Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 02:39 pm GMT

PDB ID	:	3ZWP
Title	:	Crystal structure of ADP ribosyl cyclase complexed with ara-2'F-ADP- ribose at 2.1 angstrom
Authors	:	Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.
Deposited on	:	2011-08-02
Resolution	:	2.11 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:

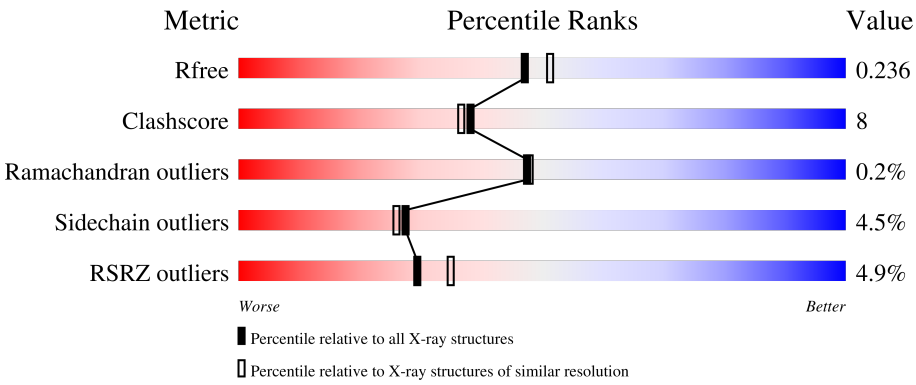
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	260	5% 78% 17%
1	B	260	% 82% 13%
1	C	260	7% 82% 13%
1	D	260	2% 79% 16%
1	E	260	3% 80% 14%

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Mol	Chain	Length	Quality of chain
1	F	260	6% 77% 18%
1	G	260	2% 78% 17%
1	H	260	13% 75% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AVU	D	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17535 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 ADP-RIBOSYL CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	2017	1291	343	369	14	0	0	0
1	B	253	2022	1294	344	370	14	0	0	0
1	C	251	2012	1288	342	368	14	0	0	0
1	D	251	2012	1288	342	368	14	0	0	0
1	E	251	2012	1288	342	368	14	0	0	0
1	F	252	2017	1291	343	369	14	0	0	0
1	G	251	2012	1288	342	368	14	0	0	0
1	H	251	2012	1288	342	368	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P29241
A	0	ALA	-	expression tag	UNP P29241
B	-1	ALA	-	expression tag	UNP P29241
B	0	ALA	-	expression tag	UNP P29241
C	-1	ALA	-	expression tag	UNP P29241
C	0	ALA	-	expression tag	UNP P29241
D	-1	ALA	-	expression tag	UNP P29241
D	0	ALA	-	expression tag	UNP P29241
E	-1	ALA	-	expression tag	UNP P29241
E	0	ALA	-	expression tag	UNP P29241
F	-1	ALA	-	expression tag	UNP P29241
F	0	ALA	-	expression tag	UNP P29241
G	-1	ALA	-	expression tag	UNP P29241

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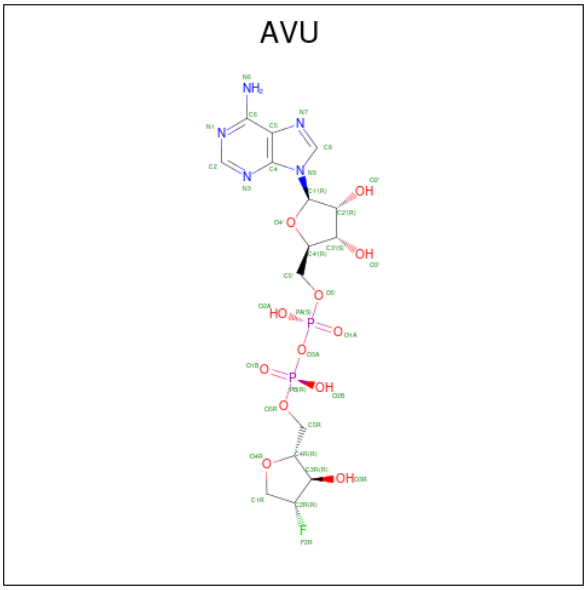
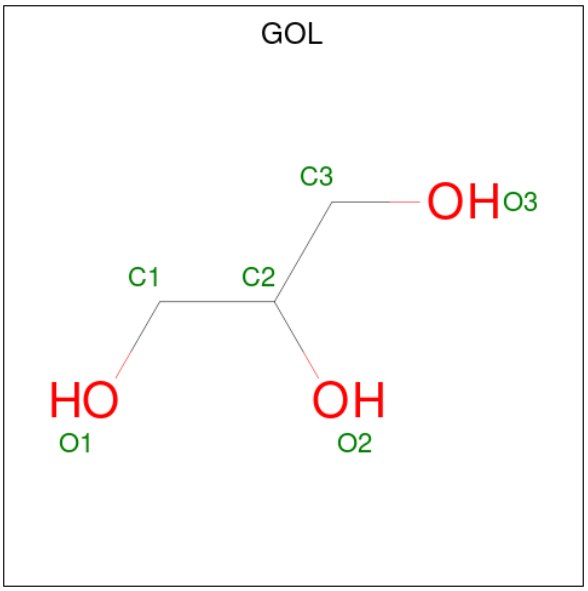
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ALA	-	expression tag	UNP P29241
H	-1	ALA	-	expression tag	UNP P29241
H	0	ALA	-	expression tag	UNP P29241

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl] methyl [(2R,3R,4R)-4-fluoro-3-hydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: AVU) (formula: $C_{15}H_{22}FN_5O_{12}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	35	15	1	5	12	2	0	0
2	B	1	35	15	1	5	12	2	0	0
2	C	1	35	15	1	5	12	2	0	0
2	D	1	35	15	1	5	12	2	0	0
2	E	1	35	15	1	5	12	2	0	0
2	F	1	35	15	1	5	12	2	0	0
2	G	1	35	15	1	5	12	2	0	0
2	H	1	35	15	1	5	12	2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	F	1	6	3	3	0	0

- Molecule 4 is water.

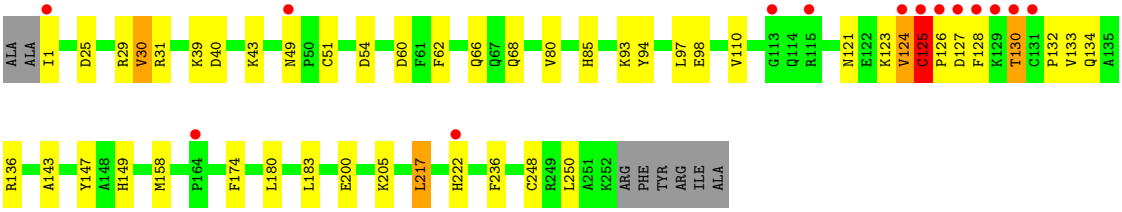
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	156	156	156	0	0
			Total	O		
4	B	221	221	221	0	0
			Total	O		
4	C	179	179	179	0	0
			Total	O		
4	D	177	177	177	0	0
			Total	O		
4	E	140	140	140	0	0
			Total	O		
4	F	67	67	67	0	0
			Total	O		
4	G	136	136	136	0	0
			Total	O		
4	H	45	45	45	0	0

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.

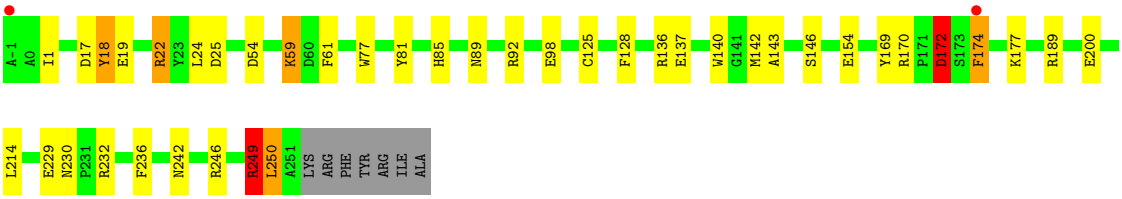
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain A:



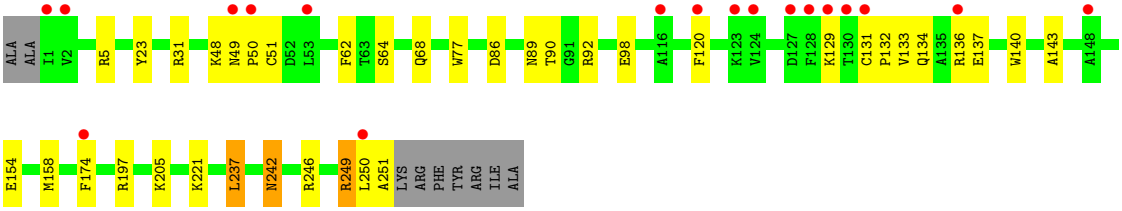
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain B:



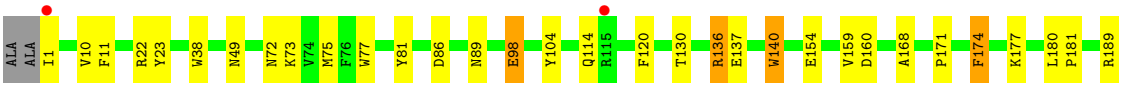
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain C:



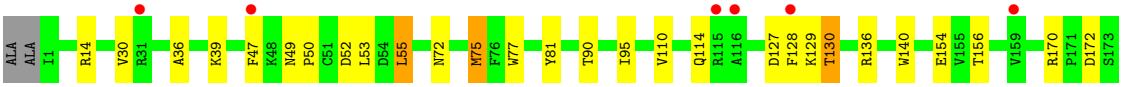
• Molecule 1: ADP-RIBOSYL CYCLASE

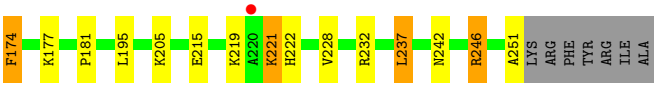
Chain D:



• Molecule 1: ADP-RIBOSYL CYCLASE

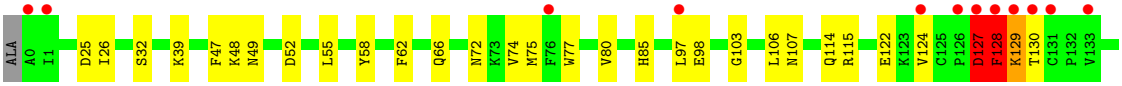
Chain E:





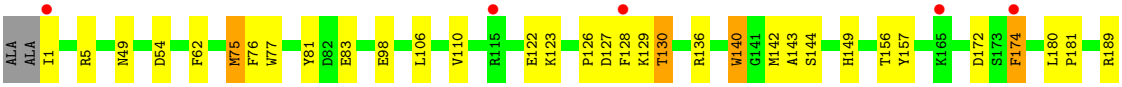
• Molecule 1: ADP-RIBOSYL CYCLASE

Chain F:



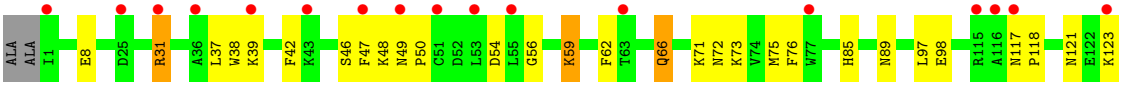
• Molecule 1: ADP-RIBOSYL CYCLASE

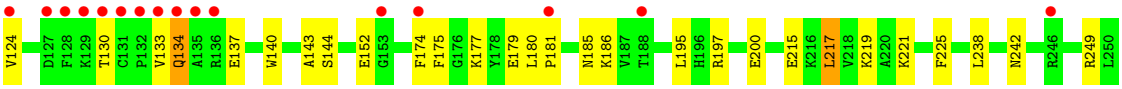
Chain G:



• Molecule 1: ADP-RIBOSYL CYCLASE

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.03Å 77.61Å 140.22Å 87.91° 89.24° 88.16°	Depositor
Resolution (Å)	30.00 – 2.11 29.88 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.11) 76.3 (29.88-2.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.241 0.184 , 0.236	Depositor DCC
R_{free} test set	5773 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l 0.021 for -h,k,-l 0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17535	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: AVU, GOL

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	1.12	5/2069 (0.2%)	1.00	5/2800 (0.2%)
1	B	1.35	10/2074 (0.5%)	1.06	7/2807 (0.2%)
1	C	1.18	2/2064 (0.1%)	0.98	5/2793 (0.2%)
1	D	1.27	11/2064 (0.5%)	1.00	5/2793 (0.2%)
1	E	1.09	4/2064 (0.2%)	0.92	2/2793 (0.1%)
1	F	0.92	0/2069	0.82	0/2800
1	G	1.23	8/2064 (0.4%)	0.99	5/2793 (0.2%)
1	H	0.89	1/2064 (0.0%)	0.81	1/2793 (0.0%)
All	All	1.14	41/16532 (0.2%)	0.95	30/22372 (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	F	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	140	TRP	CB-CG	10.01	1.68	1.50
1	D	174	PHE	CE1-CZ	7.96	1.52	1.37
1	B	172	ASP	CB-CG	7.50	1.67	1.51
1	C	98	GLU	CB-CG	7.49	1.66	1.52
1	G	174	PHE	CE1-CZ	7.22	1.51	1.37
1	D	140	TRP	CB-CG	6.75	1.62	1.50
1	C	140	TRP	CB-CG	6.68	1.62	1.50
1	B	174	PHE	CE2-CZ	5.98	1.48	1.37
1	D	98	GLU	CB-CG	5.95	1.63	1.52
1	D	104	TYR	CD1-CE1	5.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	PHE	CE2-CZ	5.79	1.48	1.37
1	B	140	TRP	CE3-CZ3	5.64	1.48	1.38
1	A	94	TYR	CD1-CE1	5.57	1.47	1.39
1	D	174	PHE	CG-CD2	5.57	1.47	1.38
1	G	144	SER	CA-CB	5.55	1.61	1.52
1	G	110	VAL	CB-CG1	5.48	1.64	1.52
1	B	140	TRP	CB-CG	5.48	1.60	1.50
1	A	125	CYS	CB-SG	-5.48	1.72	1.81
1	E	174	PHE	CE1-CZ	5.44	1.47	1.37
1	G	172	ASP	CB-CG	5.44	1.63	1.51
1	G	174	PHE	CG-CD2	5.43	1.46	1.38
1	A	200	GLU	CG-CD	5.43	1.60	1.51
1	A	25	ASP	CB-CG	5.40	1.63	1.51
1	E	110	VAL	CB-CG1	5.38	1.64	1.52
1	B	143	ALA	CA-CB	5.34	1.63	1.52
1	D	140	TRP	CE3-CZ3	5.29	1.47	1.38
1	G	83	GLU	CB-CG	5.19	1.62	1.52
1	H	200	GLU	CG-CD	5.18	1.59	1.51
1	B	19	GLU	CD-OE2	-5.16	1.20	1.25
1	D	23	TYR	CG-CD2	5.16	1.45	1.39
1	B	18	TYR	CG-CD1	5.15	1.45	1.39
1	B	61	PHE	CE1-CZ	5.15	1.47	1.37
1	D	38	TRP	CG-CD1	5.14	1.44	1.36
1	D	11	PHE	CE2-CZ	5.09	1.47	1.37
1	D	10	VAL	CB-CG2	5.04	1.63	1.52
1	B	146	SER	CB-OG	-5.04	1.35	1.42
1	E	174	PHE	CG-CD2	5.04	1.46	1.38
1	G	208	ALA	CA-CB	5.02	1.62	1.52
1	A	248	CYS	CB-SG	-5.01	1.73	1.81
1	E	140	TRP	CB-CG	5.01	1.59	1.50
1	B	174	PHE	CG-CD1	5.01	1.46	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	172	ASP	CB-CG-OD1	10.18	127.46	118.30
1	B	249	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	C	197	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	D	136	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	249	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	D	177	LYS	CD-CE-NZ	-6.77	96.14	111.70
1	G	195	LEU	CB-CG-CD1	-6.50	99.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	172	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	25	ASP	CB-CG-OD1	6.39	124.05	118.30
1	G	142	MET	CG-SD-CE	6.26	110.22	100.20
1	B	22	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	86	ASP	CB-CG-OD2	5.86	123.57	118.30
1	H	197	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	G	195	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	D	160	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	54	ASP	CB-CG-OD1	5.78	123.50	118.30
1	G	172	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	29	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	D	160	ASP	CB-CG-OD1	5.46	123.21	118.30
1	E	14	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	22	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	92	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	125	CYS	CA-CB-SG	-5.43	104.23	114.00
1	C	249	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	55	LEU	CB-CG-CD1	5.31	120.03	111.00
1	C	5	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	54	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	30	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	B	24	LEU	CB-CG-CD1	-5.06	102.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	127	ASP	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	2017	0	1970	37	1
1	B	2022	0	1978	31	0
1	C	2012	0	1968	28	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2012	0	1968	32	0
1	E	2012	0	1968	26	0
1	F	2017	0	1973	29	0
1	G	2012	0	1968	27	0
1	H	2012	0	1968	35	0
2	A	35	0	19	5	0
2	B	35	0	19	0	0
2	C	35	0	19	2	0
2	D	35	0	19	10	0
2	E	35	0	19	3	0
2	F	35	0	19	4	0
2	G	35	0	19	2	0
2	H	35	0	19	3	0
3	C	6	0	8	2	0
3	D	6	0	8	1	0
3	F	6	0	8	0	0
4	A	156	0	0	14	0
4	B	221	0	0	6	0
4	C	179	0	0	6	0
4	D	177	0	0	17	0
4	E	140	0	0	3	0
4	F	67	0	0	5	0
4	G	136	0	0	5	0
4	H	45	0	0	0	0
All	All	17535	0	15937	246	1

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 8.

All (246) 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:G:127:ASP:O	1:G:130:THR:HG22	1.28	1.29
1:C:132:PRO:HB2	1:C:134:GLN:NE2	1.65	1.10
1:G:98:GLU:OE2	2:G:301:AVU:N6	1.89	1.05
2:D:301:AVU:O5R	4:D:2172:HOH:O	1.77	1.01
1:D:73:LYS:NZ	4:D:2083:HOH:O	1.95	0.99
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.23	0.97
1:G:127:ASP:O	1:G:130:THR:CG2	2.15	0.94
1:H:31:ARG:HG3	1:H:31:ARG:HH11	1.32	0.93
1:A:174:PHE:CE2	2:A:301:AVU:H2'	2.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:AVU:H8	4:D:2174:HOH:O	1.69	0.92
1:A:66:GLN:OE1	4:A:2063:HOH:O	1.91	0.88
1:E:127:ASP:O	1:E:130:THR:HG23	1.74	0.88
1:G:5:ARG:NH1	4:G:2007:HOH:O	2.06	0.87
1:C:251:ALA:O	4:C:2178:HOH:O	1.93	0.86
1:H:117:ASN:HD22	1:H:118:PRO:HA	1.42	0.85
1:C:132:PRO:HB2	1:C:134:GLN:HE22	1.44	0.82
1:E:128:PHE:O	1:E:136:ARG:HD3	1.80	0.82
2:E:301:AVU:O5R	4:E:2139:HOH:O	1.97	0.82
1:G:149:HIS:ND1	4:G:2101:HOH:O	2.11	0.82
1:D:140:TRP:CG	2:D:301:AVU:H2	2.16	0.81
1:G:49:ASN:HB2	4:G:2040:HOH:O	1.80	0.80
1:H:31:ARG:HH11	1:H:31:ARG:CG	1.94	0.79
1:A:222:HIS:ND1	4:A:2133:HOH:O	2.16	0.79
1:B:246:ARG:NH2	1:B:249:ARG:NH2	2.30	0.78
3:D:1253:GOL:H32	4:D:2100:HOH:O	1.84	0.78
1:G:75:MET:HE1	1:G:156:THR:HG22	1.66	0.78
1:F:128:PHE:CE1	4:F:2019:HOH:O	2.39	0.76
1:H:180:LEU:HD21	1:H:217:LEU:HD22	1.65	0.76
1:D:77:TRP:NE1	4:D:2085:HOH:O	1.86	0.76
1:A:68:GLN:HG3	4:A:2066:HOH:O	1.84	0.76
1:G:128:PHE:O	1:G:136:ARG:CD	2.35	0.75
1:C:132:PRO:HB2	1:C:134:GLN:HE21	1.48	0.74
1:H:117:ASN:ND2	1:H:118:PRO:HA	2.01	0.74
1:B:174:PHE:HE1	1:B:177:LYS:HZ1	1.37	0.73
1:C:205:LYS:NZ	4:C:2139:HOH:O	2.21	0.73
1:C:137:GLU:HG2	1:C:174:PHE:CZ	2.25	0.72
1:F:85:HIS:NE2	1:F:98:GLU:OE1	2.21	0.72
1:F:174:PHE:CE2	2:F:301:AVU:H2'	2.25	0.70
1:A:51:CYS:SG	1:A:132:PRO:HD2	2.30	0.70
1:A:130:THR:O	4:A:2103:HOH:O	2.07	0.70
1:F:128:PHE:CD1	4:F:2019:HOH:O	2.46	0.68
1:A:132:PRO:HB2	1:A:134:GLN:NE2	2.09	0.68
1:D:242:ASN:ND2	4:D:2170:HOH:O	2.25	0.68
1:B:250:LEU:O	4:B:2220:HOH:O	2.13	0.67
1:D:86:ASP:HB2	4:D:2093:HOH:O	1.94	0.67
1:A:39:LYS:HE2	4:A:2052:HOH:O	1.95	0.65
1:G:128:PHE:O	1:G:136:ARG:HD2	1.94	0.65
1:E:222:HIS:ND1	4:E:2128:HOH:O	2.29	0.65
1:H:215:GLU:O	1:H:219:LYS:HG2	1.96	0.65
1:H:140:TRP:HB2	1:H:174:PHE:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:HIS:NE2	1:H:98:GLU:OE1	2.28	0.63
1:H:152:GLU:OE2	1:H:186:LYS:HD3	2.00	0.61
1:E:246:ARG:C	1:E:246:ARG:HD3	2.21	0.61
1:A:147:TYR:HA	4:A:2063:HOH:O	2.00	0.60
2:D:301:AVU:H5'A	4:D:2174:HOH:O	2.02	0.60
1:G:212:LEU:HG	1:G:216:LYS:HE2	1.82	0.60
1:F:174:PHE:CD2	2:F:301:AVU:H2'	2.36	0.60
1:G:77:TRP:CH2	1:G:81:TYR:HD2	2.19	0.60
1:H:75:MET:HG2	1:H:76:PHE:N	2.17	0.60
1:C:246:ARG:HD3	4:C:2175:HOH:O	2.01	0.59
1:F:80:VAL:HG21	1:F:158:MET:HG2	1.84	0.59
1:B:77:TRP:NE1	4:B:2111:HOH:O	1.98	0.59
1:E:49:ASN:CG	1:E:50:PRO:HD2	2.23	0.59
1:A:250:LEU:HD12	1:B:232:ARG:NH1	2.18	0.59
1:F:49:ASN:HB2	1:F:52:ASP:HB2	1.83	0.58
1:G:140:TRP:HB3	1:G:174:PHE:HE2	1.68	0.58
1:E:172:ASP:O	1:E:177:LYS:HE2	2.04	0.58
4:A:2023:HOH:O	1:B:17:ASP:OD2	2.17	0.58
1:E:36:ALA:HA	1:E:39:LYS:HD2	1.84	0.58
1:F:137:GLU:HG2	1:F:174:PHE:CZ	2.38	0.58
1:A:174:PHE:CE2	2:A:301:AVU:C2'	2.83	0.56
1:D:77:TRP:CH2	1:D:81:TYR:HD2	2.22	0.56
1:H:174:PHE:CD2	2:H:301:AVU:H2'	2.41	0.56
1:H:121:ASN:OD1	1:H:124:VAL:O	2.24	0.56
1:A:123:LYS:HA	4:A:2102:HOH:O	2.04	0.56
1:G:174:PHE:HB2	2:G:301:AVU:PB	2.46	0.56
1:C:134:GLN:NE2	1:C:134:GLN:H	2.04	0.56
1:A:1:ILE:HG23	1:A:125:CYS:HB3	1.87	0.56
1:A:174:PHE:CD2	2:A:301:AVU:H2'	2.40	0.56
1:B:77:TRP:CH2	1:B:81:TYR:HD2	2.24	0.55
1:H:56:GLY:O	1:H:59:LYS:HB2	2.06	0.55
1:D:171:PRO:HB3	1:E:129:LYS:HG2	1.89	0.55
1:B:246:ARG:CZ	1:B:249:ARG:NH2	2.70	0.54
1:A:93:LYS:HE3	4:A:2098:HOH:O	2.07	0.54
1:D:140:TRP:CD2	2:D:301:AVU:H2	2.42	0.54
1:E:215:GLU:O	1:E:219:LYS:HG2	2.08	0.54
1:C:131:CYS:HB3	1:C:132:PRO:HD2	1.90	0.53
1:H:195:LEU:HD11	1:H:238:LEU:HD21	1.89	0.53
1:E:77:TRP:CZ3	2:E:301:AVU:H5'	2.44	0.53
1:F:127:ASP:HB3	1:F:129:LYS:HG3	1.91	0.53
1:H:49:ASN:OD1	1:H:50:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:CG	1:H:31:ARG:NH1	2.62	0.52
1:D:154:GLU:HG2	1:D:189:ARG:HB3	1.91	0.52
1:A:80:VAL:HG21	1:A:158:MET:HG2	1.91	0.52
1:A:40:ASP:HA	1:A:43:LYS:HE2	1.92	0.52
1:E:47:PHE:HA	1:E:114:GLN:O	2.10	0.52
1:E:77:TRP:CH2	1:E:81:TYR:HD2	2.27	0.52
1:F:55:LEU:O	1:F:55:LEU:HG	2.09	0.52
1:D:198:LEU:HD22	1:D:247:GLU:HB2	1.91	0.52
1:B:137:GLU:OE2	1:B:177:LYS:NZ	2.43	0.52
1:C:242:ASN:ND2	4:C:2172:HOH:O	2.35	0.52
1:G:140:TRP:CB	1:G:174:PHE:HE2	2.23	0.52
1:G:196:HIS:CG	1:G:202:ILE:HD12	2.44	0.52
1:D:72:ASN:HA	1:D:154:GLU:O	2.10	0.51
1:E:77:TRP:NE1	4:E:2063:HOH:O	2.24	0.51
1:H:144:SER:OG	1:H:179:GLU:OE2	2.28	0.51
1:B:246:ARG:NH2	1:B:249:ARG:HH22	2.09	0.50
1:D:174:PHE:CE1	4:D:2127:HOH:O	2.55	0.50
1:H:31:ARG:HG3	1:H:31:ARG:NH1	2.13	0.50
1:E:128:PHE:O	1:E:136:ARG:CD	2.56	0.49
1:G:128:PHE:O	1:G:136:ARG:HD3	2.12	0.49
1:C:68:GLN:HG2	4:C:2059:HOH:O	2.11	0.49
1:F:246:ARG:HD2	1:F:249:ARG:NE	2.27	0.49
1:C:62:PHE:CZ	1:C:143:ALA:HB2	2.47	0.49
1:A:149:HIS:ND1	4:A:2107:HOH:O	2.35	0.49
1:F:214:LEU:O	1:F:218:VAL:HG23	2.13	0.48
1:F:175:PHE:HA	1:F:179:GLU:HB2	1.95	0.48
1:F:127:ASP:HB2	1:F:130:THR:HG23	1.94	0.48
1:H:181:PRO:HA	1:H:221:LYS:NZ	2.28	0.48
1:B:142:MET:HE1	4:B:2168:HOH:O	2.13	0.48
1:D:174:PHE:CD1	4:D:2127:HOH:O	2.65	0.48
1:C:48:LYS:O	1:C:49:ASN:C	2.51	0.48
1:C:250:LEU:HD11	1:D:236:PHE:CZ	2.48	0.48
1:C:49:ASN:ND2	1:C:51:CYS:H	2.10	0.48
1:D:140:TRP:CD1	2:D:301:AVU:H2	2.49	0.48
1:A:147:TYR:CA	4:A:2063:HOH:O	2.59	0.48
1:C:49:ASN:HD22	1:C:51:CYS:H	1.62	0.48
1:A:147:TYR:N	4:A:2063:HOH:O	2.47	0.48
1:F:25:ASP:OD1	1:F:26:ILE:HG13	2.13	0.48
1:A:128:PHE:O	1:A:136:ARG:HD3	2.15	0.47
1:H:133:VAL:O	1:H:137:GLU:HG3	2.14	0.47
1:A:126:PRO:O	1:A:128:PHE:HD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ASN:CG	1:C:50:PRO:HD2	2.35	0.47
1:C:137:GLU:HG2	1:C:174:PHE:HZ	1.73	0.47
1:D:49:ASN:HB3	4:D:2055:HOH:O	2.13	0.47
1:B:128:PHE:HA	4:B:2040:HOH:O	2.13	0.47
1:D:77:TRP:CE2	4:D:2085:HOH:O	2.52	0.47
2:H:301:AVU:H3'	2:H:301:AVU:O5R	2.15	0.47
1:B:249:ARG:HG2	1:B:249:ARG:NH1	2.00	0.47
1:C:174:PHE:CD2	2:C:301:AVU:H2'	2.50	0.47
1:B:154:GLU:HG2	1:B:189:ARG:HB3	1.96	0.47
1:D:200:GLU:OE1	1:D:200:GLU:HA	2.15	0.47
1:A:133:VAL:HA	1:A:136:ARG:NH2	2.30	0.46
1:D:159:VAL:HG21	1:D:168:ALA:HB1	1.97	0.46
1:A:127:ASP:O	1:A:130:THR:HB	2.16	0.46
1:A:128:PHE:C	1:A:130:THR:H	2.17	0.46
1:F:47:PHE:HA	1:F:114:GLN:O	2.16	0.46
1:A:121:ASN:HD21	1:A:124:VAL:HG13	1.80	0.46
1:B:18:TYR:HA	1:B:22:ARG:HG2	1.96	0.46
1:B:59:LYS:HB2	1:B:59:LYS:HE3	1.76	0.46
1:G:180:LEU:HB3	1:G:181:PRO:HD3	1.98	0.46
1:A:250:LEU:HD23	1:B:250:LEU:HD12	1.97	0.45
1:F:48:LYS:NZ	4:F:2017:HOH:O	2.48	0.45
1:H:46:SER:C	1:H:48:LYS:H	2.19	0.45
1:A:98:GLU:OE2	2:A:301:AVU:N6	2.48	0.45
1:C:90:THR:HG22	3:C:1253:GOL:H12	1.99	0.45
1:A:236:PHE:O	1:B:236:PHE:HB3	2.15	0.45
1:H:42:PHE:O	1:H:46:SER:HB3	2.16	0.45
1:D:216:LYS:HB2	1:D:216:LYS:HE3	1.42	0.45
1:E:221:LYS:O	1:E:222:HIS:HB2	2.16	0.45
1:F:97:LEU:HD23	1:F:97:LEU:O	2.16	0.45
1:C:129:LYS:HG3	1:C:136:ARG:NH2	2.32	0.45
1:E:174:PHE:HB2	2:E:301:AVU:PB	2.56	0.45
1:G:54:ASP:HB2	4:G:2045:HOH:O	2.17	0.45
2:H:301:AVU:O3'	2:H:301:AVU:O1B	2.33	0.45
1:C:23:TYR:CZ	3:C:1253:GOL:H11	2.53	0.44
1:F:58:TYR:HD1	4:F:2021:HOH:O	2.01	0.44
1:F:72:ASN:HA	1:F:154:GLU:O	2.18	0.44
1:G:218:VAL:HG13	1:G:223:PHE:HB2	2.00	0.44
1:D:171:PRO:HG3	1:E:129:LYS:HD3	2.00	0.44
1:E:72:ASN:HA	1:E:154:GLU:O	2.18	0.44
1:F:77:TRP:HA	1:F:158:MET:O	2.18	0.44
1:F:137:GLU:HG2	1:F:174:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:ARG:NH2	1:F:244:ASN:ND2	2.66	0.44
1:B:142:MET:CE	4:B:2168:HOH:O	2.66	0.44
1:B:170:ARG:HD2	1:B:172:ASP:OD2	2.18	0.44
1:A:62:PHE:CZ	1:A:143:ALA:HB2	2.53	0.44
1:B:170:ARG:HD2	1:B:170:ARG:HH11	1.65	0.44
1:H:215:GLU:HB2	1:H:225:PHE:CE2	2.53	0.44
1:A:1:ILE:HG12	1:A:110:VAL:HG11	2.00	0.43
1:D:174:PHE:HB2	2:D:301:AVU:PB	2.57	0.43
1:G:250:LEU:HD23	1:G:250:LEU:HA	1.76	0.43
1:H:8:GLU:HG3	1:H:38:TRP:CE2	2.53	0.43
1:H:59:LYS:NZ	1:H:59:LYS:HB3	2.33	0.43
1:A:85:HIS:NE2	1:A:98:GLU:OE1	2.45	0.43
1:D:130:THR:O	1:E:181:PRO:HB3	2.17	0.43
1:D:241:ASP:HB3	4:D:2169:HOH:O	2.17	0.43
1:F:174:PHE:CE2	2:F:301:AVU:C2'	2.98	0.43
1:G:62:PHE:CZ	1:G:143:ALA:HB2	2.53	0.43
1:E:75:MET:HE1	1:E:156:THR:HG22	2.00	0.43
1:D:217:LEU:O	1:D:220:ALA:HB3	2.18	0.43
1:C:221:LYS:HD2	4:C:2123:HOH:O	2.18	0.43
4:A:2085:HOH:O	1:B:92:ARG:NH2	2.52	0.43
1:B:137:GLU:CD	1:B:177:LYS:HZ2	2.22	0.43
1:D:114:GLN:HG2	1:D:120:PHE:C	2.39	0.43
1:D:213:ASP:HA	1:D:216:LYS:HE2	2.00	0.43
1:D:1:ILE:N	4:D:2001:HOH:O	2.51	0.43
2:F:301:AVU:H2	4:F:2040:HOH:O	2.18	0.43
1:G:76:PHE:O	1:G:157:TYR:HA	2.19	0.43
1:B:169:TYR:CD1	1:B:214:LEU:HD13	2.54	0.43
1:B:232:ARG:NH2	4:B:2212:HOH:O	2.52	0.43
1:B:18:TYR:HA	1:B:22:ARG:CG	2.48	0.42
1:E:52:ASP:O	1:E:53:LEU:HD23	2.19	0.42
1:C:49:ASN:OD1	1:C:50:PRO:HD2	2.19	0.42
1:D:180:LEU:HB3	1:D:181:PRO:HD3	2.01	0.42
1:C:237:LEU:HD12	1:D:237:LEU:HD23	2.01	0.42
2:D:301:AVU:H8	4:D:2176:HOH:O	2.18	0.42
1:H:54:ASP:HA	1:H:134:GLN:O	2.20	0.42
1:H:144:SER:OG	1:H:179:GLU:CG	2.67	0.42
1:C:77:TRP:HA	1:C:158:MET:O	2.18	0.42
1:F:246:ARG:O	1:F:249:ARG:HG3	2.20	0.42
2:D:301:AVU:C8	4:D:2176:HOH:O	2.67	0.42
2:D:301:AVU:H2'	4:D:2172:HOH:O	2.20	0.42
1:E:251:ALA:HB2	1:F:250:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:PRO:HA	1:G:221:LYS:HE3	2.01	0.42
1:B:1:ILE:HB	1:B:125:CYS:O	2.20	0.42
1:C:249:ARG:CZ	1:C:249:ARG:HB2	2.48	0.42
1:H:137:GLU:CD	1:H:177:LYS:HZ1	2.22	0.42
1:H:37:LEU:HD23	1:H:37:LEU:HA	1.78	0.42
1:A:180:LEU:HD12	1:A:183:LEU:HD12	2.02	0.41
1:H:140:TRP:CB	1:H:174:PHE:HE2	2.31	0.41
1:H:249:ARG:HB3	1:H:249:ARG:NH1	2.35	0.41
1:D:81:TYR:OH	1:D:98:GLU:HG2	2.20	0.41
1:A:180:LEU:HD21	1:A:217:LEU:HD13	2.02	0.41
1:B:128:PHE:HB2	1:B:136:ARG:HG3	2.01	0.41
1:G:189:ARG:HD3	1:G:226:ASP:OD2	2.20	0.41
1:H:62:PHE:CZ	1:H:143:ALA:HB2	2.55	0.41
1:F:103:GLY:O	1:F:107:ASN:HB2	2.21	0.41
1:H:133:VAL:HG13	1:H:134:GLN:N	2.36	0.41
1:D:136:ARG:HG2	1:D:137:GLU:HG3	2.03	0.41
1:C:174:PHE:CE2	2:C:301:AVU:O2'	2.55	0.41
1:E:205:LYS:HB3	1:E:205:LYS:HE3	1.91	0.41
1:H:71:LYS:O	1:H:72:ASN:HB2	2.19	0.41
1:A:49:ASN:C	1:A:51:CYS:H	2.25	0.40
1:B:85:HIS:NE2	1:B:98:GLU:OE1	2.55	0.40
1:E:237:LEU:HD13	1:F:240:SER:OG	2.20	0.40
1:A:132:PRO:HB2	1:A:134:GLN:HE22	1.84	0.40
1:E:170:ARG:HH11	1:E:170:ARG:HD2	1.64	0.40
1:F:62:PHE:O	1:F:66:GLN:HB2	2.21	0.40
1:G:77:TRP:NE1	4:G:2064:HOH:O	2.30	0.40
1:H:62:PHE:O	1:H:66:GLN:HB2	2.20	0.40
1:A:66:GLN:CD	4:A:2063:HOH:O	2.50	0.40
1:G:126:PRO:HB2	1:G:130:THR:CG2	2.50	0.40
2:A:301:AVU:O1B	2:A:301:AVU:O3'	2.38	0.40
1:B:229:GLU:O	1:B:230:ASN:C	2.59	0.40
1:G:126:PRO:HB2	1:G:130:THR:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH1	1:C:154:GLU:OE1[1_545]	1.93	0.27

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	250/260 (96%)	235 (94%)	15 (6%)	0	100	100
1	B	251/260 (96%)	247 (98%)	4 (2%)	0	100	100
1	C	249/260 (96%)	239 (96%)	9 (4%)	1 (0%)	34	32
1	D	249/260 (96%)	240 (96%)	9 (4%)	0	100	100
1	E	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
1	F	250/260 (96%)	242 (97%)	7 (3%)	1 (0%)	34	32
1	G	249/260 (96%)	244 (98%)	5 (2%)	0	100	100
1	H	249/260 (96%)	239 (96%)	8 (3%)	2 (1%)	19	14
All	All	1996/2080 (96%)	1927 (96%)	65 (3%)	4 (0%)	47	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	128	PHE
1	C	133	VAL
1	H	47	PHE
1	H	175	PHE

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	220/226 (97%)	213 (97%)	7 (3%)	39	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/226 (97%)	213 (97%)	7 (3%)	39	40
1	C	220/226 (97%)	214 (97%)	6 (3%)	44	47
1	D	220/226 (97%)	215 (98%)	5 (2%)	50	53
1	E	220/226 (97%)	208 (94%)	12 (6%)	21	18
1	F	220/226 (97%)	201 (91%)	19 (9%)	10	6
1	G	220/226 (97%)	209 (95%)	11 (5%)	24	22
1	H	220/226 (97%)	207 (94%)	13 (6%)	19	16
All	All	1760/1808 (97%)	1680 (96%)	80 (4%)	27	26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	97	LEU
1	A	124	VAL
1	A	125	CYS
1	A	130	THR
1	A	205	LYS
1	A	217	LEU
1	B	59	LYS
1	B	89	ASN
1	B	172	ASP
1	B	200	GLU
1	B	242	ASN
1	B	249	ARG
1	B	250	LEU
1	C	31	ARG
1	C	64	SER
1	C	89	ASN
1	C	120	PHE
1	C	237	LEU
1	C	242	ASN
1	D	75	MET
1	D	89	ASN
1	D	201	LYS
1	D	221	LYS
1	D	246	ARG
1	E	30	VAL
1	E	55	LEU
1	E	75	MET

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Mol	Chain	Res	Type
1	E	90	THR
1	E	95	ILE
1	E	130	THR
1	E	195	LEU
1	E	221	LYS
1	E	228	VAL
1	E	237	LEU
1	E	242	ASN
1	E	246	ARG
1	F	32	SER
1	F	39	LYS
1	F	74	VAL
1	F	75	MET
1	F	106	LEU
1	F	115	ARG
1	F	122	GLU
1	F	124	VAL
1	F	127	ASP
1	F	128	PHE
1	F	129	LYS
1	F	170	ARG
1	F	184	THR
1	F	186	LYS
1	F	201	LYS
1	F	205	LYS
1	F	217	LEU
1	F	242	ASN
1	F	249	ARG
1	G	1	ILE
1	G	75	MET
1	G	106	LEU
1	G	122	GLU
1	G	123	LYS
1	G	129	LYS
1	G	130	THR
1	G	211	LEU
1	G	237	LEU
1	G	242	ASN
1	G	246	ARG
1	H	31	ARG
1	H	39	LYS
1	H	59	LYS

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Mol	Chain	Res	Type
1	H	66	GLN
1	H	73	LYS
1	H	89	ASN
1	H	97	LEU
1	H	123	LYS
1	H	130	THR
1	H	134	GLN
1	H	185	ASN
1	H	217	LEU
1	H	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	107	ASN
1	B	89	ASN
1	B	242	ASN
1	C	49	ASN
1	C	89	ASN
1	C	117	ASN
1	C	134	GLN
1	D	89	ASN
1	D	107	ASN
1	D	117	ASN
1	D	242	ASN
1	E	89	ASN
1	E	242	ASN
1	F	89	ASN
1	F	242	ASN
1	F	244	ASN
1	G	89	ASN
1	G	117	ASN
1	G	242	ASN
1	H	89	ASN
1	H	117	ASN
1	H	185	ASN
1	H	242	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	AVU	B	301	1	33,38,38	1.12	3 (9%)	37,58,58	1.76	8 (21%)
2	AVU	G	301	1	33,38,38	1.04	2 (6%)	37,58,58	1.58	5 (13%)
2	AVU	C	301	1	33,38,38	1.23	3 (9%)	37,58,58	2.25	13 (35%)
3	GOL	F	1253	-	5,5,5	0.28	0	5,5,5	0.49	0
2	AVU	D	301	1	33,38,38	0.97	2 (6%)	37,58,58	1.50	5 (13%)
2	AVU	E	301	1	33,38,38	1.06	3 (9%)	37,58,58	1.66	8 (21%)
3	GOL	C	1253	-	5,5,5	0.63	0	5,5,5	1.11	0
2	AVU	A	301	1	33,38,38	0.97	2 (6%)	37,58,58	1.47	4 (10%)
2	AVU	F	301	1	33,38,38	1.09	3 (9%)	37,58,58	1.83	11 (29%)
2	AVU	H	301	1	33,38,38	0.97	2 (6%)	37,58,58	1.67	8 (21%)
3	GOL	D	1253	-	5,5,5	0.56	0	5,5,5	0.53	0

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	AVU	B	301	1	-	5/18/51/51	0/4/4/4
2	AVU	G	301	1	-	4/18/51/51	0/4/4/4
2	AVU	C	301	1	-	3/18/51/51	0/4/4/4
3	GOL	F	1253	-	-	2/4/4/4	-
2	AVU	D	301	1	-	6/18/51/51	0/4/4/4
2	AVU	E	301	1	-	4/18/51/51	0/4/4/4
3	GOL	C	1253	-	-	1/4/4/4	-
2	AVU	A	301	1	-	5/18/51/51	0/4/4/4
2	AVU	F	301	1	-	2/18/51/51	0/4/4/4
2	AVU	H	301	1	-	4/18/51/51	0/4/4/4
3	GOL	D	1253	-	-	3/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	AVU	O4'-C1'	3.33	1.45	1.41
2	B	301	AVU	O4'-C1'	2.99	1.45	1.41
2	F	301	AVU	O4'-C1'	2.98	1.45	1.41
2	G	301	AVU	O4'-C1'	2.95	1.45	1.41
2	D	301	AVU	O4'-C1'	2.94	1.45	1.41
2	A	301	AVU	O4'-C1'	2.92	1.45	1.41
2	D	301	AVU	PB-O5R	2.62	1.69	1.59
2	C	301	AVU	C2'-C1'	-2.55	1.49	1.53
2	E	301	AVU	PB-O5R	2.45	1.69	1.59
2	C	301	AVU	PB-O5R	2.43	1.69	1.59
2	E	301	AVU	F2R-C2R	-2.41	1.34	1.40
2	A	301	AVU	C2-N3	2.41	1.36	1.32
2	H	301	AVU	O4'-C1'	2.35	1.44	1.41
2	H	301	AVU	F2R-C2R	-2.32	1.35	1.40
2	G	301	AVU	O4R-C1R	-2.26	1.38	1.43
2	F	301	AVU	C2'-C1'	-2.24	1.50	1.53
2	F	301	AVU	F2R-C2R	-2.21	1.35	1.40
2	E	301	AVU	O4'-C1'	2.20	1.44	1.41
2	B	301	AVU	O4R-C1R	-2.14	1.39	1.43
2	B	301	AVU	C2-N3	2.04	1.35	1.32

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	AVU	N3-C2-N1	-5.94	119.39	128.68
2	F	301	AVU	N3-C2-N1	-5.51	120.06	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	AVU	N3-C2-N1	-5.40	120.23	128.68
2	B	301	AVU	N3-C2-N1	-5.31	120.39	128.68
2	H	301	AVU	N3-C2-N1	-5.23	120.50	128.68
2	E	301	AVU	N3-C2-N1	-5.10	120.71	128.68
2	C	301	AVU	F2R-C2R-C3R	5.00	113.08	108.57
2	D	301	AVU	N3-C2-N1	-4.98	120.90	128.68
2	C	301	AVU	N3-C2-N1	-4.80	121.17	128.68
2	C	301	AVU	C1'-N9-C4	-4.77	118.26	126.64
2	C	301	AVU	C2R-C3R-C4R	4.60	108.37	102.34
2	F	301	AVU	C1'-N9-C4	-4.29	119.10	126.64
2	C	301	AVU	C3'-C2'-C1'	4.23	107.34	100.98
2	C	301	AVU	O3R-C3R-C2R	-4.10	96.57	111.44
2	B	301	AVU	O5R-C5R-C4R	3.86	122.29	108.99
2	H	301	AVU	O4R-C4R-C3R	3.62	107.91	104.70
2	F	301	AVU	C2R-C3R-C4R	3.52	106.96	102.34
2	E	301	AVU	C1'-N9-C4	-3.44	120.59	126.64
2	A	301	AVU	C1'-N9-C4	-3.30	120.85	126.64
2	H	301	AVU	F2R-C2R-C3R	-3.24	105.65	108.57
2	B	301	AVU	C2R-C3R-C4R	3.16	106.48	102.34
2	E	301	AVU	PB-O3A-PA	-3.14	122.07	132.83
2	E	301	AVU	C2R-C3R-C4R	3.11	106.42	102.34
2	G	301	AVU	C3'-C2'-C1'	3.05	105.57	100.98
2	H	301	AVU	C1'-N9-C4	-3.01	121.35	126.64
2	A	301	AVU	C2R-C3R-C4R	2.85	106.08	102.34
2	F	301	AVU	O4R-C1R-C2R	2.82	109.24	104.88
2	C	301	AVU	C4-C5-N7	-2.80	106.48	109.40
2	F	301	AVU	O3R-C3R-C2R	-2.70	101.67	111.44
2	B	301	AVU	C3'-C2'-C1'	2.64	104.96	100.98
2	H	301	AVU	O5'-C5'-C4'	-2.64	99.91	108.99
2	B	301	AVU	F2R-C2R-C3R	2.63	110.95	108.57
2	C	301	AVU	O2'-C2'-C1'	-2.62	101.17	110.85
2	D	301	AVU	C2R-C3R-C4R	2.50	105.61	102.34
2	C	301	AVU	O2A-PA-O1A	2.48	124.48	112.24
2	D	301	AVU	C1'-N9-C4	-2.47	122.30	126.64
2	F	301	AVU	O2A-PA-O1A	2.46	124.42	112.24
2	E	301	AVU	C1R-C2R-C3R	2.46	107.13	104.21
2	F	301	AVU	O2'-C2'-C3'	-2.45	103.88	111.82
2	H	301	AVU	O4'-C4'-C5'	2.42	117.33	109.37
2	F	301	AVU	O3'-C3'-C2'	-2.33	104.30	111.82
2	G	301	AVU	C2R-C3R-C4R	2.26	105.30	102.34
2	F	301	AVU	O4'-C4'-C5'	2.26	116.80	109.37
2	C	301	AVU	C5-C6-N6	2.25	123.77	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	AVU	C5'-C4'-C3'	-2.23	106.83	115.18
2	B	301	AVU	O4'-C4'-C3'	2.22	109.50	105.11
2	E	301	AVU	C1R-O4R-C4R	2.22	113.34	108.16
2	C	301	AVU	C1R-O4R-C4R	2.20	113.30	108.16
2	F	301	AVU	C2-N1-C6	2.19	122.50	118.75
2	D	301	AVU	C4-C5-N7	-2.19	107.12	109.40
2	B	301	AVU	N6-C6-N1	2.17	123.08	118.57
2	E	301	AVU	O2A-PA-O1A	2.15	122.85	112.24
2	E	301	AVU	O3R-C3R-C4R	-2.15	104.85	111.05
2	G	301	AVU	O2A-PA-O1A	2.13	122.75	112.24
2	A	301	AVU	C4-C5-N7	-2.11	107.20	109.40
2	H	301	AVU	C1R-C2R-C3R	2.10	106.70	104.21
2	G	301	AVU	O3R-C3R-C2R	-2.09	103.88	111.44
2	F	301	AVU	O5'-C5'-C4'	-2.09	101.81	108.99
2	C	301	AVU	O5R-C5R-C4R	2.07	116.13	108.99
2	B	301	AVU	PB-O3A-PA	-2.07	125.72	132.83
2	D	301	AVU	C2-N1-C6	2.04	122.25	118.75
2	C	301	AVU	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	AVU	C5'-O5'-PA-O2A
2	B	301	AVU	O4'-C4'-C5'-O5'
2	B	301	AVU	C4R-C5R-O5R-PB
2	C	301	AVU	C4R-C5R-O5R-PB
2	D	301	AVU	PB-O3A-PA-O5'
2	D	301	AVU	C5'-O5'-PA-O3A
3	D	1253	GOL	O1-C1-C2-C3
3	F	1253	GOL	C1-C2-C3-O3
2	D	301	AVU	O4'-C4'-C5'-O5'
2	G	301	AVU	C3'-C4'-C5'-O5'
2	G	301	AVU	O4'-C4'-C5'-O5'
2	D	301	AVU	C3'-C4'-C5'-O5'
2	A	301	AVU	C4R-C5R-O5R-PB
2	D	301	AVU	C4R-C5R-O5R-PB
3	F	1253	GOL	O2-C2-C3-O3
2	E	301	AVU	C4R-C5R-O5R-PB
2	G	301	AVU	C4R-C5R-O5R-PB
3	D	1253	GOL	O1-C1-C2-O2
2	B	301	AVU	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	F	301	AVU	C4R-C5R-O5R-PB
2	A	301	AVU	PB-O3A-PA-O5'
2	B	301	AVU	PB-O3A-PA-O5'
2	C	301	AVU	PB-O3A-PA-O5'
2	G	301	AVU	PB-O3A-PA-O5'
2	B	301	AVU	C3'-C4'-C5'-O5'
2	E	301	AVU	C4'-C5'-O5'-PA
3	C	1253	GOL	O2-C2-C3-O3
2	H	301	AVU	C4R-C5R-O5R-PB
2	D	301	AVU	C5'-O5'-PA-O1A
3	D	1253	GOL	C1-C2-C3-O3
2	A	301	AVU	O4'-C4'-C5'-O5'
2	C	301	AVU	O4'-C4'-C5'-O5'
2	E	301	AVU	PA-O3A-PB-O2B
2	H	301	AVU	PA-O3A-PB-O1B
2	H	301	AVU	PA-O3A-PB-O2B
2	A	301	AVU	C5'-O5'-PA-O1A
2	E	301	AVU	O4'-C4'-C5'-O5'
2	F	301	AVU	O4'-C4'-C5'-O5'
2	H	301	AVU	O4'-C4'-C5'-O5'

There are no ring outliers.

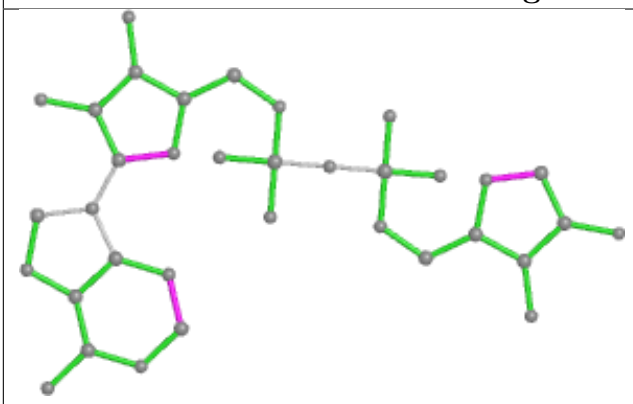
9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	AVU	2	0
2	C	301	AVU	2	0
2	D	301	AVU	10	0
2	E	301	AVU	3	0
3	C	1253	GOL	2	0
2	A	301	AVU	5	0
2	F	301	AVU	4	0
2	H	301	AVU	3	0
3	D	1253	GOL	1	0

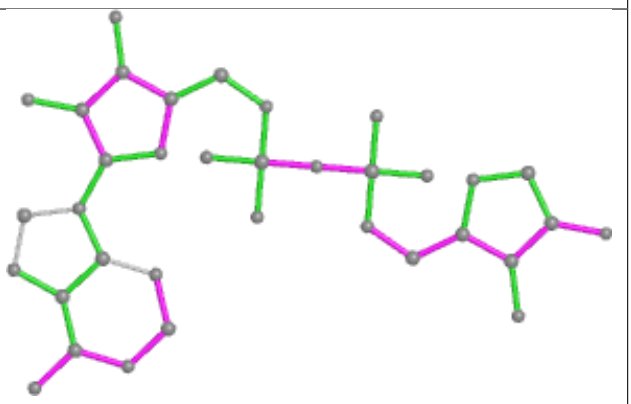
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

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

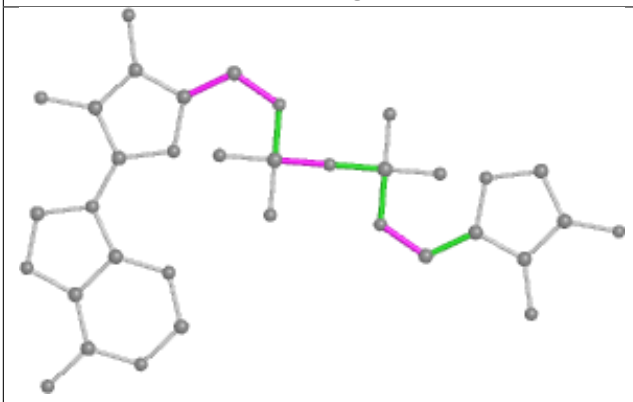
Ligand AVU B 301



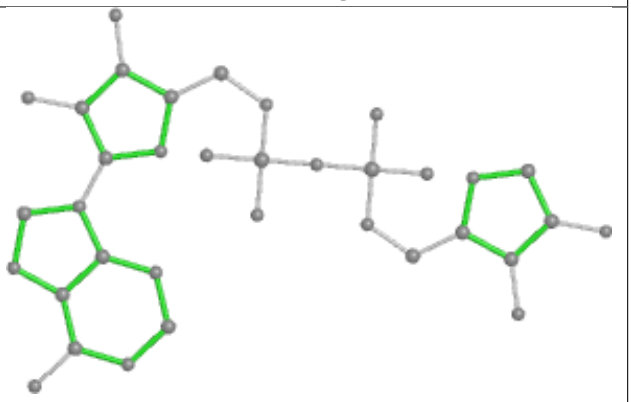
Bond lengths



Bond angles

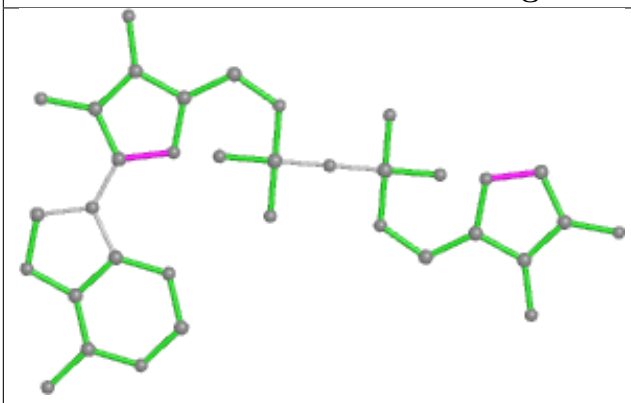


Torsions

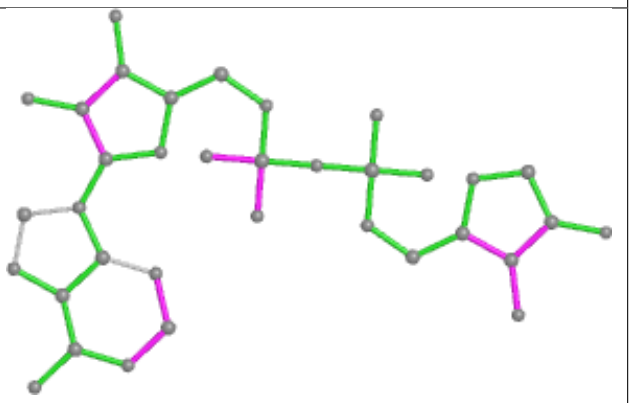


Rings

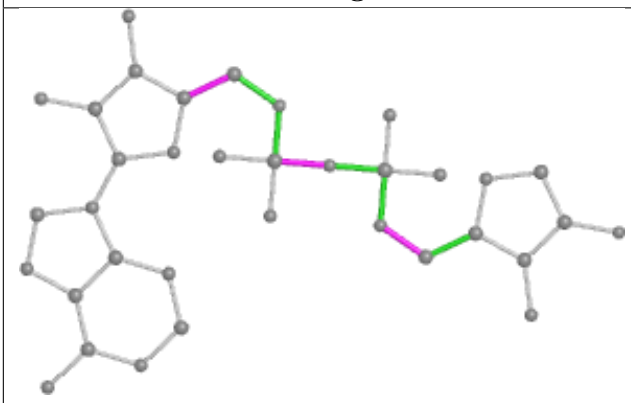
Ligand AVU G 301



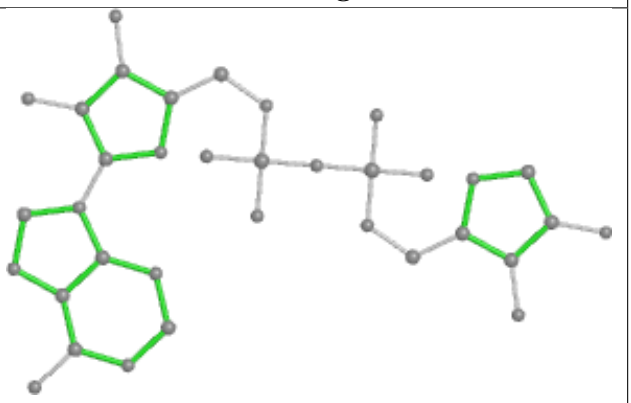
Bond lengths



Bond angles

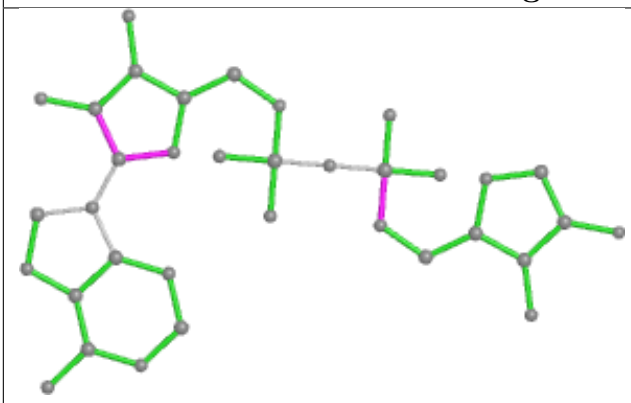


Torsions

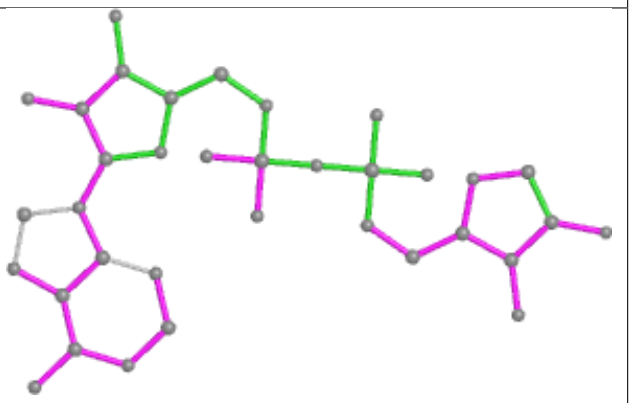


Rings

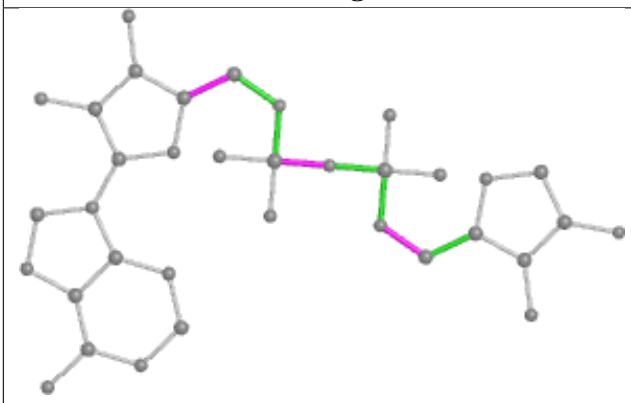
Ligand AVU C 301



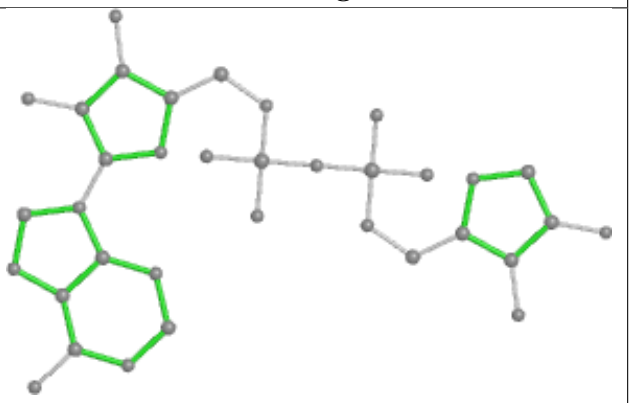
Bond lengths



Bond angles

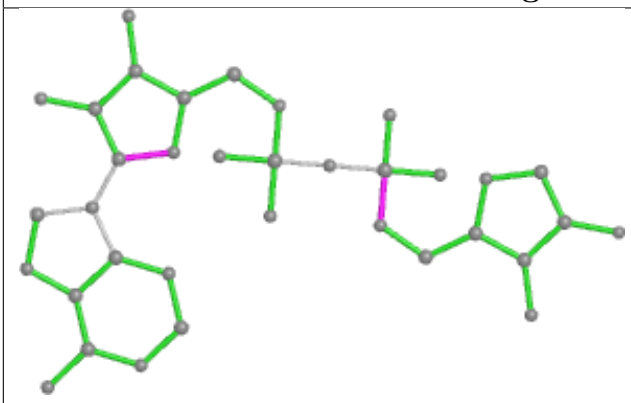


Torsions



Rings

Ligand AVU D 301



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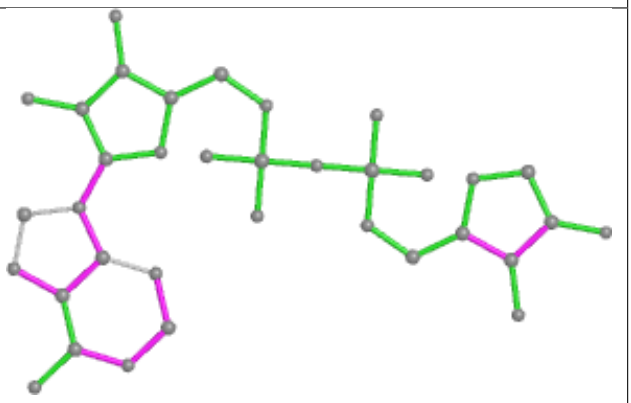
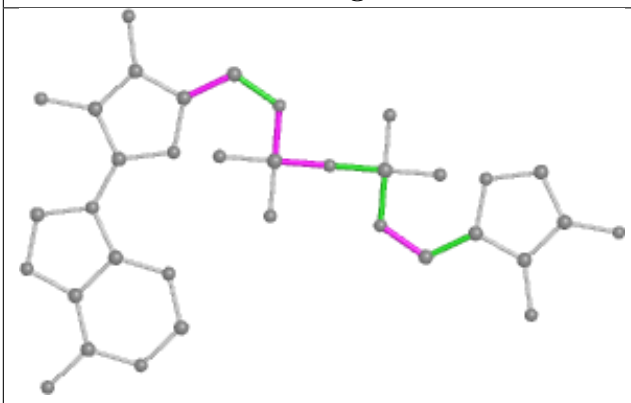
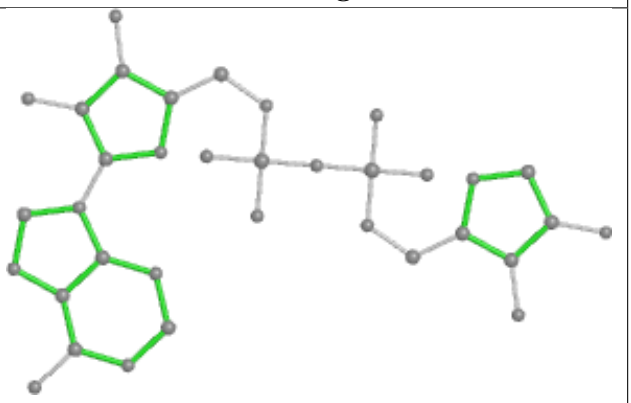


Bond angles

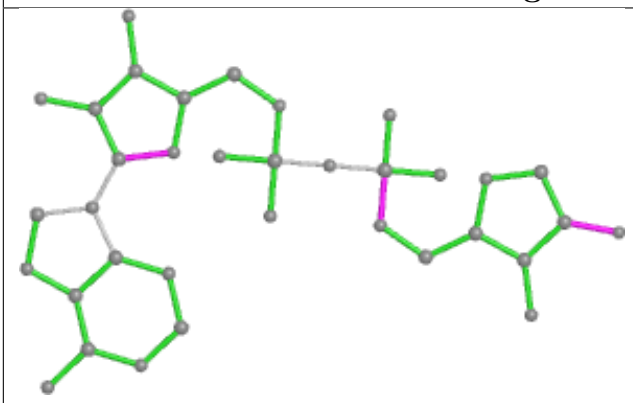


Torsions

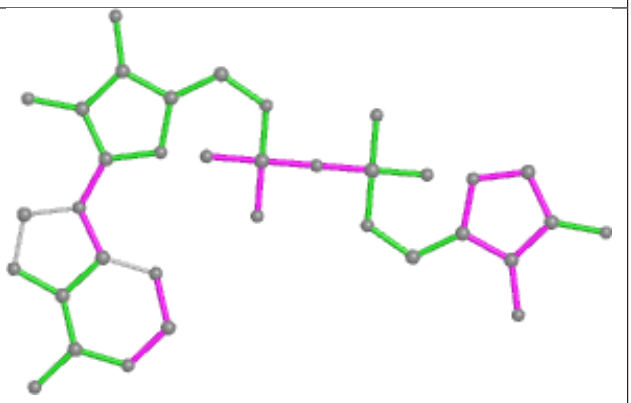


Rings

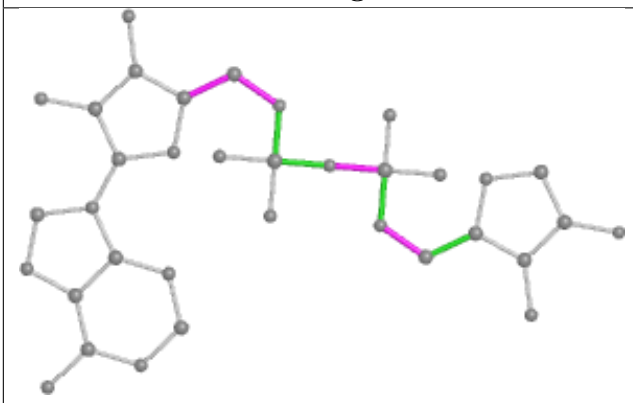
Ligand AVU E 301



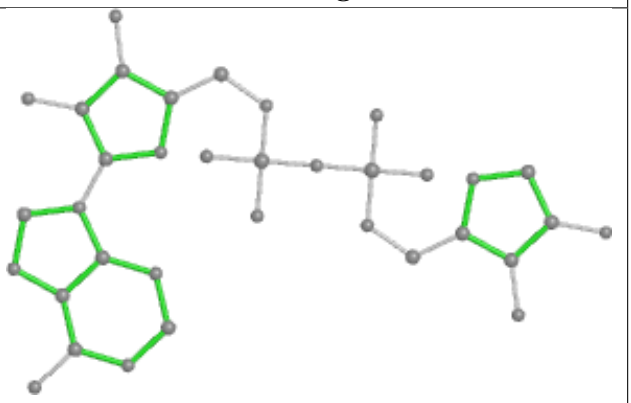
Bond lengths



Bond angles

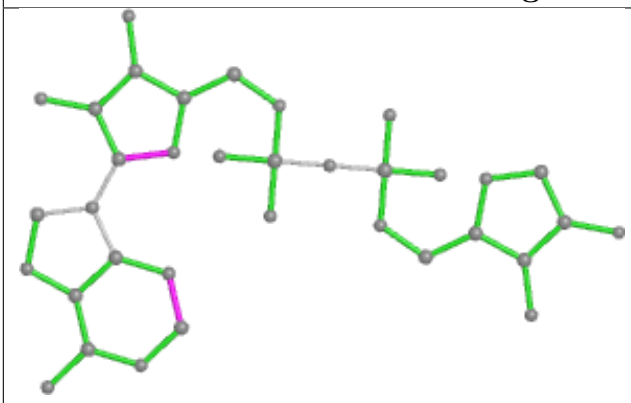


Torsions

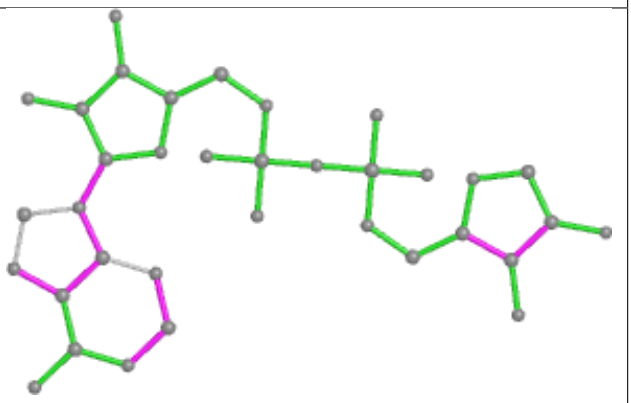


Rings

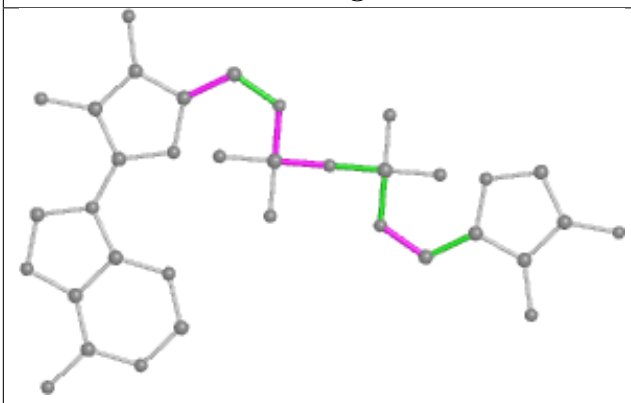
Ligand AVU A 301



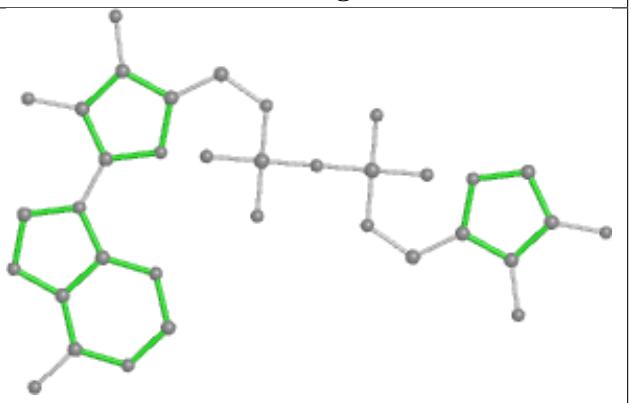
Bond lengths



Bond angles

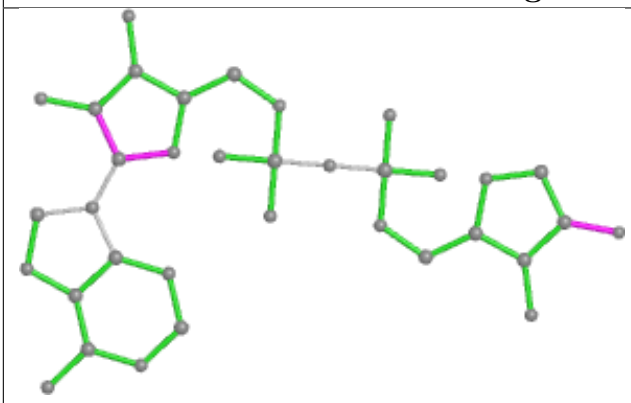


Torsions

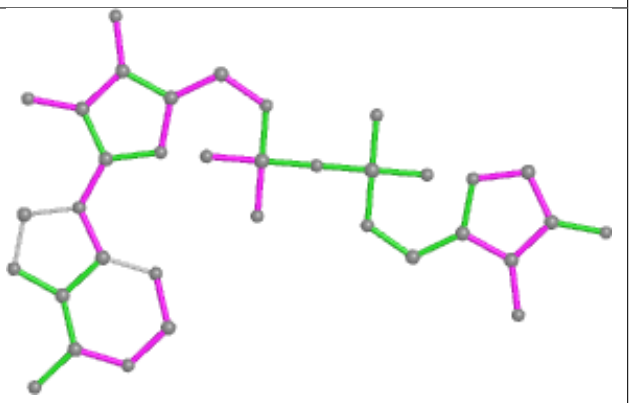


Rings

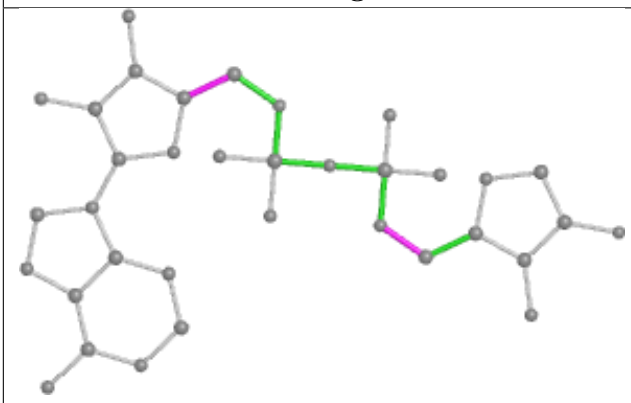
Ligand AVU F 301



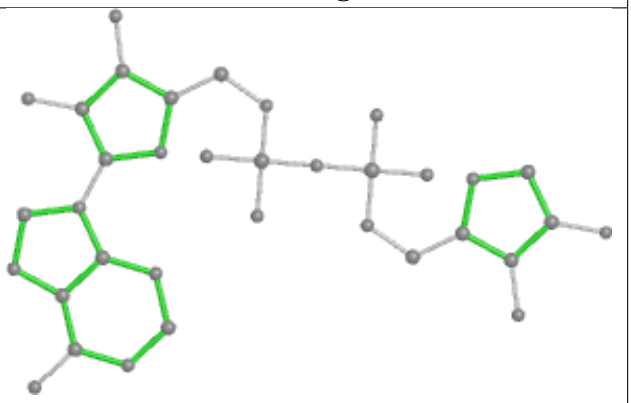
Bond lengths



Bond angles

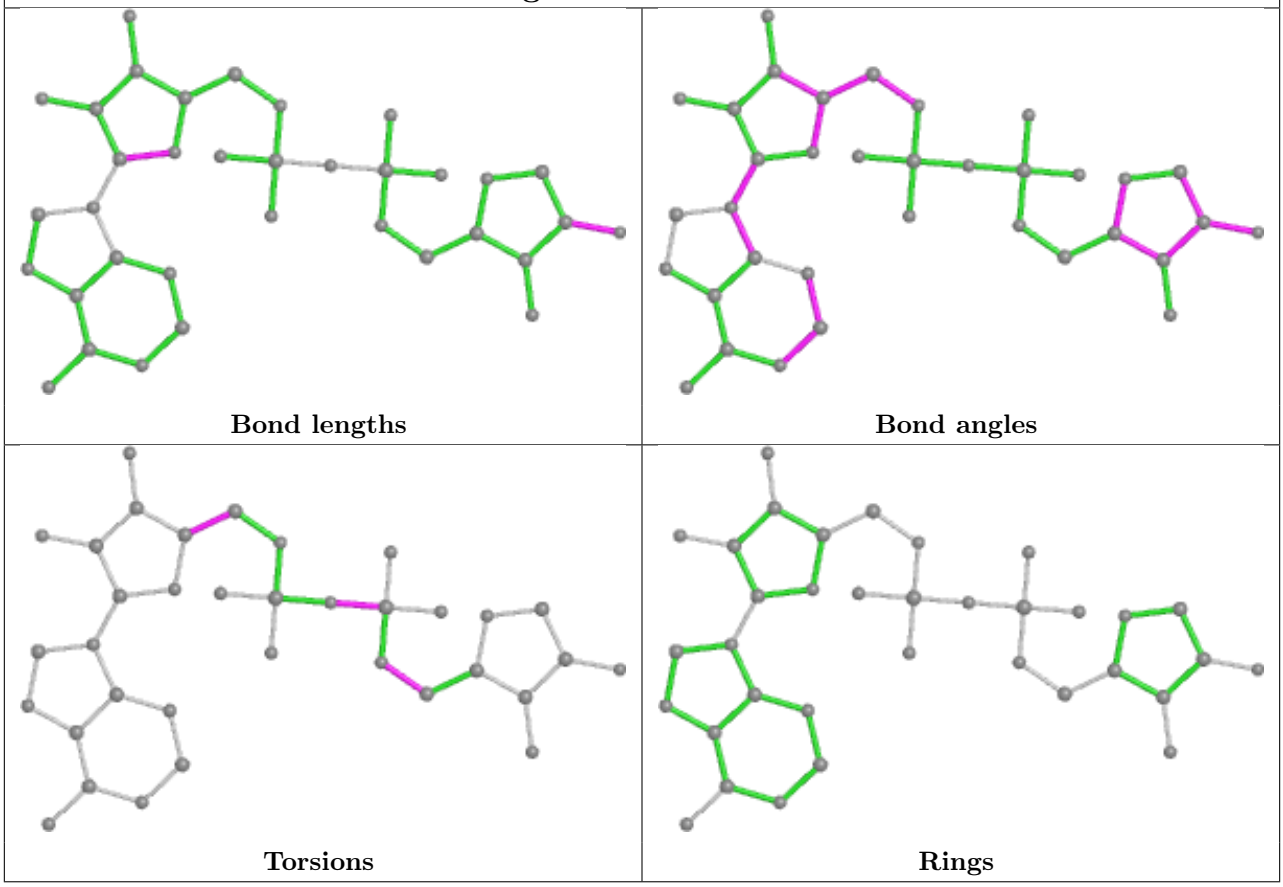


Torsions



Rings

Ligand AVU H 301



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	252/260 (96%)	0.11	14 (5%)	24	29	21, 42, 74, 90	0
1	B	253/260 (97%)	-0.27	2 (0%)	86	88	19, 30, 49, 55	0
1	C	251/260 (96%)	0.08	18 (7%)	15	19	21, 33, 70, 86	0
1	D	251/260 (96%)	-0.19	4 (1%)	72	76	19, 34, 54, 63	0
1	E	251/260 (96%)	-0.10	7 (2%)	53	59	25, 40, 59, 71	0
1	F	252/260 (96%)	0.31	16 (6%)	20	24	33, 53, 78, 95	0
1	G	251/260 (96%)	-0.15	5 (1%)	65	69	22, 36, 56, 64	0
1	H	251/260 (96%)	0.64	33 (13%)	3	4	40, 69, 98, 113	0
All	All	2012/2080 (96%)	0.05	99 (4%)	29	35	19, 40, 80, 113	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	PHE	8.7
1	F	128	PHE	7.5
1	C	128	PHE	6.2
1	A	128	PHE	5.8
1	H	47	PHE	5.6
1	H	43	LYS	4.8
1	A	127	ASP	4.5
1	E	47	PHE	4.5
1	F	130	THR	4.5
1	F	0	ALA	4.1
1	H	130	THR	4.0
1	H	134	GLN	3.9
1	F	1	ILE	3.9
1	H	63	THR	3.9
1	A	126	PRO	3.7
1	A	49	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1	ILE	3.6
1	F	174	PHE	3.6
1	H	127	ASP	3.6
1	F	133	VAL	3.5
1	H	1	ILE	3.4
1	H	49	ASN	3.4
1	H	116	ALA	3.3
1	H	124	VAL	3.3
1	F	129	LYS	3.3
1	E	115	ARG	3.3
1	E	128	PHE	3.2
1	F	126	PRO	3.2
1	C	130	THR	3.2
1	H	39	LYS	3.1
1	A	130	THR	3.0
1	E	31	ARG	2.9
1	H	188	THR	2.9
1	D	115	ARG	2.9
1	H	129	LYS	2.9
1	H	51	CYS	2.9
1	F	127	ASP	2.9
1	A	129	LYS	2.9
1	H	123	LYS	2.9
1	H	174	PHE	2.8
1	C	123	LYS	2.8
1	H	153	GLY	2.8
1	C	1	ILE	2.8
1	C	129	LYS	2.8
1	C	131	CYS	2.7
1	A	124	VAL	2.7
1	H	181	PRO	2.7
1	H	132	PRO	2.7
1	C	2	VAL	2.6
1	C	127	ASP	2.6
1	H	135	ALA	2.6
1	F	131	CYS	2.6
1	G	115	ARG	2.6
1	C	136	ARG	2.6
1	G	1	ILE	2.6
1	H	246	ARG	2.6
1	G	165	LYS	2.6
1	G	128	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	131	CYS	2.6
1	H	131	CYS	2.6
1	A	164	PRO	2.5
1	F	97	LEU	2.5
1	E	116	ALA	2.5
1	F	76	PHE	2.5
1	H	117	ASN	2.5
1	A	125	CYS	2.5
1	C	174	PHE	2.5
1	B	174	PHE	2.4
1	F	157	TYR	2.4
1	C	49	ASN	2.4
1	A	115	ARG	2.4
1	C	50	PRO	2.4
1	H	77	TRP	2.4
1	H	55	LEU	2.4
1	D	250	LEU	2.3
1	A	113	GLY	2.3
1	D	251	ALA	2.3
1	C	124	VAL	2.3
1	H	133	VAL	2.3
1	H	115	ARG	2.3
1	C	148	ALA	2.3
1	D	1	ILE	2.3
1	E	159	VAL	2.2
1	C	116	ALA	2.2
1	C	250	LEU	2.2
1	H	136	ARG	2.2
1	G	174	PHE	2.1
1	B	-1	ALA	2.1
1	H	31	ARG	2.1
1	E	220	ALA	2.1
1	H	25	ASP	2.1
1	H	53	LEU	2.1
1	C	120	PHE	2.1
1	F	188	THR	2.1
1	H	36	ALA	2.1
1	A	222	HIS	2.1
1	F	244	ASN	2.0
1	C	53	LEU	2.0
1	F	124	VAL	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)

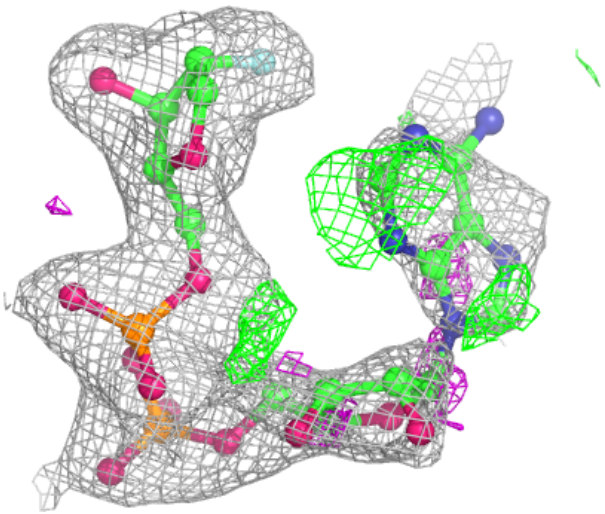
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

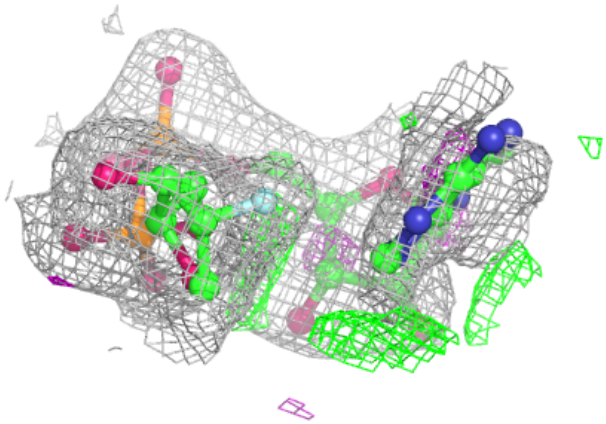
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	F	1253	6/6	0.79	0.26	67,68,70,71	0
2	AVU	G	301	35/35	0.91	0.18	30,58,97,98	0
2	AVU	C	301	35/35	0.93	0.14	31,53,84,87	0
2	AVU	E	301	35/35	0.93	0.12	28,55,84,84	0
2	AVU	A	301	35/35	0.93	0.13	49,61,87,89	0
2	AVU	B	301	35/35	0.93	0.16	30,56,78,81	0
2	AVU	D	301	35/35	0.94	0.14	36,60,94,94	0
2	AVU	H	301	35/35	0.95	0.15	67,72,90,91	0
3	GOL	C	1253	6/6	0.95	0.09	29,40,46,48	0
3	GOL	D	1253	6/6	0.95	0.11	35,46,52,53	0
2	AVU	F	301	35/35	0.95	0.18	47,59,71,71	0

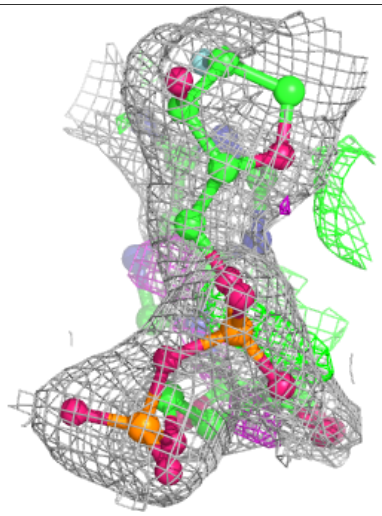
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AVU G 301:

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

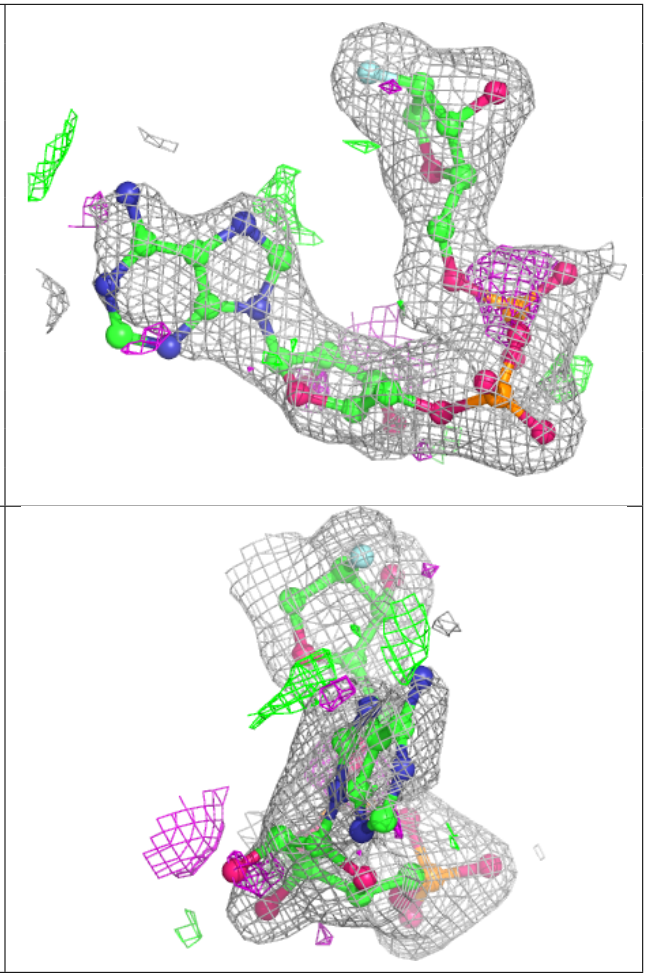






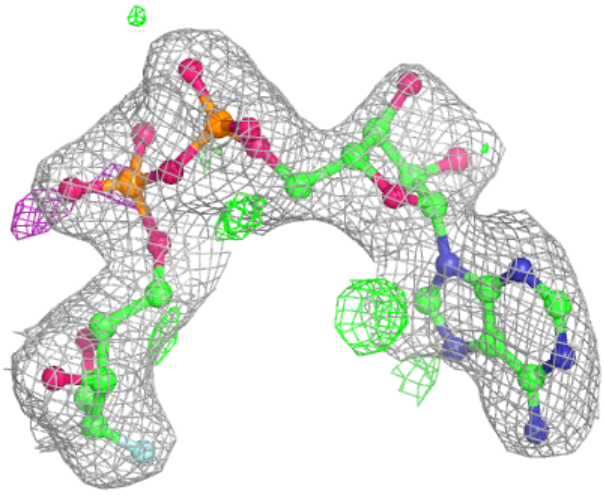
Electron density around AVU C 301:

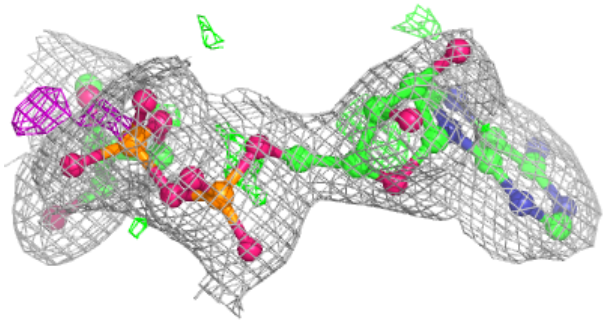
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

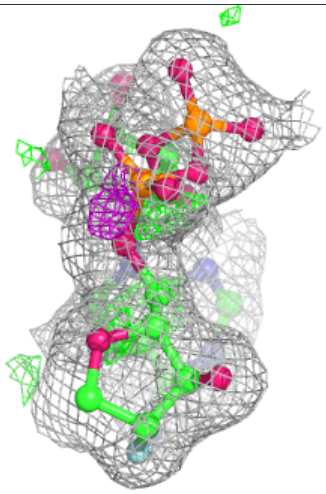


Electron density around AVU E 301:

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

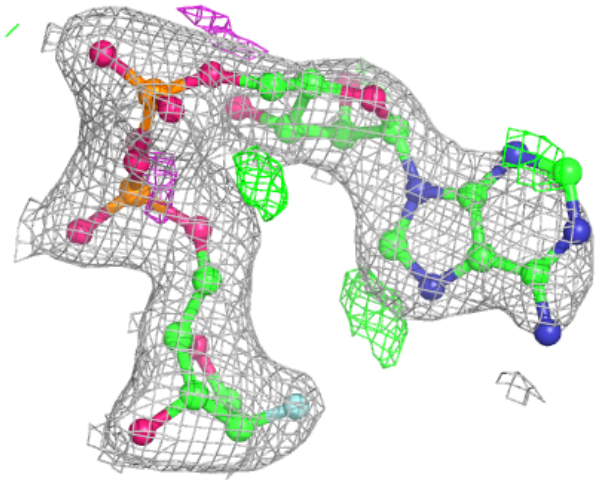


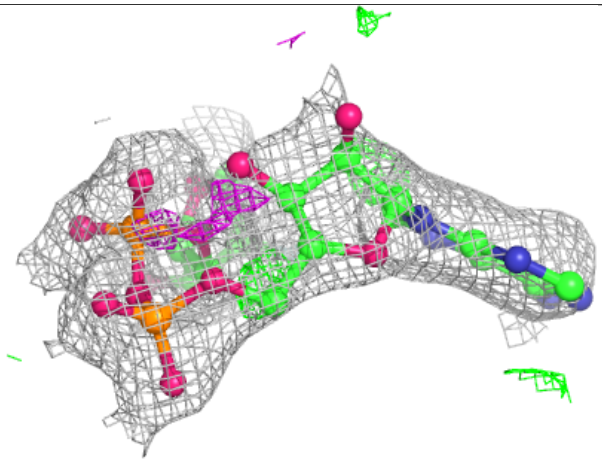


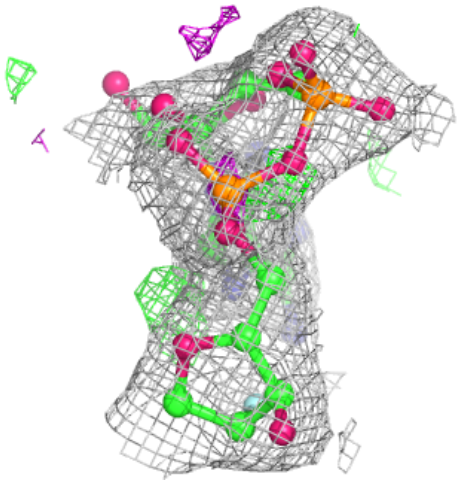


Electron density around AVU A 301:

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

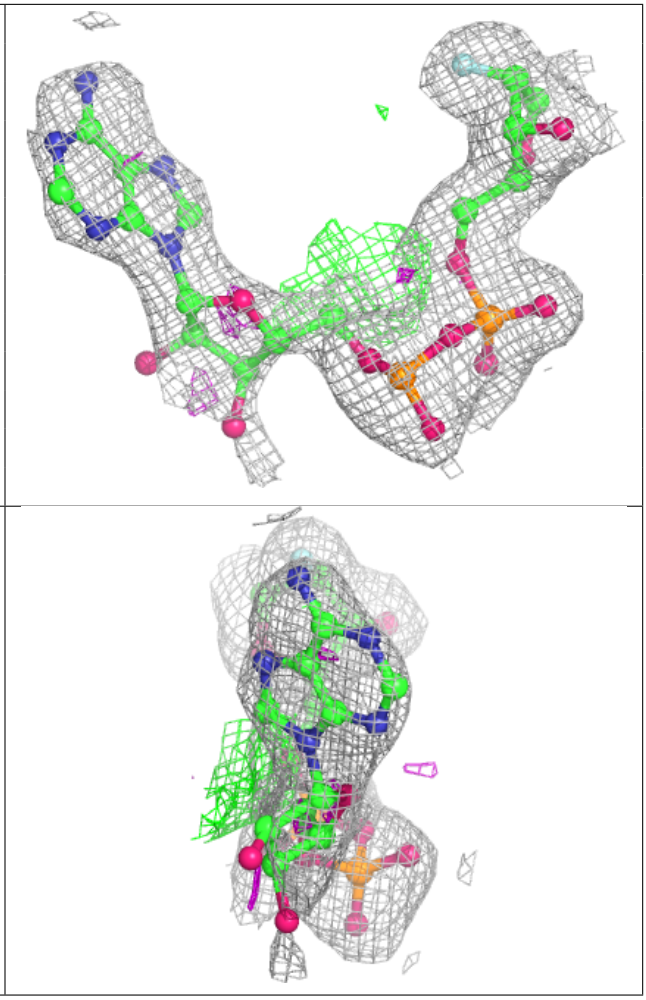






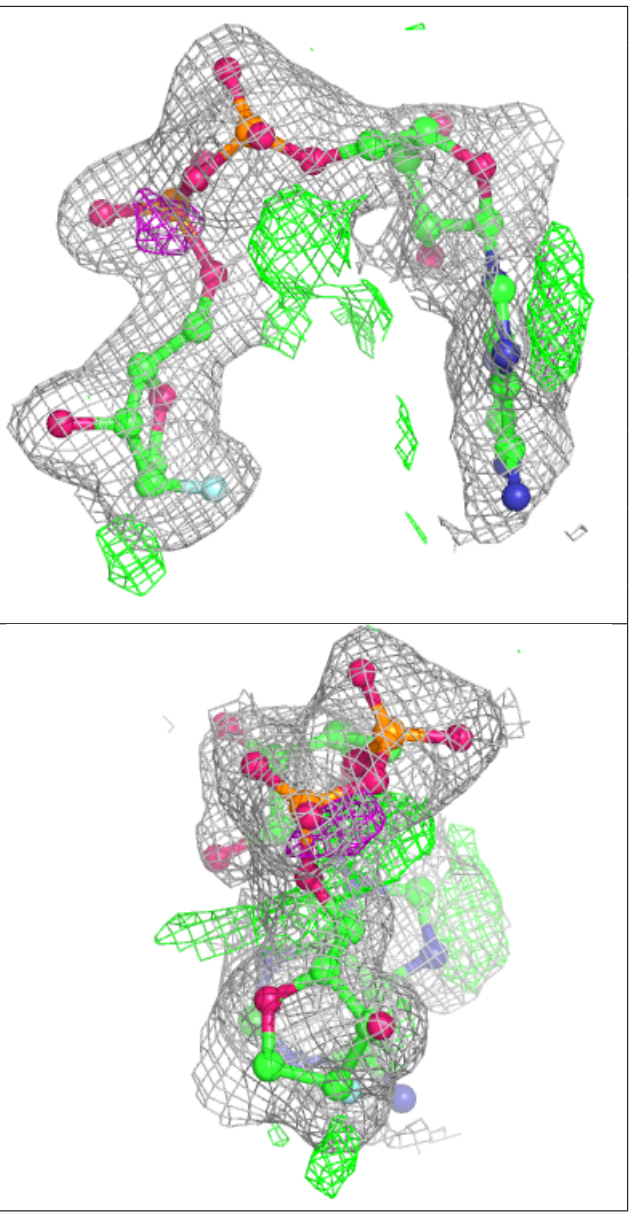
Electron density around AVU B 301:

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



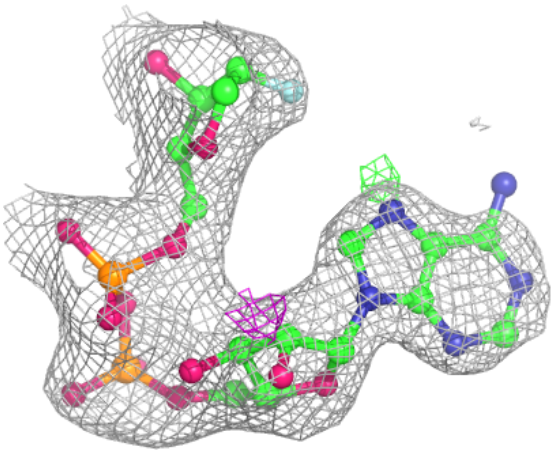
Electron density around AVU D 301:

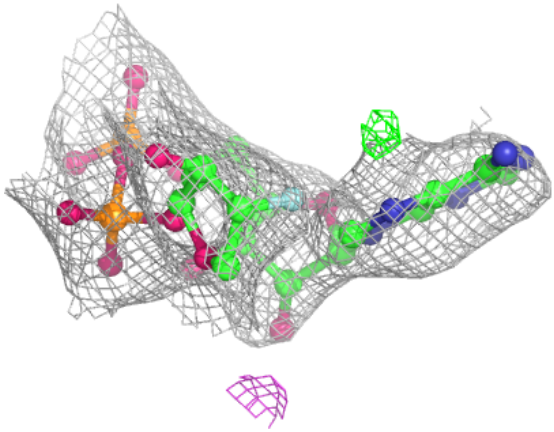
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

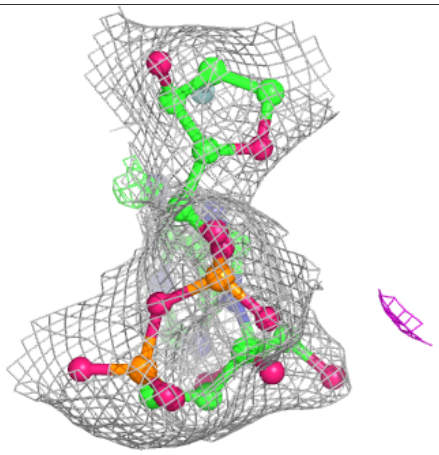


Electron density around AVU H 301:

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

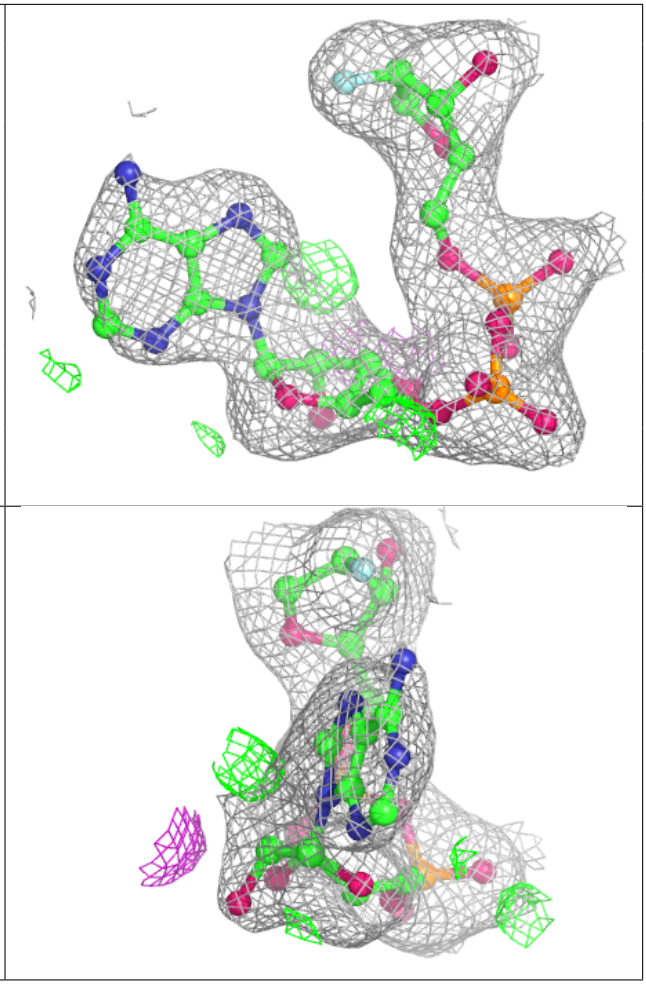






Electron density around AVU F 301:

$2mF_o$-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.