51
1:L:38:LYS:HG2	1:L:40:LEU:HD22	1.93	0.51
1:B:100:PRO:HG2	1:F:102:THR:HG22	1.93	0.51
1:F:11:LYS:HB3	1:F:12:PRO:CD	2.40	0.51
1:A:51:TYR:CD1	1:A:54:LEU:HD12	2.46	0.51
1:A:35:VAL:HG13	1:A:138:ILE:HG23	1.93	0.50
1:C:141:TRP:CD1	1:F:71:PRO:HG3	2.46	0.50
1:M:90:LEU:O	1:M:104:ARG:HD2	2.11	0.50
1:B:12:PRO:HD3	1:B:72:ILE:HG22	1.93	0.50
1:C:80:LYS:HD3	3:E:253:HOH:O	2.11	0.50
1:D:55:CYS:HA	1:D:60:PHE:CD1	2.47	0.50
1:G:61:PRO:HD2	1:G:62:ALA:HB3	1.92	0.50
1:I:145:SER:HB3	1:J:144:HIS:CD2	2.47	0.50
1:C:76:VAL:HG22	1:C:129:ILE:HG12	1.94	0.50
1:G:12:PRO:HD3	1:G:72:ILE:HG22	1.94	0.50
1:J:32:TYR:CD1	1:J:82:VAL:HG13	2.46	0.50
1:L:37:LEU:HD13	1:L:75:MET:HG2	1.94	0.50
1:J:90:LEU:HD22	1:J:116:CYS:SG	2.52	0.50
1:H:50:HIS:O	1:H:51:TYR:CB	2.60	0.50
1:G:90:LEU:HG	1:G:116:CYS:SG	2.52	0.49
1:A:93:THR:CG2	2:A:152:AMP:H4'	2.40	0.49
1:K:134:LYS:O	1:K:137:GLU:HG2	2.12	0.49
1:D:95:PRO:HA	1:D:98:SER:OG	2.12	0.49
1:L:32:TYR:CD1	1:L:82:VAL:HG13	2.47	0.49
1:J:51:TYR:CD2	1:J:63:LEU:HD13	2.48	0.49
1:G:50:HIS:HD2	1:G:132:TRP:HE1	1.60	0.49
1:M:82:VAL:O	1:M:86:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:90:LEU:HG	1:N:116[A]:CYS:SG	2.53	0.48
1:C:71:PRO:HG2	1:F:141:TRP:CD1	2.48	0.48
1:J:71:PRO:HG2	1:K:141:TRP:CG	2.48	0.48
1:A:95:PRO:HA	1:A:98:SER:HB2	1.96	0.48
1:C:26:ARG:HD3	1:C:29:ARG:HH21	1.79	0.48
1:J:63:LEU:HD12	1:J:64:VAL:H	1.78	0.48
1:J:141:TRP:CG	1:K:71:PRO:HG2	2.48	0.48
1:G:122:VAL:HG23	1:G:123:GLU:N	2.28	0.47
1:M:35:VAL:HG13	1:M:138:ILE:HG23	1.95	0.47
1:B:40:LEU:H	1:B:40:LEU:HD23	1.79	0.47
1:H:50:HIS:O	1:H:51:TYR:CD2	2.67	0.47
1:I:150:TYR:HA	1:K:110:ASP:OD2	2.14	0.47
1:D:79:GLY:O	1:D:82:VAL:HG22	2.14	0.47
1:G:71:PRO:HG3	1:H:141:TRP:CG	2.50	0.47
1:L:85:SER:HA	1:L:88:VAL:HB	1.96	0.47
1:B:66:TYR:CE1	1:B:113:ARG:CZ	2.98	0.47
1:I:35:VAL:HG22	1:I:139:ALA:O	2.14	0.47
1:K:9:ALA:HA	1:K:73:VAL:O	2.14	0.47
1:L:143:SER:C	1:L:145:SER:H	2.16	0.47
1:M:90:LEU:HG	1:M:116[A]:CYS:SG	2.55	0.47
1:A:6:THR:HB	1:A:83:VAL:HG22	1.95	0.47
1:H:60:PHE:N	1:H:61:PRO:HD2	2.30	0.47
1:A:51:TYR:CZ	1:A:63:LEU:HD12	2.50	0.47
1:H:82:VAL:O	1:H:86:GLY:N	2.37	0.47
1:C:6:THR:HB	1:C:83:VAL:HG22	1.95	0.47
1:I:11:LYS:HB3	1:I:12:PRO:HD2	1.97	0.47
1:D:71:PRO:HG3	1:E:141:TRP:CD1	2.50	0.46
1:G:44:THR:O	1:G:47:ALA:HB3	2.14	0.46
1:A:71:PRO:HG3	1:B:141:TRP:CD1	2.50	0.46
1:B:90:LEU:HG	1:B:116[A]:CYS:SG	2.55	0.46
1:C:135:ALA:O	1:C:136:ASP:C	2.54	0.46
1:D:32:TYR:HD1	1:D:79:GLY:HA3	1.80	0.46
1:G:119:SER:HB3	1:G:128:GLU:OE1	2.15	0.46
1:A:5:ARG:HD3	3:A:180:HOH:O	2.15	0.46
1:H:33:LYS:HG3	1:H:141:TRP:CZ2	2.50	0.46
1:J:143:SER:O	1:J:145:SER:N	2.48	0.46
1:F:59:PHE:CZ	2:F:152:AMP:H2'	2.51	0.46
1:A:109:VAL:HG11	1:E:150:TYR:CE1	2.49	0.46
1:A:37:LEU:HB2	1:B:39:ILE:CD1	2.46	0.46
1:I:98:SER:OG	1:I:104:ARG:HB2	2.15	0.46
1:J:141:TRP:CD2	1:K:71:PRO:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:VAL:HG12	1:D:76:VAL:HB	1.98	0.45
1:I:52:LYS:HB3	1:I:52:LYS:HE2	1.78	0.45
1:J:90:LEU:HD23	1:J:103:ILE:CD1	2.46	0.45
1:K:87:ARG:CZ	1:K:120:ASP:HB3	2.46	0.45
1:A:141:TRP:CG	1:B:71:PRO:HG3	2.51	0.45
1:F:11:LYS:HB3	1:F:12:PRO:HD2	1.98	0.45
1:E:134:LYS:O	1:E:137:GLU:HB2	2.16	0.45
1:G:109:VAL:CG2	3:G:277:HOH:O	2.40	0.45
1:K:90:LEU:HG	1:K:116[A]:CYS:SG	2.56	0.45
1:I:37:LEU:HD12	1:I:75:MET:HG2	1.99	0.45
1:B:102:THR:HG22	1:D:100:PRO:HG2	1.99	0.45
1:I:93:THR:HG21	2:I:152:AMP:H4'	1.99	0.45
1:J:5:ARG:NH2	1:J:138:ILE:HG21	2.32	0.45
1:C:51:TYR:O	1:C:52:LYS:C	2.56	0.45
1:G:42:PRO:HG2	1:G:67:PHE:O	2.17	0.45
1:K:86:GLY:O	1:K:90:LEU:HD13	2.16	0.45
1:M:93:THR:HG21	2:M:152:AMP:H4'	1.99	0.45
1:B:111:VAL:CG2	2:B:152:AMP:H1'	2.47	0.44
1:L:2:SER:HB3	1:L:80:LYS:HA	1.99	0.44
1:H:84:LYS:O	1:H:88:VAL:HG23	2.17	0.44
1:G:59:PHE:CD1	1:G:63:LEU:HD12	2.53	0.44
1:H:51:TYR:H	1:H:52:LYS:NZ	2.16	0.44
1:C:47:ALA:HB3	1:C:64:VAL:HG13	1.99	0.44
1:G:139:ALA:O	1:G:141:TRP:HD1	2.00	0.44
1:K:26:ARG:HD3	3:K:254:HOH:O	2.17	0.44
1:G:59:PHE:CZ	2:G:152:AMP:H2'	2.53	0.44
1:M:76:VAL:HG22	1:M:129:ILE:HG12	2.00	0.44
1:I:71:PRO:HG3	1:L:141:TRP:CD2	2.52	0.44
1:A:6:THR:OG1	1:A:119:SER:HB2	2.18	0.44
1:I:10:VAL:HG23	1:I:75:MET:CE	2.47	0.44
1:L:83:VAL:HG21	1:L:122:VAL:HA	1.99	0.44
1:K:52:LYS:HG3	1:K:53:ASP:N	2.33	0.43
1:A:90:LEU:HG	1:A:116[A]:CYS:SG	2.58	0.43
1:C:16:GLN:HB3	1:F:144:HIS:HD1	1.83	0.43
1:G:59:PHE:HD1	1:G:63:LEU:HD12	1.83	0.43
1:H:11:LYS:NZ	3:H:261:HOH:O	2.51	0.43
1:M:71:PRO:HG2	1:N:141:TRP:CD1	2.54	0.43
1:H:11:LYS:HB3	1:H:12:PRO:CD	2.48	0.43
1:J:40:LEU:HD23	1:J:40:LEU:C	2.37	0.43
1:N:11:LYS:HB3	1:N:12:PRO:CD	2.48	0.43
1:A:36:ALA:HB1	1:A:133:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:LYS:HE2	1:J:132:TRP:O	2.18	0.43
1:C:49:GLY:O	1:C:127:ARG:NH2	2.50	0.43
1:F:89:LEU:O	1:F:103:ILE:HD12	2.18	0.43
1:G:93:THR:HA	1:G:104:ARG:NH1	2.33	0.43
1:I:7:PHE:CZ	1:I:9:ALA:HB2	2.54	0.43
1:I:32:TYR:CD1	1:I:82:VAL:CG1	3.02	0.43
1:L:83:VAL:HG13	1:L:119:SER:O	2.18	0.43
1:M:54:LEU:CD1	2:M:152:AMP:H5'1	2.48	0.43
1:N:95:PRO:O	1:N:96:ALA:C	2.57	0.43
1:H:134:LYS:HB3	1:H:135:ALA:H	1.55	0.43
1:A:87:ARG:HB3	3:A:225:HOH:O	2.19	0.42
1:C:22:GLU:HG2	1:C:107:PHE:CZ	2.53	0.42
1:G:51:TYR:O	1:G:60:PHE:HE2	2.02	0.42
1:K:54:LEU:HD13	1:K:59:PHE:CE1	2.51	0.42
1:B:70:GLY:HA3	3:B:266:HOH:O	2.19	0.42
1:N:32:TYR:CD1	1:N:82:VAL:CG1	3.01	0.42
1:D:141:TRP:CD2	1:E:71:PRO:HG2	2.53	0.42
1:L:32:TYR:CE1	1:L:82:VAL:HG13	2.54	0.42
1:M:71:PRO:HG2	1:N:141:TRP:CG	2.54	0.42
1:B:34:LEU:HD11	1:B:37:LEU:HD22	2.02	0.42
1:F:4:GLU:HG2	1:F:82:VAL:HG23	2.01	0.42
1:F:9:ALA:HA	1:F:73:VAL:O	2.19	0.42
1:I:3:SER:O	1:I:4:GLU:C	2.58	0.42
1:I:26:ARG:HG2	1:I:29:ARG:HH21	1.85	0.42
1:I:35:VAL:HG12	1:I:76:VAL:HB	2.02	0.42
1:A:63:LEU:HD22	3:A:201:HOH:O	2.20	0.42
1:A:90:LEU:HD12	1:A:103:ILE:CD1	2.45	0.42
1:A:144:HIS:CD2	1:F:144:HIS:CD2	3.08	0.42
1:C:23:ILE:HG12	1:C:103:ILE:HG12	2.01	0.42
1:E:29:ARG:HE	1:E:29:ARG:HB3	1.05	0.42
1:F:26:ARG:HD3	3:F:159:HOH:O	2.18	0.42
1:L:10:VAL:HB	1:L:73:VAL:HB	2.02	0.42
1:L:117:HIS:CG	1:L:118:GLY:N	2.87	0.42
1:M:43:THR:OG1	1:M:46:GLN:HG3	2.20	0.42
1:E:19:LEU:O	1:E:23:ILE:HD12	2.20	0.42
1:J:5:ARG:NH1	1:J:78:GLU:OE2	2.51	0.42
1:L:12:PRO:HG3	1:L:72:ILE:HG22	2.02	0.42
1:C:32:TYR:HH	1:C:85:SER:HG	1.68	0.42
1:M:32:TYR:CE1	1:M:82:VAL:HG13	2.54	0.42
1:I:30:LYS:O	1:I:30:LYS:HG3	2.20	0.42
1:E:32:TYR:CD1	1:E:82:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ARG:HD3	1:F:114:ASN:HB2	2.02	0.42
1:D:32:TYR:CD1	1:D:79:GLY:HA3	2.55	0.41
1:N:13:ASP:O	1:N:17:ARG:HG3	2.20	0.41
1:J:32:TYR:CE1	1:J:82:VAL:HG13	2.54	0.41
1:L:11:LYS:HE2	1:L:117:HIS:HB2	2.01	0.41
1:I:34:LEU:HD21	1:I:37:LEU:HD13	2.01	0.41
1:K:37:LEU:O	1:K:38:LYS:HB3	2.21	0.41
1:E:35:VAL:HG12	1:E:76:VAL:O	2.20	0.41
1:M:28:GLU:OE2	1:N:18:GLY:HA2	2.19	0.41
1:E:13:ASP:N	1:E:13:ASP:OD1	2.54	0.41
1:I:37:LEU:HG	1:L:37:LEU:HG	2.01	0.41
1:I:93:THR:O	1:I:95:PRO:HD3	2.20	0.41
1:M:36:ALA:O	1:M:75:MET:HA	2.20	0.41
1:M:134:LYS:O	1:M:137:GLU:HB2	2.20	0.41
1:H:52:LYS:HA	1:H:52:LYS:HD3	1.89	0.41
1:A:51:TYR:HD1	1:A:54:LEU:HD12	1.85	0.41
1:C:90:LEU:HD12	1:C:103:ILE:HD13	2.01	0.41
1:E:26:ARG:HD3	3:E:154:HOH:O	2.21	0.41
1:B:80:LYS:O	1:B:81:ASN:CB	2.69	0.41
1:C:37:LEU:O	1:C:38:LYS:HB3	2.21	0.41
1:I:36:ALA:O	1:I:75:MET:HA	2.21	0.41
1:A:34:LEU:HD11	1:A:37:LEU:HD22	2.03	0.41
1:C:4:GLU:N	3:C:221:HOH:O	2.54	0.41
1:I:71:PRO:HG3	1:L:141:TRP:CD1	2.55	0.41
1:J:95:PRO:HB2	1:J:109:VAL:O	2.21	0.41
1:L:102:THR:O	1:L:103:ILE:C	2.58	0.41
1:A:37:LEU:HB2	1:B:39:ILE:HD13	2.02	0.41
1:A:81:ASN:O	1:A:82:VAL:C	2.59	0.41
1:B:13:ASP:HB3	1:B:66:TYR:OH	2.21	0.41
1:C:4:GLU:HG2	1:C:82:VAL:HG23	2.03	0.41
1:C:37:LEU:HG	1:F:37:LEU:HG	2.02	0.41
1:C:117:HIS:ND1	2:C:152:AMP:O1P	2.50	0.41
1:H:34:LEU:HD11	1:H:37:LEU:HD22	2.03	0.41
1:K:54:LEU:HD11	2:K:152:AMP:H5'2	2.03	0.41
1:C:38:LYS:CE	3:C:355:HOH:O	2.65	0.40
1:F:39:ILE:O	1:F:39:ILE:HG23	2.21	0.40
1:K:134:LYS:C	1:K:136:ASP:N	2.74	0.40
1:E:11:LYS:HD2	3:E:316:HOH:O	2.21	0.40
1:K:11:LYS:HB3	1:K:12:PRO:HD2	2.03	0.40
1:N:51:TYR:O	1:N:60:PHE:HE1	2.04	0.40
1:A:55:CYS:HA	1:A:60:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:PHE:HB3	1:C:61:PRO:CD	2.52	0.40
1:J:6:THR:O	1:J:76:VAL:HA	2.21	0.40
1:J:36:ALA:O	1:J:75:MET:HA	2.22	0.40
1:N:11:LYS:HE3	1:N:116[A]:CYS:O	2.22	0.40
1:N:40:LEU:HD23	1:N:40:LEU:O	2.21	0.40
1:C:7:PHE:CE1	1:C:74:CYS:HB3	2.57	0.40
1:G:9:ALA:O	1:G:116:CYS:HA	2.22	0.40
1:H:9:ALA:HA	1:H:73:VAL:O	2.20	0.40
1:I:36:ALA:HB1	1:I:133:PHE:CE1	2.57	0.40
1:I:51:TYR:O	1:I:52:LYS:C	2.60	0.40
1:J:11:LYS:HB3	1:J:12:PRO:CD	2.52	0.40
1:A:51:TYR:CE2	1:A:63:LEU:HD12	2.56	0.40
1:A:104:ARG:HH11	1:A:104:ARG:HD2	1.74	0.40
1:C:11:LYS:NZ	2:C:152:AMP:O3P	2.54	0.40
1:G:47:ALA:HB3	1:G:64:VAL:HG13	2.03	0.40
1:K:13:ASP:OD1	1:K:13:ASP:N	2.52	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 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	149/151 (99%)	144 (97%)	4 (3%)	1 (1%)	22 41
1	B	148/151 (98%)	137 (93%)	8 (5%)	3 (2%)	7 13
1	C	147/151 (97%)	135 (92%)	10 (7%)	2 (1%)	11 21
1	D	148/151 (98%)	137 (93%)	11 (7%)	0	100 100
1	E	149/151 (99%)	142 (95%)	6 (4%)	1 (1%)	22 41
1	F	149/151 (99%)	134 (90%)	12 (8%)	3 (2%)	7 13
1	G	147/151 (97%)	135 (92%)	10 (7%)	2 (1%)	11 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	144/151 (95%)	127 (88%)	12 (8%)	5 (4%)	3	5
1	I	149/151 (99%)	141 (95%)	6 (4%)	2 (1%)	12	23
1	J	146/151 (97%)	140 (96%)	2 (1%)	4 (3%)	5	8
1	K	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
1	L	121/151 (80%)	109 (90%)	7 (6%)	5 (4%)	3	3
1	M	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
1	N	149/151 (99%)	143 (96%)	5 (3%)	1 (1%)	22	41
All	All	2042/2114 (97%)	1908 (93%)	105 (5%)	29 (1%)	11	21

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	123	GLU
1	F	3	SER
1	F	137	GLU
1	H	4	GLU
1	H	51	TYR
1	J	115	VAL
1	L	122	VAL
1	G	115	VAL
1	H	115	VAL
1	H	134	LYS
1	I	52	LYS
1	J	56	SER
1	J	144	HIS
1	N	115	VAL
1	B	144	HIS
1	C	136	ASP
1	L	135	ALA
1	A	115	VAL
1	B	115	VAL
1	G	63	LEU
1	J	52	LYS
1	L	81	ASN
1	H	57	LYS
1	I	115	VAL
1	L	144	HIS
1	B	81	ASN
1	F	115	VAL
1	C	35	VAL

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Mol	Chain	Res	Type
1	L	115	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	126/126 (100%)	114 (90%)	12 (10%)	8 15
1	B	125/126 (99%)	110 (88%)	15 (12%)	5 9
1	C	124/126 (98%)	111 (90%)	13 (10%)	7 12
1	D	125/126 (99%)	116 (93%)	9 (7%)	14 27
1	E	126/126 (100%)	116 (92%)	10 (8%)	12 23
1	F	126/126 (100%)	112 (89%)	14 (11%)	6 10
1	G	124/126 (98%)	111 (90%)	13 (10%)	7 12
1	H	123/126 (98%)	105 (85%)	18 (15%)	3 5
1	I	126/126 (100%)	110 (87%)	16 (13%)	4 7
1	J	123/126 (98%)	108 (88%)	15 (12%)	5 8
1	K	125/126 (99%)	118 (94%)	7 (6%)	21 40
1	L	103/126 (82%)	88 (85%)	15 (15%)	3 5
1	M	125/126 (99%)	112 (90%)	13 (10%)	7 12
1	N	126/126 (100%)	112 (89%)	14 (11%)	6 10
All	All	1727/1764 (98%)	1543 (89%)	184 (11%)	6 11

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	35	VAL
1	A	44	THR
1	A	63	LEU
1	A	82	VAL
1	A	84	LYS

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Mol	Chain	Res	Type
1	A	90	LEU
1	A	98	SER
1	A	115	VAL
1	A	122	VAL
1	A	126	GLU
1	A	147	SER
1	B	5	ARG
1	B	29	ARG
1	B	34	LEU
1	B	35	VAL
1	B	38	LYS
1	B	39	ILE
1	B	40	LEU
1	B	52	LYS
1	B	55[A]	CYS
1	B	55[B]	CYS
1	B	56	SER
1	B	82	VAL
1	B	84	LYS
1	B	136	ASP
1	B	140	SER
1	C	34	LEU
1	C	35	VAL
1	C	65	LYS
1	C	80	LYS
1	C	82	VAL
1	C	85	SER
1	C	90	LEU
1	C	103	ILE
1	C	122	VAL
1	C	124	SER
1	C	134	LYS
1	C	146	VAL
1	C	151	GLU
1	D	2	SER
1	D	34	LEU
1	D	35	VAL
1	D	82	VAL
1	D	120	ASP
1	D	122	VAL
1	D	124	SER
1	D	147	SER

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Mol	Chain	Res	Type
1	D	151	GLU
1	E	29	ARG
1	E	34	LEU
1	E	44	THR
1	E	45	GLU
1	E	82	VAL
1	E	90	LEU
1	E	122	VAL
1	E	136	ASP
1	E	147	SER
1	E	149	ILE
1	F	3	SER
1	F	34	LEU
1	F	44	THR
1	F	52	LYS
1	F	53	ASP
1	F	54	LEU
1	F	82	VAL
1	F	85	SER
1	F	87	ARG
1	F	90	LEU
1	F	98	SER
1	F	136	ASP
1	F	142	THR
1	F	146	VAL
1	G	3	SER
1	G	29	ARG
1	G	34	LEU
1	G	40	LEU
1	G	52	LYS
1	G	53	ASP
1	G	63	LEU
1	G	82	VAL
1	G	84	LYS
1	G	115	VAL
1	G	119	SER
1	G	136	ASP
1	G	147	SER
1	H	4	GLU
1	H	5	ARG
1	H	34	LEU
1	H	35	VAL

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Mol	Chain	Res	Type
1	H	44	THR
1	H	45	GLU
1	H	52	LYS
1	H	65	LYS
1	H	75	MET
1	H	82	VAL
1	H	84	LYS
1	H	87	ARG
1	H	110	ASP
1	H	115	VAL
1	H	124	SER
1	H	126	GLU
1	H	134	LYS
1	H	140	SER
1	I	30	LYS
1	I	34	LEU
1	I	35	VAL
1	I	40	LEU
1	I	44	THR
1	I	56	SER
1	I	82	VAL
1	I	84	LYS
1	I	85	SER
1	I	87	ARG
1	I	115	VAL
1	I	122	VAL
1	I	134	LYS
1	I	136	ASP
1	I	138	ILE
1	I	145	SER
1	J	3	SER
1	J	34	LEU
1	J	38	LYS
1	J	40	LEU
1	J	55	CYS
1	J	63	LEU
1	J	82	VAL
1	J	84	LYS
1	J	115	VAL
1	J	122	VAL
1	J	124	SER
1	J	136	ASP

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Mol	Chain	Res	Type
1	J	140	SER
1	J	143	SER
1	J	147	SER
1	K	34	LEU
1	K	35	VAL
1	K	56	SER
1	K	82	VAL
1	K	84	LYS
1	K	127	ARG
1	K	147	SER
1	L	33	LYS
1	L	34	LEU
1	L	41	GLN
1	L	82	VAL
1	L	85	SER
1	L	87	ARG
1	L	93	THR
1	L	97	ASP
1	L	115	VAL
1	L	120	ASP
1	L	123	GLU
1	L	127	ARG
1	L	134	LYS
1	L	142	THR
1	L	146	VAL
1	M	11	LYS
1	M	34	LEU
1	M	35	VAL
1	M	38	LYS
1	M	40	LEU
1	M	44	THR
1	M	52	LYS
1	M	82	VAL
1	M	84	LYS
1	M	90	LEU
1	M	122	VAL
1	M	127	ARG
1	M	147	SER
1	N	34	LEU
1	N	35	VAL
1	N	40	LEU
1	N	45	GLU

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Mol	Chain	Res	Type
1	N	53	ASP
1	N	54	LEU
1	N	82	VAL
1	N	90	LEU
1	N	110	ASP
1	N	115	VAL
1	N	122	VAL
1	N	123	GLU
1	N	136	ASP
1	N	138	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	D	48	GLN
1	E	41	GLN
1	F	81	ASN
1	G	50	HIS
1	H	50	HIS
1	I	41	GLN
1	J	50	HIS
1	K	81	ASN
1	K	94	ASN
1	L	41	GLN
1	M	50	HIS
1	N	48	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AMP	C	152	-	22,25,25	1.27	2 (9%)	25,38,38	1.33	4 (16%)
2	AMP	B	152	-	22,25,25	1.21	3 (13%)	25,38,38	1.25	4 (16%)
2	AMP	F	152	-	22,25,25	1.28	3 (13%)	25,38,38	1.44	5 (20%)
2	AMP	D	152	-	22,25,25	1.26	2 (9%)	25,38,38	1.43	3 (12%)
2	AMP	G	152	-	22,25,25	1.17	2 (9%)	25,38,38	1.72	8 (32%)
2	AMP	K	152	-	22,25,25	1.12	2 (9%)	25,38,38	1.48	3 (12%)
2	AMP	A	152	-	22,25,25	1.40	3 (13%)	25,38,38	1.51	3 (12%)
2	AMP	N	152	-	22,25,25	1.04	1 (4%)	25,38,38	1.40	3 (12%)
2	AMP	J	152	-	22,25,25	1.32	2 (9%)	25,38,38	1.46	2 (8%)
2	AMP	E	152	-	22,25,25	1.25	3 (13%)	25,38,38	1.58	6 (24%)
2	AMP	H	152	-	22,25,25	1.15	2 (9%)	25,38,38	1.41	4 (16%)
2	AMP	I	152	-	22,25,25	1.19	2 (9%)	25,38,38	1.32	3 (12%)
2	AMP	M	152	-	22,25,25	1.30	3 (13%)	25,38,38	1.50	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
2	AMP	C	152	-	-	6/6/26/26	0/3/3/3
2	AMP	B	152	-	-	5/6/26/26	0/3/3/3
2	AMP	F	152	-	-	5/6/26/26	0/3/3/3
2	AMP	D	152	-	-	4/6/26/26	0/3/3/3
2	AMP	G	152	-	-	6/6/26/26	0/3/3/3
2	AMP	K	152	-	-	6/6/26/26	0/3/3/3
2	AMP	A	152	-	-	3/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	N	152	-	-	6/6/26/26	0/3/3/3
2	AMP	J	152	-	-	6/6/26/26	0/3/3/3
2	AMP	E	152	-	-	5/6/26/26	0/3/3/3
2	AMP	H	152	-	-	5/6/26/26	0/3/3/3
2	AMP	I	152	-	-	3/6/26/26	0/3/3/3
2	AMP	M	152	-	-	3/6/26/26	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	152	AMP	C2-N3	3.27	1.37	1.32
2	A	152	AMP	C5-C4	3.26	1.49	1.40
2	C	152	AMP	C2-N3	3.16	1.37	1.32
2	E	152	AMP	C5-C4	3.12	1.49	1.40
2	J	152	AMP	C5-C4	3.10	1.49	1.40
2	F	152	AMP	C5-C4	3.05	1.49	1.40
2	B	152	AMP	C5-C4	2.99	1.48	1.40
2	I	152	AMP	C5-C4	2.93	1.48	1.40
2	H	152	AMP	C5-C4	2.91	1.48	1.40
2	C	152	AMP	C5-C4	2.84	1.48	1.40
2	D	152	AMP	C5-C4	2.83	1.48	1.40
2	G	152	AMP	C5-C4	2.82	1.48	1.40
2	F	152	AMP	C2-N3	2.82	1.36	1.32
2	D	152	AMP	C2-N3	2.82	1.36	1.32
2	M	152	AMP	C5-C4	2.76	1.48	1.40
2	J	152	AMP	C2-N3	2.72	1.36	1.32
2	M	152	AMP	C2-N3	2.72	1.36	1.32
2	I	152	AMP	C2-N3	2.72	1.36	1.32
2	N	152	AMP	C5-C4	2.72	1.48	1.40
2	E	152	AMP	C2-N3	2.64	1.36	1.32
2	B	152	AMP	C2-N3	2.58	1.36	1.32
2	K	152	AMP	C5-C4	2.48	1.47	1.40
2	H	152	AMP	C2-N3	2.45	1.36	1.32
2	M	152	AMP	C2'-C1'	-2.23	1.50	1.53
2	F	152	AMP	O4'-C1'	2.21	1.44	1.41
2	A	152	AMP	C6-C5	2.17	1.51	1.43
2	B	152	AMP	O4'-C1'	2.12	1.44	1.41
2	K	152	AMP	C2-N3	2.11	1.35	1.32
2	E	152	AMP	O4'-C1'	2.07	1.44	1.41
2	G	152	AMP	O4'-C1'	2.02	1.43	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	152	AMP	N3-C2-N1	-4.03	122.37	128.68
2	A	152	AMP	C4-C5-N7	-3.94	105.29	109.40
2	E	152	AMP	N3-C2-N1	-3.90	122.58	128.68
2	G	152	AMP	C4-C5-N7	-3.72	105.53	109.40
2	J	152	AMP	C4-C5-N7	-3.66	105.58	109.40
2	D	152	AMP	C4-C5-N7	-3.49	105.77	109.40
2	M	152	AMP	P-O5'-C5'	3.45	127.78	118.30
2	G	152	AMP	N3-C2-N1	-3.39	123.38	128.68
2	D	152	AMP	N3-C2-N1	-3.37	123.41	128.68
2	N	152	AMP	C4-C5-N7	-3.33	105.93	109.40
2	H	152	AMP	C4-C5-N7	-3.29	105.97	109.40
2	K	152	AMP	P-O5'-C5'	3.23	127.20	118.30
2	J	152	AMP	N3-C2-N1	-3.12	123.80	128.68
2	F	152	AMP	N3-C2-N1	-3.03	123.94	128.68
2	I	152	AMP	P-O5'-C5'	3.00	126.55	118.30
2	N	152	AMP	N3-C2-N1	-2.99	124.00	128.68
2	H	152	AMP	N3-C2-N1	-2.98	124.02	128.68
2	F	152	AMP	O3P-P-O5'	-2.98	98.81	106.73
2	F	152	AMP	C4-C5-N7	-2.92	106.36	109.40
2	I	152	AMP	C4-C5-N7	-2.85	106.43	109.40
2	G	152	AMP	O3P-P-O5'	-2.84	99.17	106.73
2	B	152	AMP	C4-C5-N7	-2.74	106.54	109.40
2	H	152	AMP	C3'-C2'-C1'	2.65	104.97	100.98
2	B	152	AMP	P-O5'-C5'	2.64	125.58	118.30
2	E	152	AMP	O3P-P-O5'	-2.63	99.73	106.73
2	D	152	AMP	O5'-P-O1P	-2.59	99.20	106.47
2	G	152	AMP	C3'-C2'-C1'	2.56	104.84	100.98
2	E	152	AMP	O3P-P-O2P	2.54	117.36	107.64
2	A	152	AMP	O3P-P-O2P	2.50	117.19	107.64
2	E	152	AMP	C2-N1-C6	2.48	122.99	118.75
2	C	152	AMP	N3-C2-N1	-2.45	124.86	128.68
2	C	152	AMP	C1'-N9-C4	2.42	130.89	126.64
2	C	152	AMP	C4-C5-N7	-2.37	106.93	109.40
2	F	152	AMP	P-O5'-C5'	2.36	124.81	118.30
2	K	152	AMP	C2-N1-C6	2.32	122.72	118.75
2	M	152	AMP	O3'-C3'-C4'	2.28	117.65	111.05
2	I	152	AMP	N3-C2-N1	-2.28	125.12	128.68
2	G	152	AMP	P-O5'-C5'	2.26	124.53	118.30
2	C	152	AMP	N6-C6-N1	2.26	123.27	118.57
2	E	152	AMP	N6-C6-N1	2.24	123.22	118.57
2	B	152	AMP	N3-C2-N1	-2.22	125.21	128.68
2	F	152	AMP	C3'-C2'-C1'	2.19	104.27	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	152	AMP	O4'-C4'-C5'	2.18	116.54	109.37
2	G	152	AMP	O5'-C5'-C4'	2.16	116.43	108.99
2	G	152	AMP	C5-C6-N6	2.16	123.63	120.35
2	A	152	AMP	O2P-P-O5'	-2.11	101.12	106.73
2	E	152	AMP	C2'-C3'-C4'	2.08	106.69	102.64
2	H	152	AMP	P-O5'-C5'	2.06	123.97	118.30
2	G	152	AMP	C2-N1-C6	2.05	122.26	118.75
2	M	152	AMP	C4-C5-N7	-2.04	107.27	109.40
2	M	152	AMP	N6-C6-N1	2.03	122.79	118.57
2	N	152	AMP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	152	AMP	O4'-C4'-C5'-O5'
2	A	152	AMP	C3'-C4'-C5'-O5'
2	B	152	AMP	C5'-O5'-P-O1P
2	B	152	AMP	C5'-O5'-P-O2P
2	B	152	AMP	C5'-O5'-P-O3P
2	C	152	AMP	C5'-O5'-P-O2P
2	C	152	AMP	C5'-O5'-P-O3P
2	C	152	AMP	O4'-C4'-C5'-O5'
2	C	152	AMP	C3'-C4'-C5'-O5'
2	D	152	AMP	C3'-C4'-C5'-O5'
2	E	152	AMP	C5'-O5'-P-O2P
2	E	152	AMP	C5'-O5'-P-O3P
2	E	152	AMP	C3'-C4'-C5'-O5'
2	F	152	AMP	C5'-O5'-P-O2P
2	F	152	AMP	C5'-O5'-P-O3P
2	F	152	AMP	O4'-C4'-C5'-O5'
2	F	152	AMP	C3'-C4'-C5'-O5'
2	G	152	AMP	C5'-O5'-P-O2P
2	G	152	AMP	C5'-O5'-P-O3P
2	G	152	AMP	O4'-C4'-C5'-O5'
2	G	152	AMP	C3'-C4'-C5'-O5'
2	H	152	AMP	C5'-O5'-P-O1P
2	H	152	AMP	C5'-O5'-P-O2P
2	H	152	AMP	C5'-O5'-P-O3P
2	I	152	AMP	O4'-C4'-C5'-O5'
2	I	152	AMP	C3'-C4'-C5'-O5'
2	J	152	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	J	152	AMP	C5'-O5'-P-O2P
2	J	152	AMP	C5'-O5'-P-O3P
2	J	152	AMP	C3'-C4'-C5'-O5'
2	K	152	AMP	C5'-O5'-P-O2P
2	K	152	AMP	C5'-O5'-P-O3P
2	M	152	AMP	C3'-C4'-C5'-O5'
2	N	152	AMP	C5'-O5'-P-O1P
2	N	152	AMP	C5'-O5'-P-O2P
2	N	152	AMP	C5'-O5'-P-O3P
2	D	152	AMP	O4'-C4'-C5'-O5'
2	E	152	AMP	O4'-C4'-C5'-O5'
2	K	152	AMP	O4'-C4'-C5'-O5'
2	M	152	AMP	C4'-C5'-O5'-P
2	J	152	AMP	O4'-C4'-C5'-O5'
2	M	152	AMP	O4'-C4'-C5'-O5'
2	N	152	AMP	C4'-C5'-O5'-P
2	K	152	AMP	C3'-C4'-C5'-O5'
2	N	152	AMP	O4'-C4'-C5'-O5'
2	E	152	AMP	C4'-C5'-O5'-P
2	K	152	AMP	C4'-C5'-O5'-P
2	N	152	AMP	C3'-C4'-C5'-O5'
2	C	152	AMP	C5'-O5'-P-O1P
2	G	152	AMP	C5'-O5'-P-O1P
2	K	152	AMP	C5'-O5'-P-O1P
2	C	152	AMP	C4'-C5'-O5'-P
2	I	152	AMP	C4'-C5'-O5'-P
2	A	152	AMP	C4'-C5'-O5'-P
2	D	152	AMP	C4'-C5'-O5'-P
2	H	152	AMP	C4'-C5'-O5'-P
2	G	152	AMP	C4'-C5'-O5'-P
2	B	152	AMP	C4'-C5'-O5'-P
2	F	152	AMP	C4'-C5'-O5'-P
2	J	152	AMP	C4'-C5'-O5'-P
2	D	152	AMP	C5'-O5'-P-O2P
2	B	152	AMP	O4'-C4'-C5'-O5'
2	H	152	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	152	AMP	4	0

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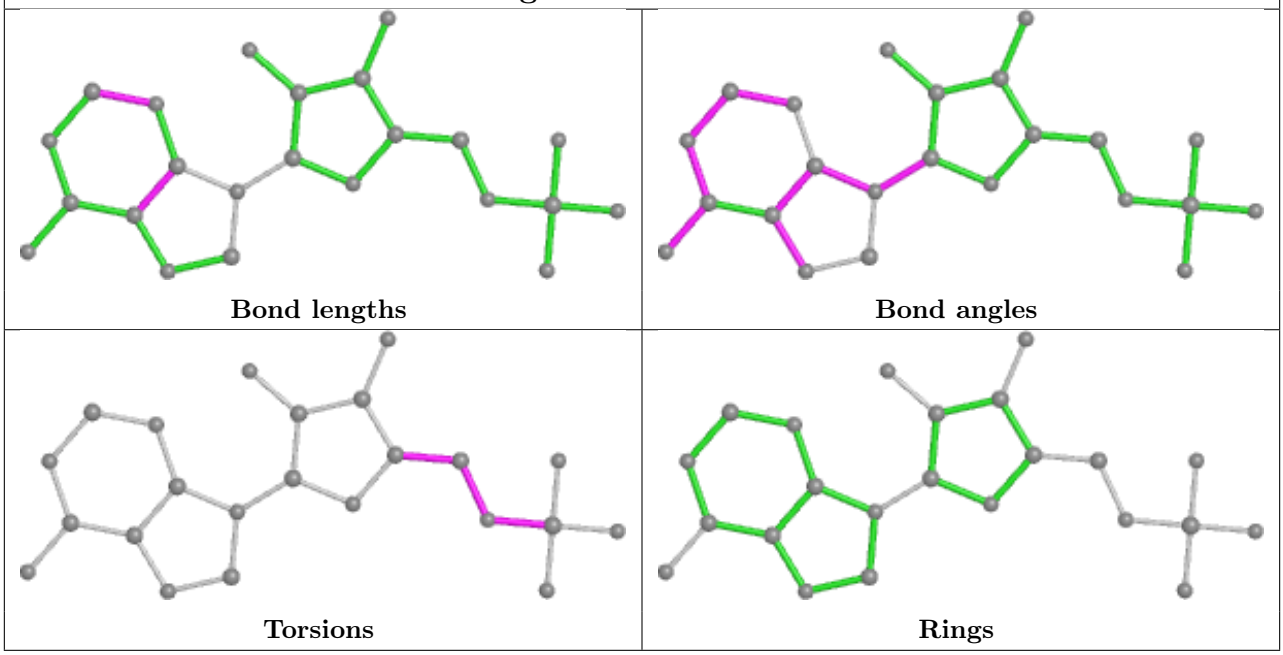
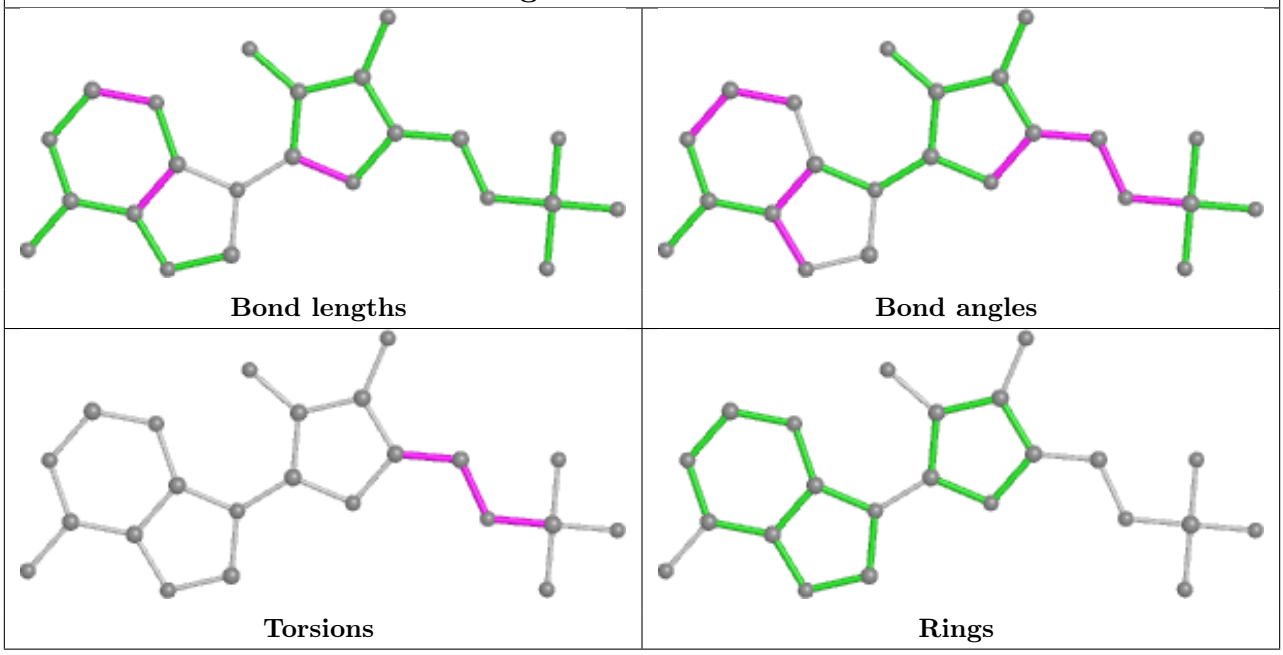
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	152	AMP	2	0
2	F	152	AMP	1	0
2	D	152	AMP	1	0
2	G	152	AMP	2	0
2	K	152	AMP	2	0
2	A	152	AMP	3	0
2	N	152	AMP	2	0
2	J	152	AMP	2	0
2	E	152	AMP	3	0
2	I	152	AMP	2	0
2	M	152	AMP	4	0

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.

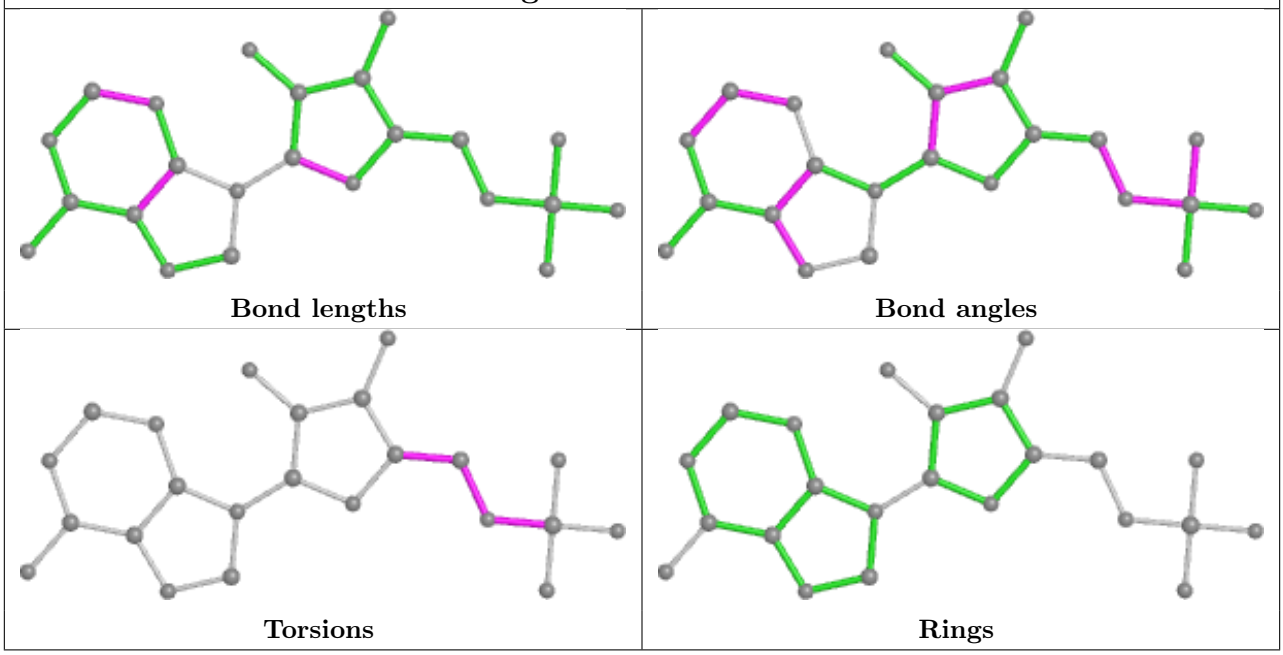
Ligand AMP C 152



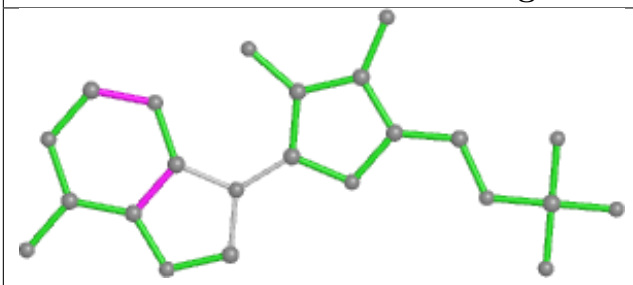
Ligand AMP B 152



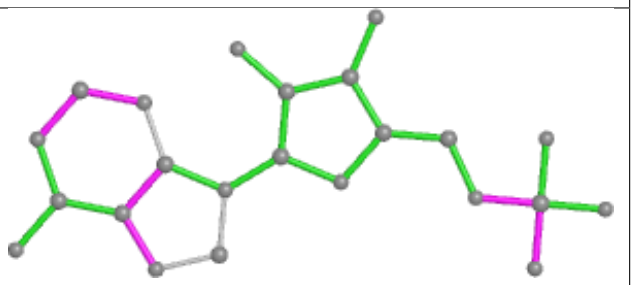
Ligand AMP F 152



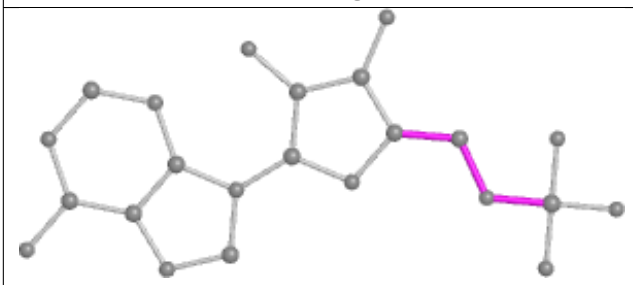
Ligand AMP D 152



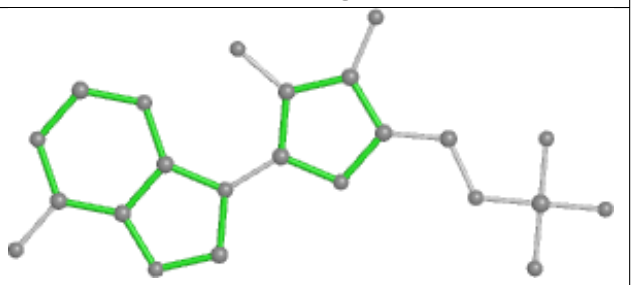
Bond lengths



Bond angles

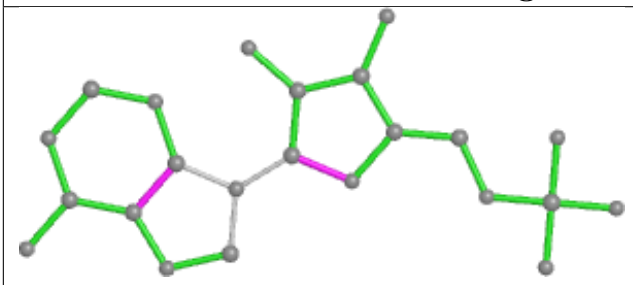


Torsions

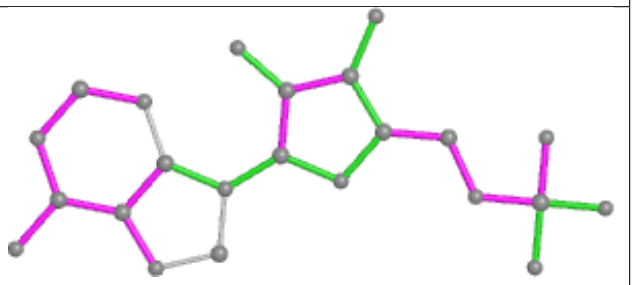


Rings

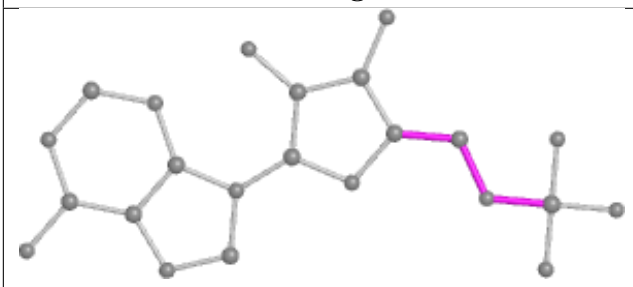
Ligand AMP G 152



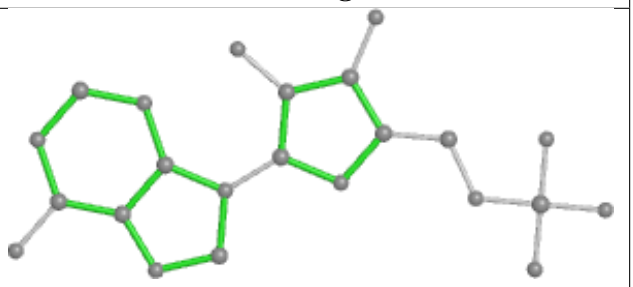
Bond lengths



Bond angles

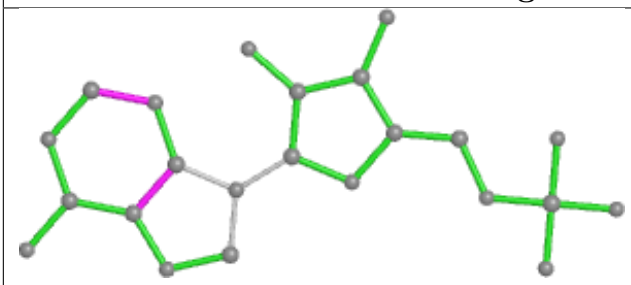


Torsions

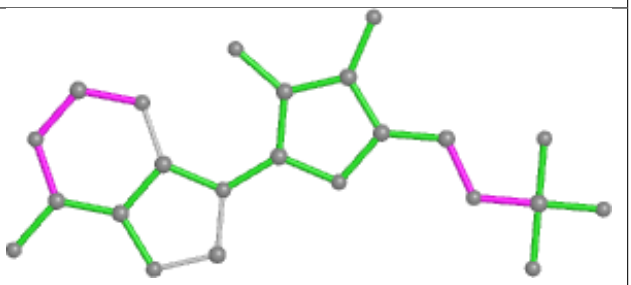


Rings

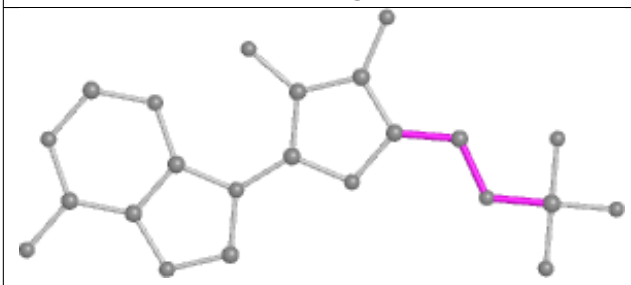
Ligand AMP K 152



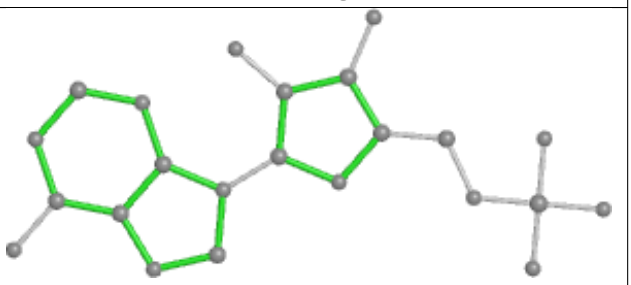
Bond lengths



Bond angles

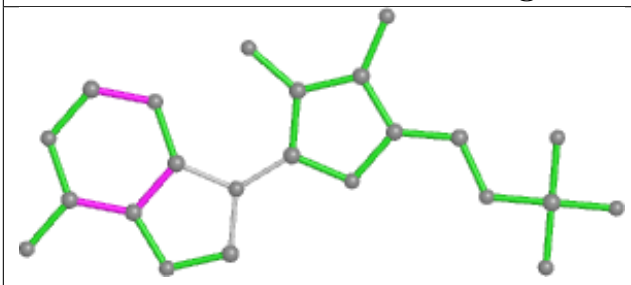


Torsions

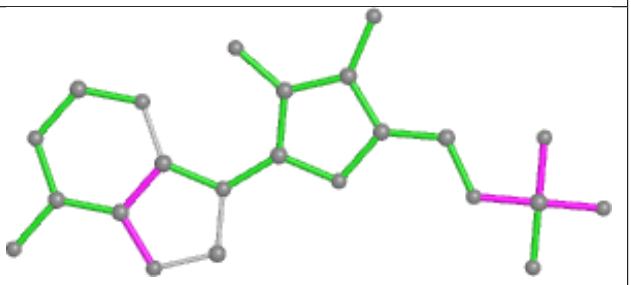


Rings

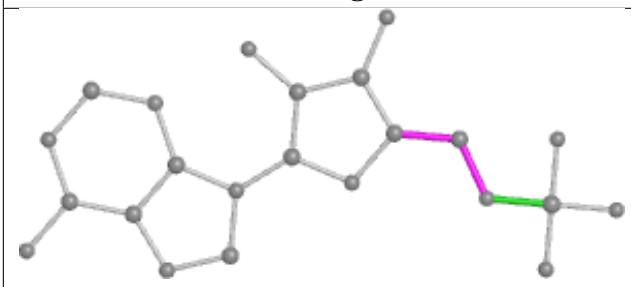
Ligand AMP A 152



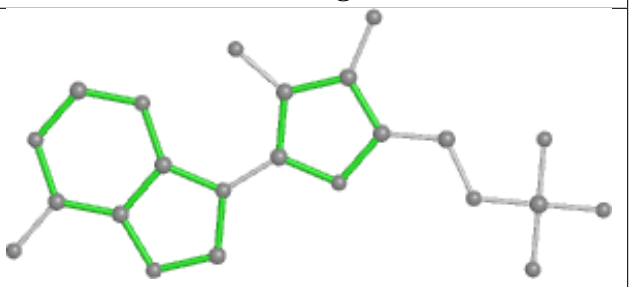
Bond lengths



Bond angles

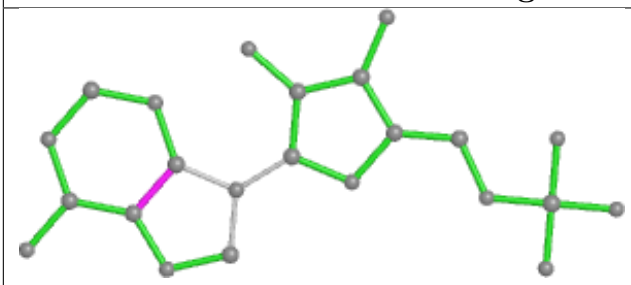


Torsions

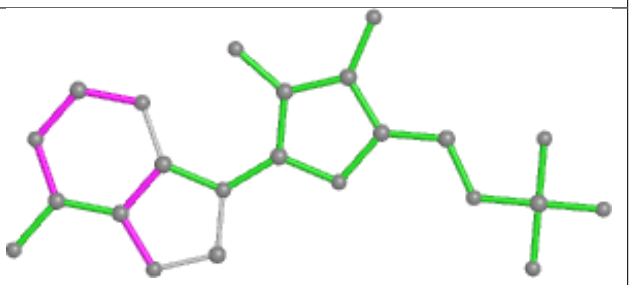


Rings

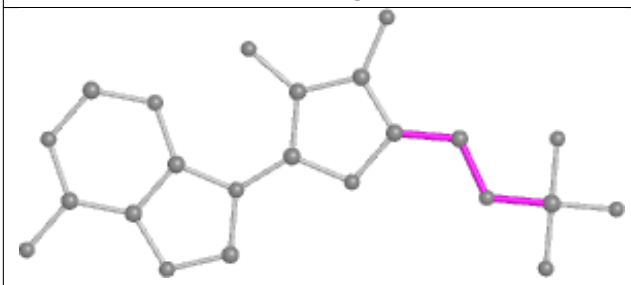
Ligand AMP N 152



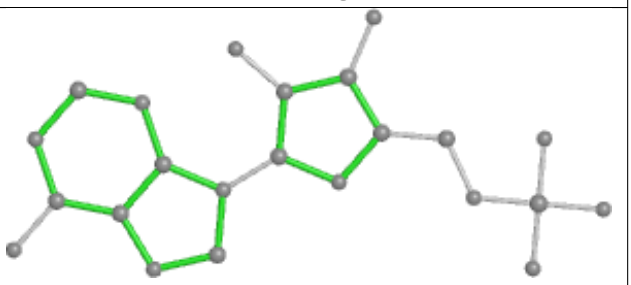
Bond lengths



Bond angles

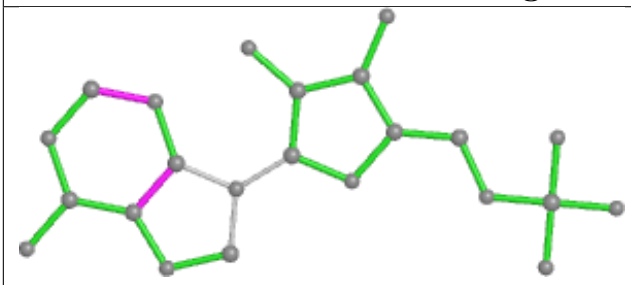


Torsions

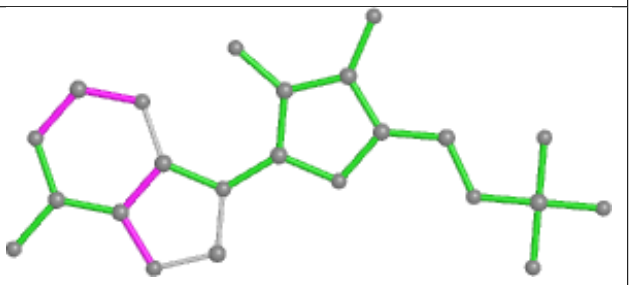


Rings

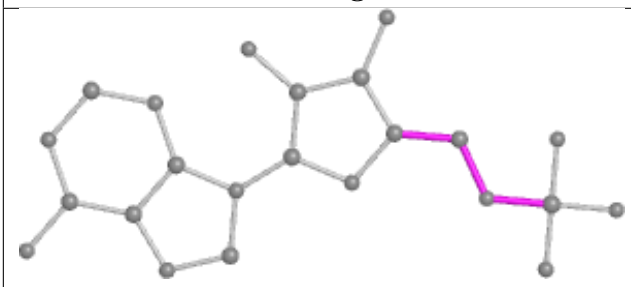
Ligand AMP J 152



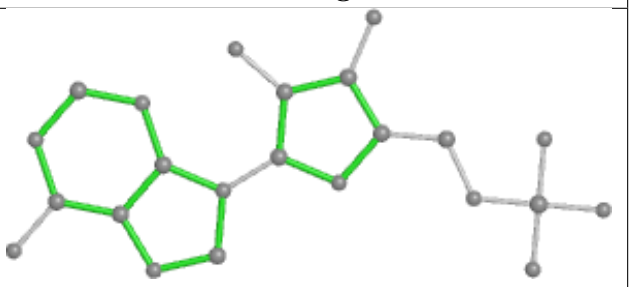
Bond lengths



Bond angles

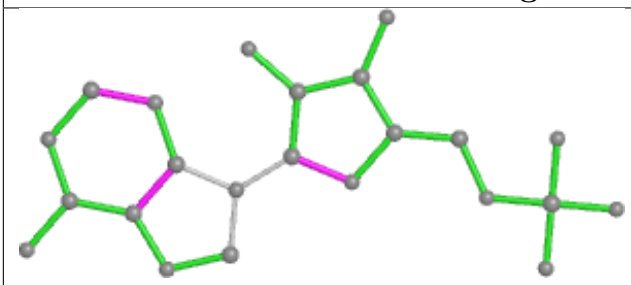


Torsions

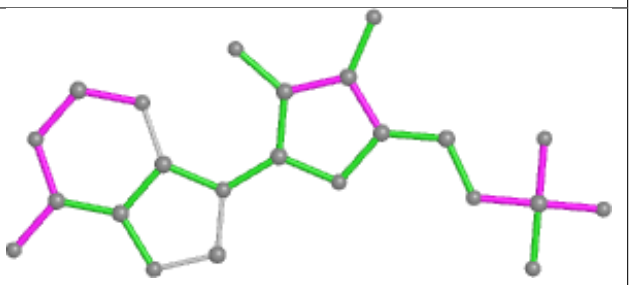


Rings

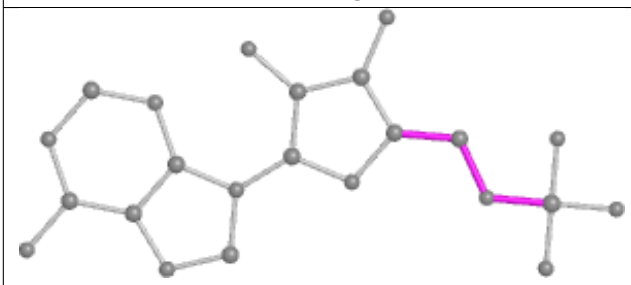
Ligand AMP E 152



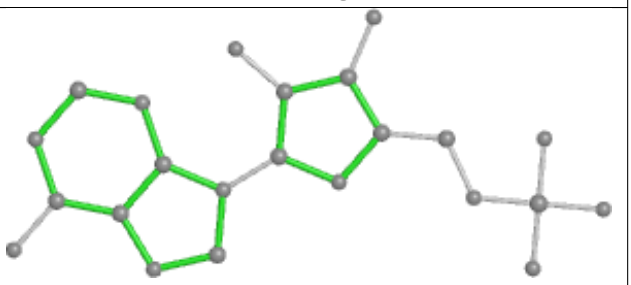
Bond lengths



Bond angles

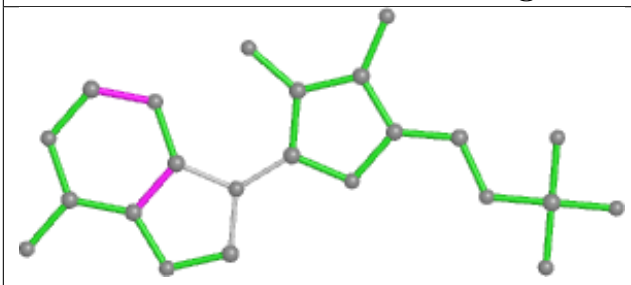


Torsions

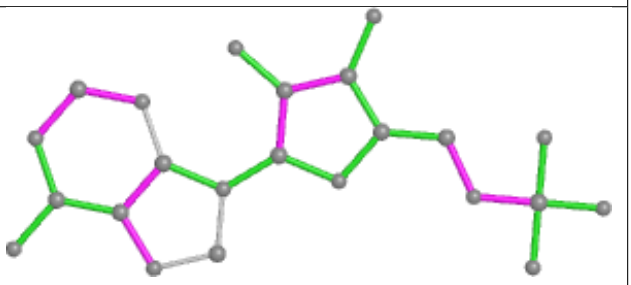


Rings

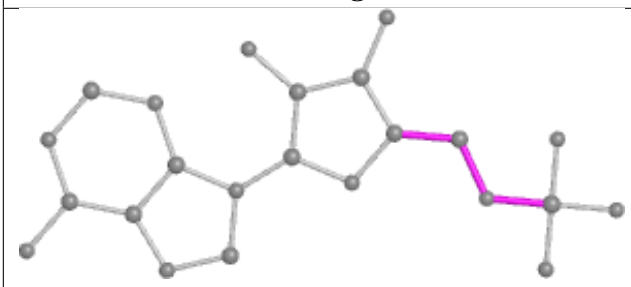
Ligand AMP H 152



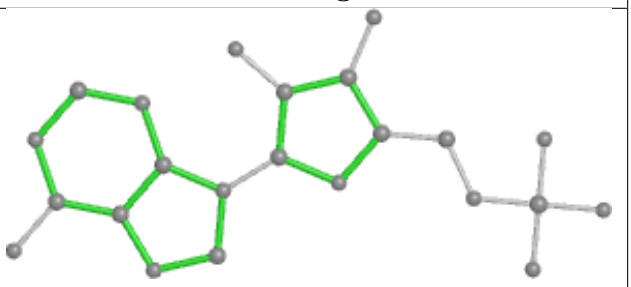
Bond lengths



Bond angles

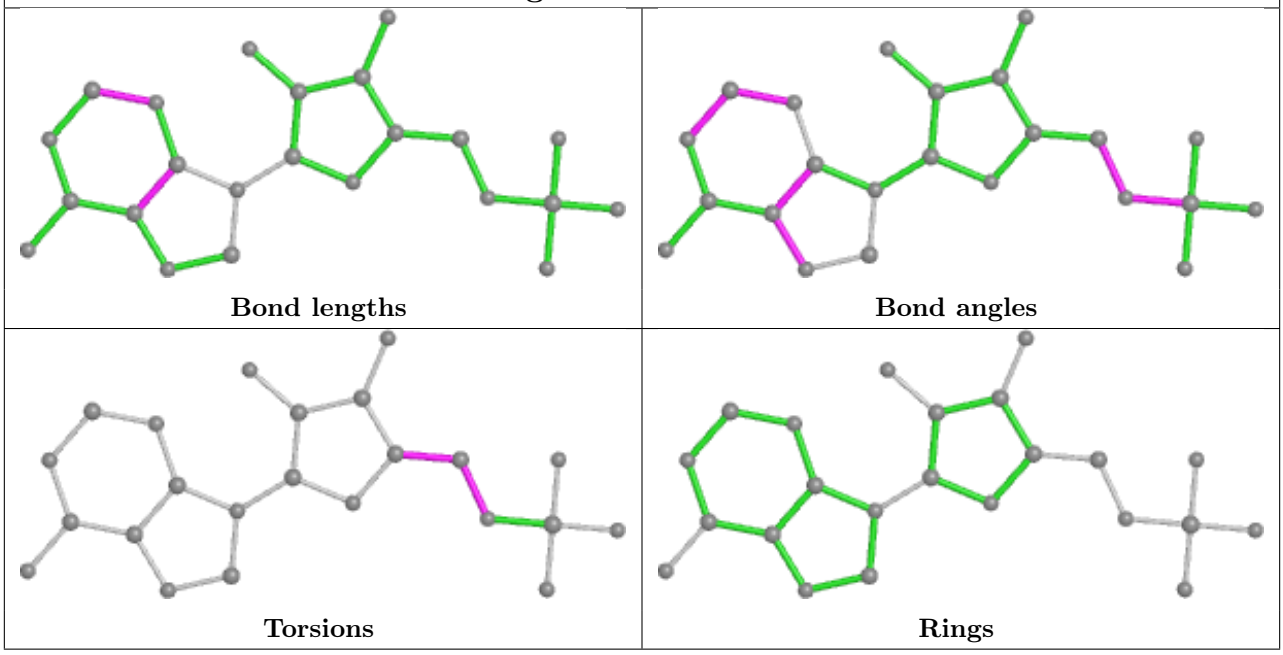


Torsions

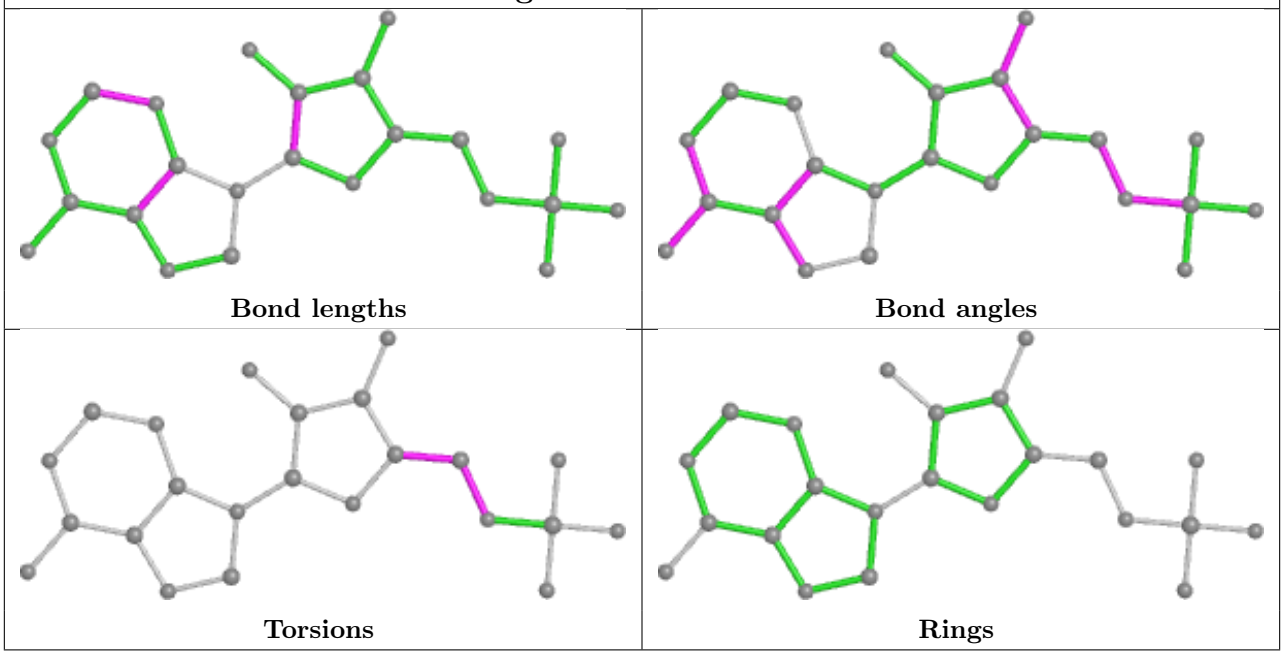


Rings

Ligand AMP I 152



Ligand AMP M 152



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	150/151 (99%)	0.02	5 (3%)	46	42	20, 33, 46, 56	10 (6%)
1	B	148/151 (98%)	-0.19	1 (0%)	87	86	19, 32, 44, 49	9 (6%)
1	C	148/151 (98%)	0.06	2 (1%)	75	73	20, 34, 46, 58	8 (5%)
1	D	150/151 (99%)	-0.05	2 (1%)	77	74	23, 34, 50, 59	8 (5%)
1	E	150/151 (99%)	0.09	2 (1%)	77	74	23, 37, 51, 57	10 (6%)
1	F	150/151 (99%)	-0.01	2 (1%)	77	74	20, 36, 52, 62	10 (6%)
1	G	149/151 (98%)	0.13	6 (4%)	38	34	28, 44, 64, 67	14 (9%)
1	H	147/151 (97%)	0.26	7 (4%)	30	26	29, 47, 68, 75	13 (8%)
1	I	150/151 (99%)	0.16	4 (2%)	54	51	29, 44, 58, 63	14 (9%)
1	J	148/151 (98%)	0.05	1 (0%)	87	86	26, 38, 53, 55	8 (5%)
1	K	149/151 (98%)	-0.15	1 (0%)	87	86	26, 38, 48, 59	7 (4%)
1	L	125/151 (82%)	0.54	11 (8%)	10	8	34, 53, 68, 72	9 (7%)
1	M	149/151 (98%)	-0.21	0	100	100	21, 30, 44, 48	8 (5%)
1	N	150/151 (99%)	0.03	3 (2%)	65	62	19, 32, 50, 57	8 (5%)
All	All	2063/2114 (97%)	0.05	47 (2%)	60	57	19, 38, 58, 75	136 (6%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	3	SER	4.8
1	A	2	SER	4.6
1	L	2	SER	4.5
1	G	55	CYS	3.9
1	L	92	ALA	3.9
1	A	29	ARG	3.7
1	H	59	PHE	3.7
1	C	151	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	3	SER	3.4
1	H	56	SER	3.4
1	G	60	PHE	3.2
1	I	140	SER	3.2
1	D	29	ARG	3.1
1	A	122	VAL	3.1
1	D	66	TYR	3.1
1	G	44	THR	3.0
1	N	3	SER	2.9
1	E	2	SER	2.8
1	F	2	SER	2.7
1	H	120	ASP	2.7
1	L	132	TRP	2.6
1	G	51	TYR	2.5
1	N	25	ALA	2.5
1	E	3	SER	2.5
1	G	61	PRO	2.5
1	I	135	ALA	2.5
1	G	151	GLU	2.5
1	N	151	GLU	2.5
1	L	130	ALA	2.4
1	J	136	ASP	2.4
1	L	120	ASP	2.3
1	L	97	ASP	2.3
1	B	66	TYR	2.3
1	F	3	SER	2.3
1	H	66	TYR	2.2
1	L	150	TYR	2.2
1	H	112	GLY	2.2
1	I	64	VAL	2.2
1	I	151	GLU	2.2
1	L	121	SER	2.2
1	H	53	ASP	2.2
1	L	122	VAL	2.1
1	A	151	GLU	2.1
1	L	40	LEU	2.1
1	K	64	VAL	2.0
1	H	60	PHE	2.0
1	C	21	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

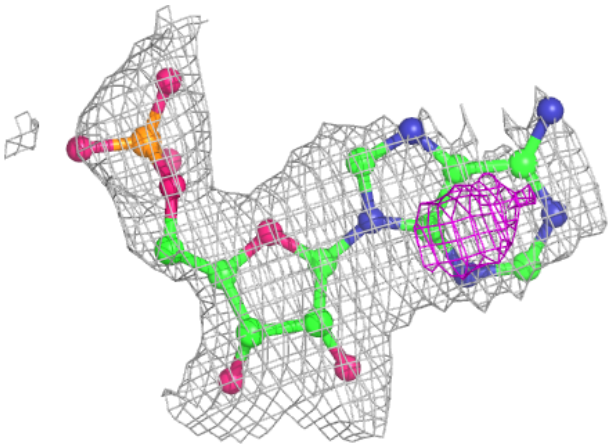
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

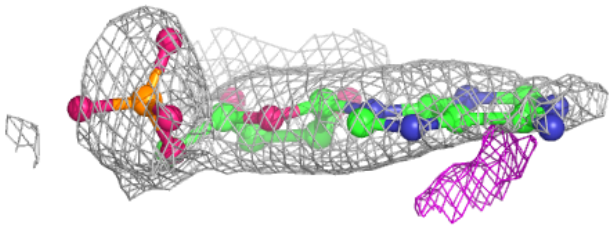
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AMP	I	152	23/23	0.78	0.27	73,75,80,81	0
2	AMP	H	152	23/23	0.79	0.35	84,86,87,88	0
2	AMP	N	152	23/23	0.80	0.24	67,71,79,80	0
2	AMP	M	152	23/23	0.83	0.28	49,58,65,65	0
2	AMP	E	152	23/23	0.83	0.26	55,58,60,63	0
2	AMP	J	152	23/23	0.84	0.24	65,67,70,70	0
2	AMP	D	152	23/23	0.84	0.22	66,67,69,70	0
2	AMP	G	152	23/23	0.84	0.26	78,80,84,84	0
2	AMP	B	152	23/23	0.85	0.26	63,68,73,74	0
2	AMP	C	152	23/23	0.86	0.26	56,60,61,64	0
2	AMP	K	152	23/23	0.86	0.23	59,65,72,72	0
2	AMP	F	152	23/23	0.88	0.23	59,69,74,75	0
2	AMP	A	152	23/23	0.88	0.28	48,52,57,57	0

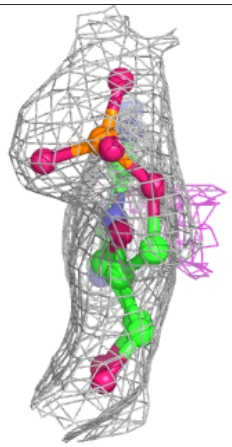
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP I 152:

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

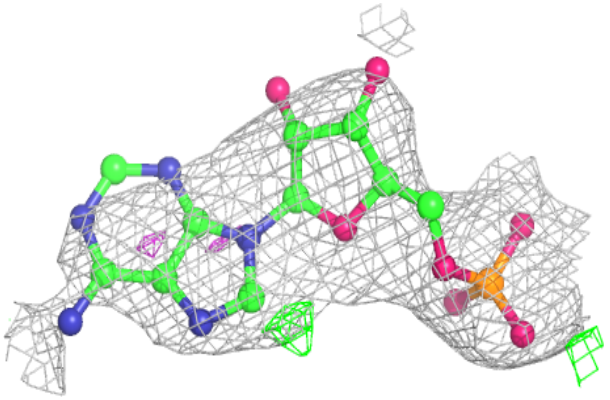


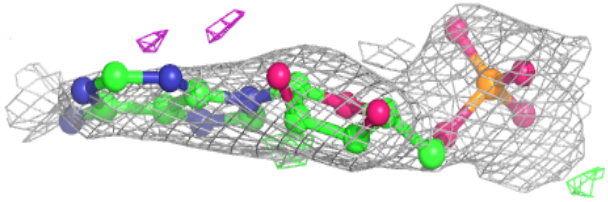


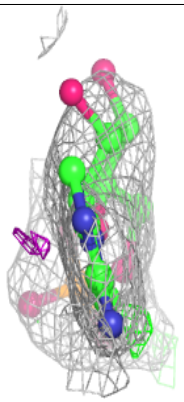


Electron density around AMP H 152:

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

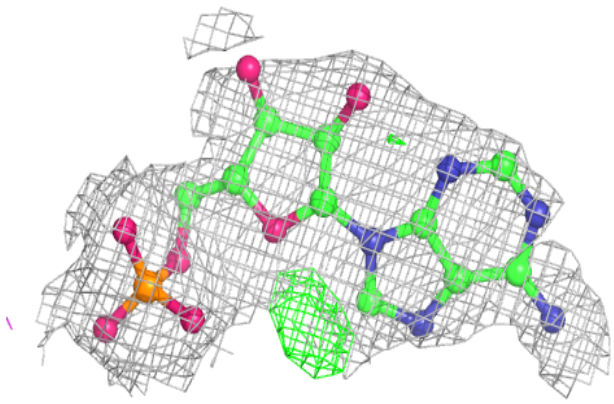


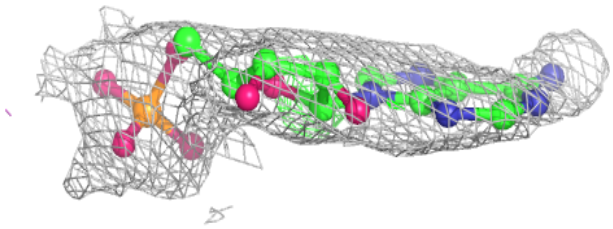


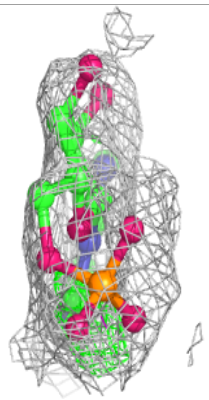


Electron density around AMP N 152:

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

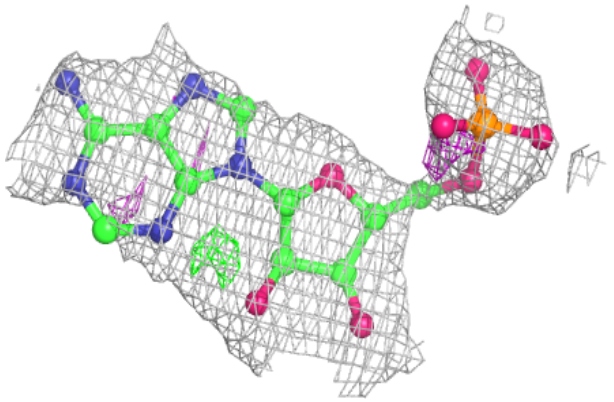


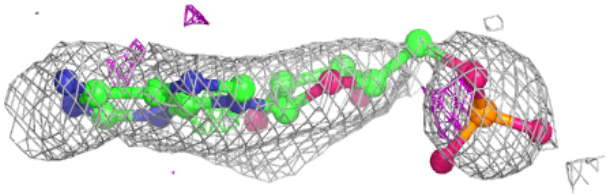


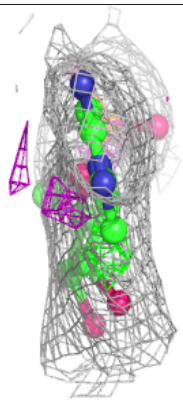


Electron density around AMP M 152:

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

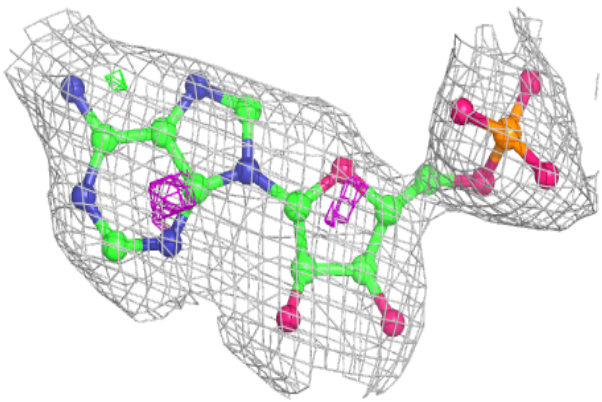


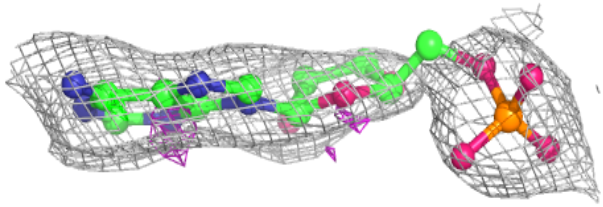


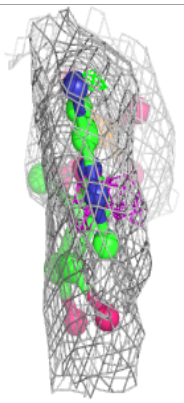


Electron density around AMP E 152:

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

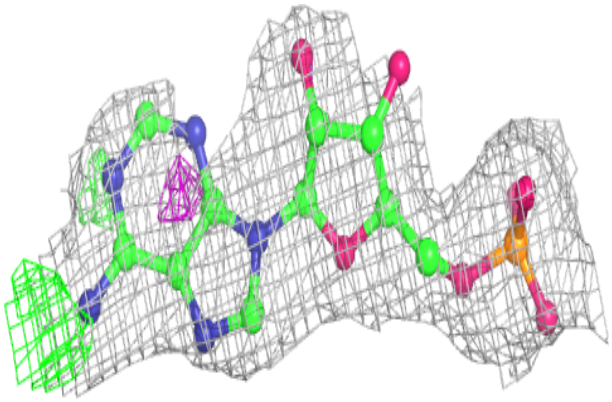


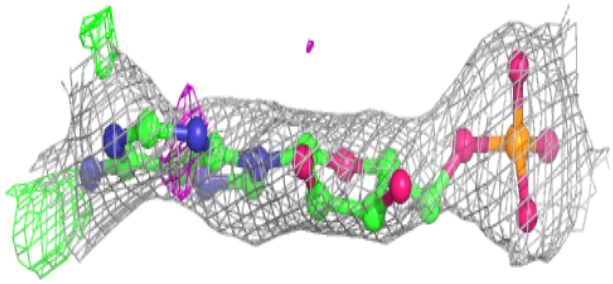


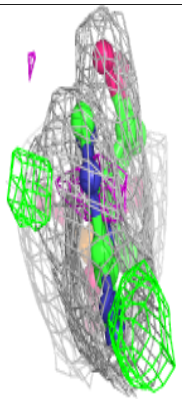


Electron density around AMP J 152:

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

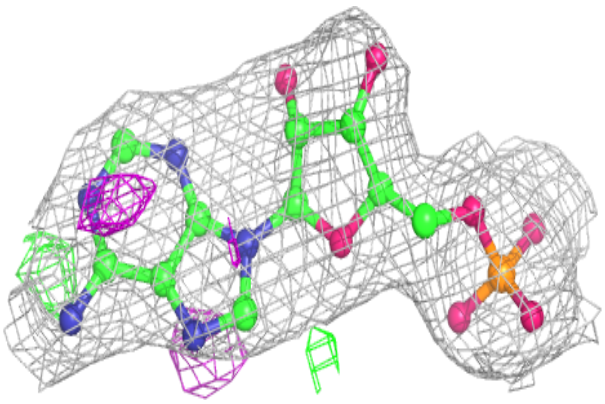


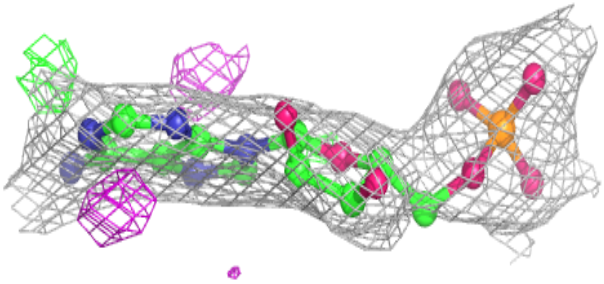


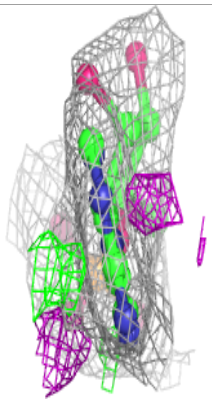


Electron density around AMP D 152:

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

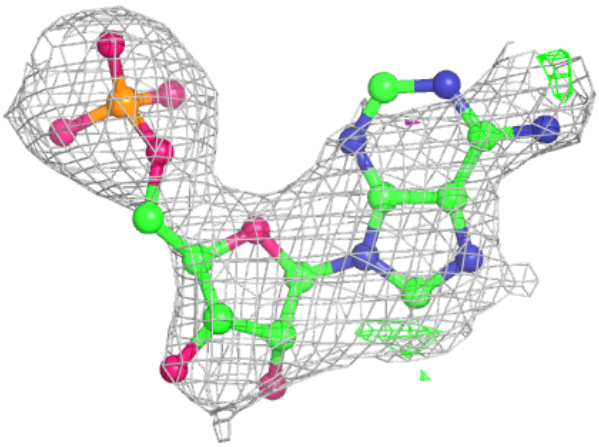


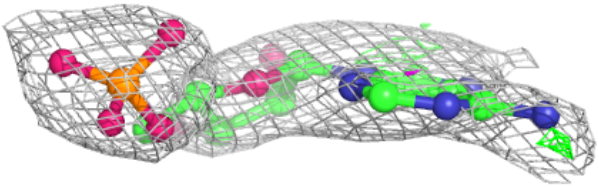


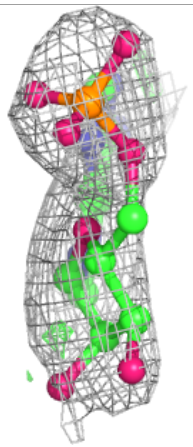


Electron density around AMP G 152:

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

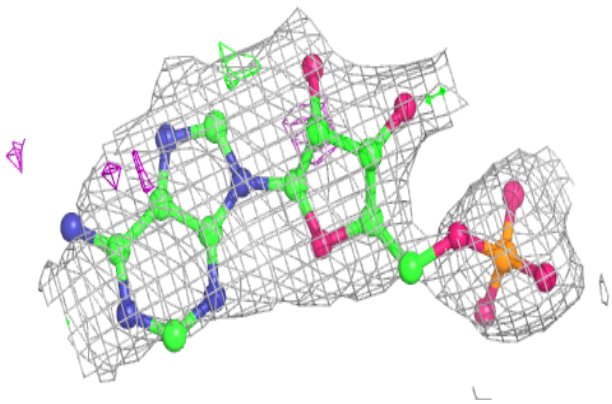


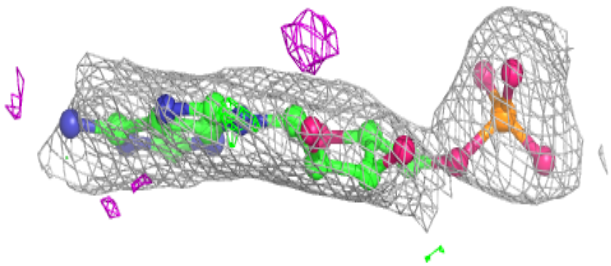


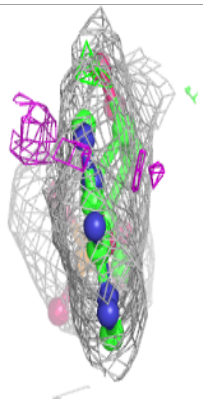


Electron density around AMP B 152:

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

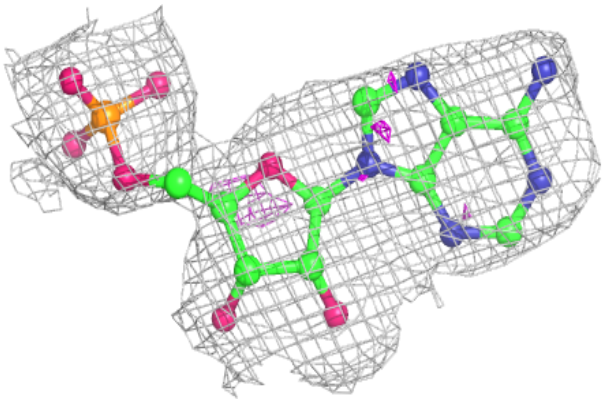


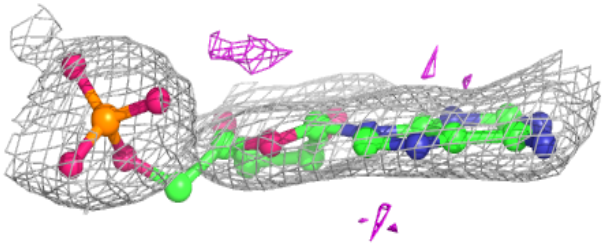


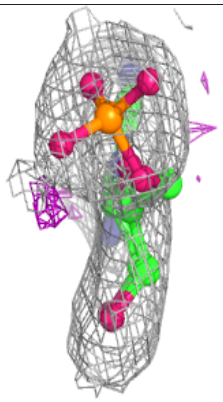


Electron density around AMP C 152:

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

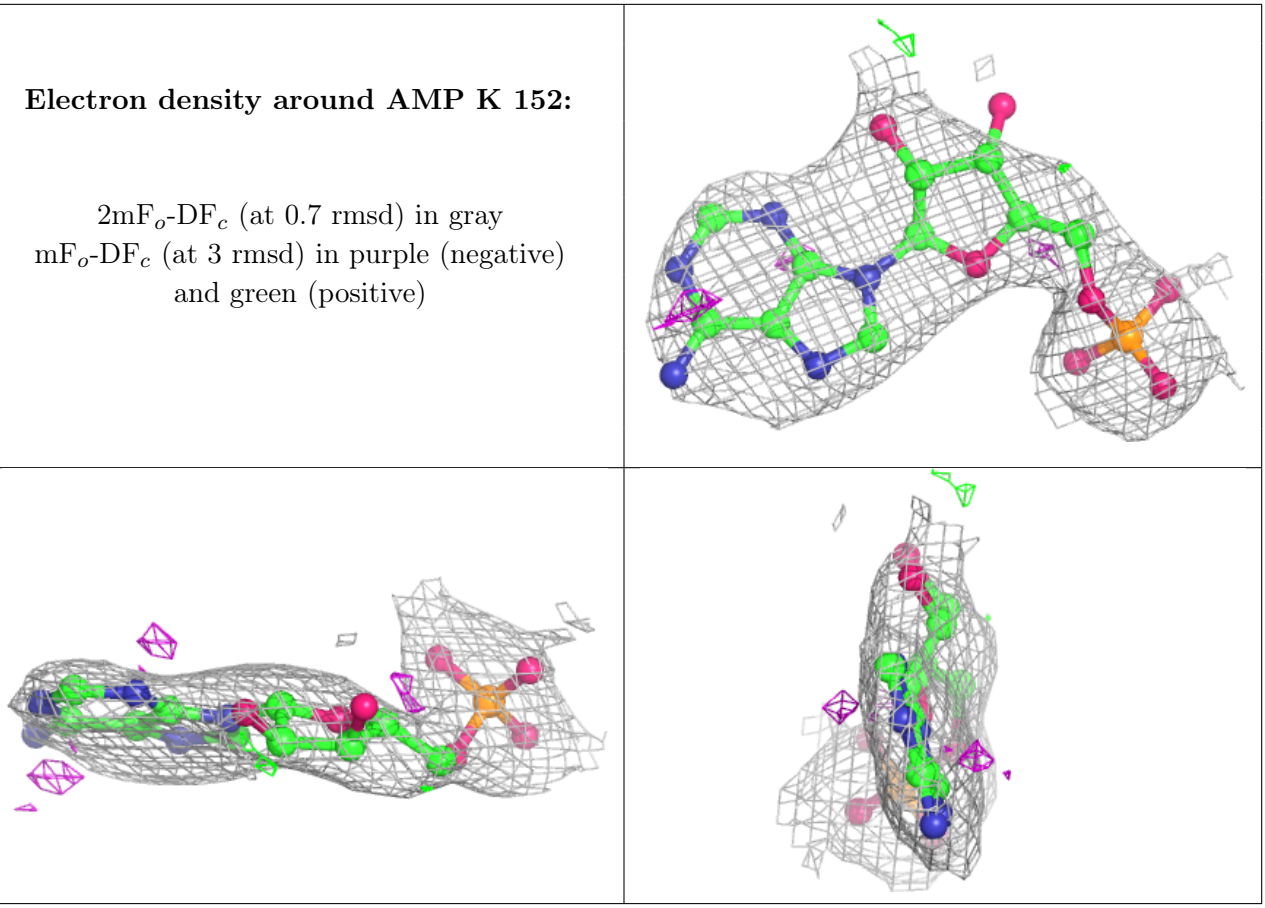






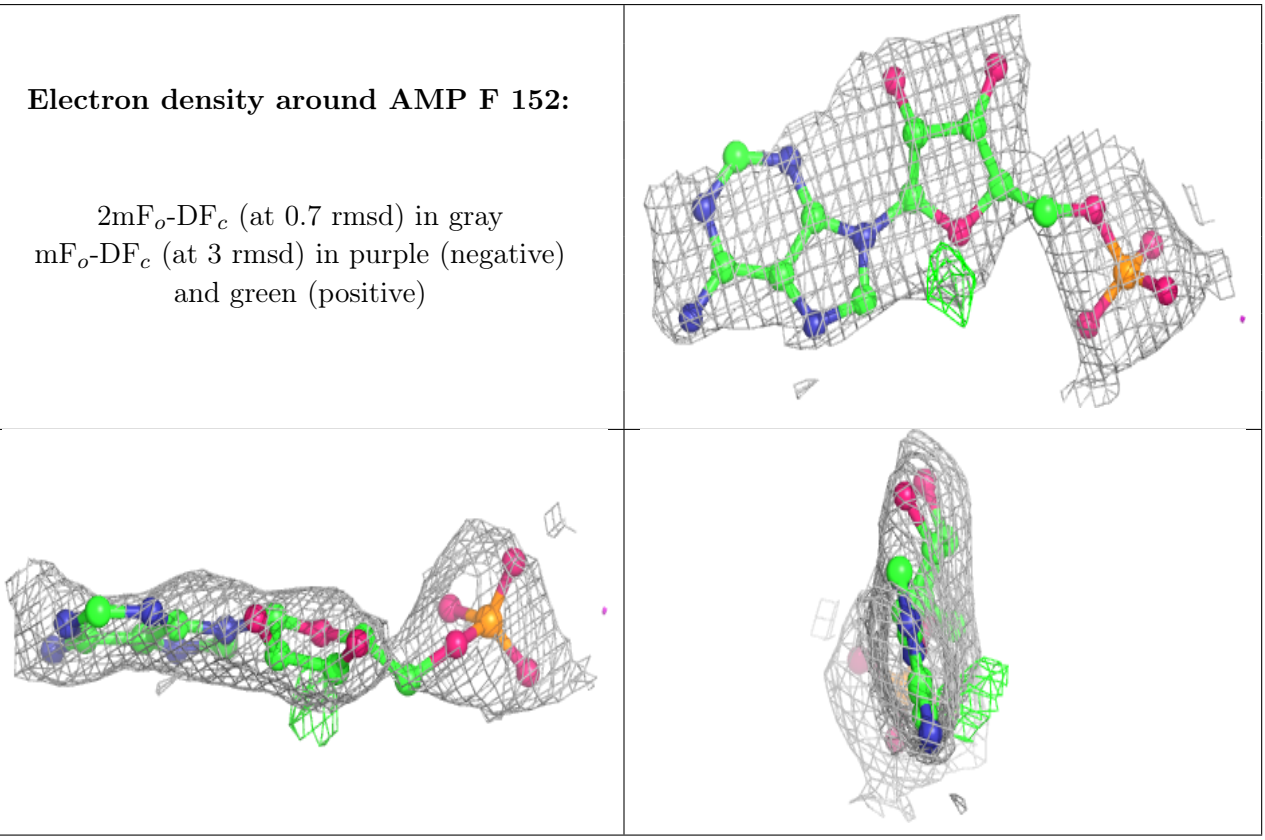
Electron density around AMP K 152:

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



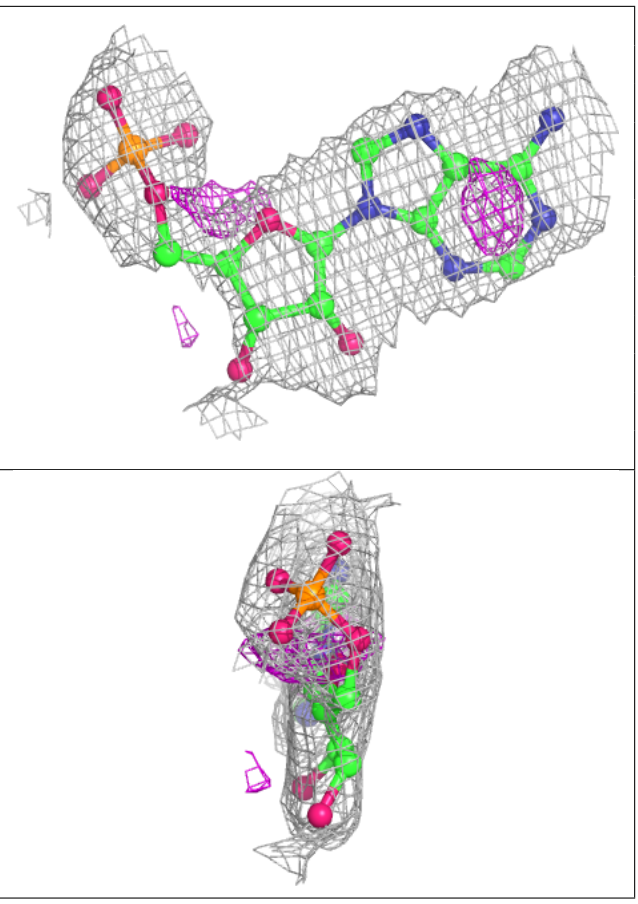
Electron density around AMP F 152:

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



Electron density around AMP A 152:

$2mF_o$-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.