



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:30 PM BST

PDB ID : 3ZWW  
Title : Crystal structure of ADP-ribosyl cyclase complexed with ara-2'F-ADP- ribose at 2.3 angstrom  
Authors : Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.  
Deposited on : 2011-08-03  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

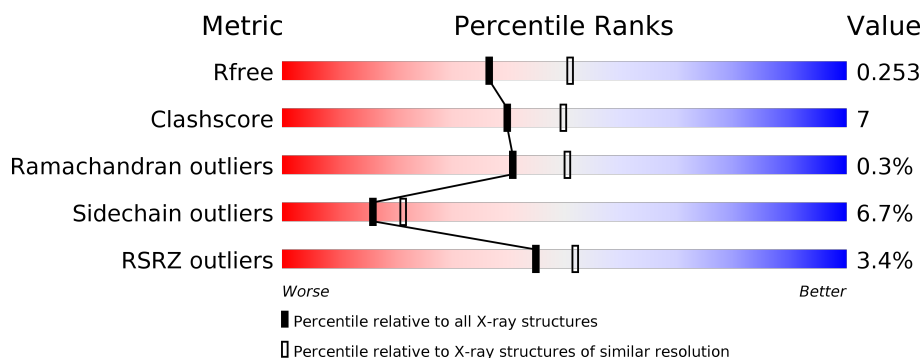
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	
1	D	260	
1	E	260	
1	F	260	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	260	<div><div>%</div><div><div></div><div>77%</div><div>18%</div><div></div><div></div></div></div>
1	H	260	<div><div>6%</div><div><div></div><div>77%</div><div>17%</div><div></div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16769 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
1	A	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	B	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	C	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	D	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	E	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	F	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	G	251	Total	C	N	O	S	0	0	0
			2012	1288	342	368	14			
1	H	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			

There are 16 discrepancies between the modelled and reference sequences:

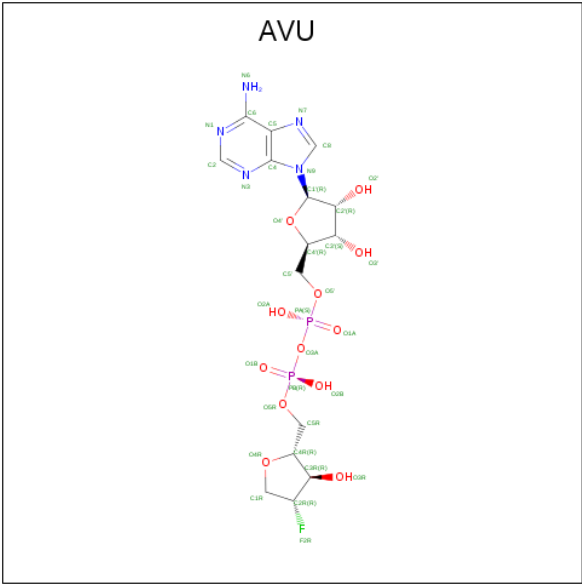
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P29241
A	0	ALA	-	expression tag	UNP P29241
B	-1	ALA	-	expression tag	UNP P29241
B	0	ALA	-	expression tag	UNP P29241
C	-1	ALA	-	expression tag	UNP P29241
C	0	ALA	-	expression tag	UNP P29241
D	-1	ALA	-	expression tag	UNP P29241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

*Continued on next page...*

Continued from previous page...

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<sub>15</sub>H<sub>22</sub>FN<sub>5</sub>O<sub>12</sub>P<sub>2</sub>).



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

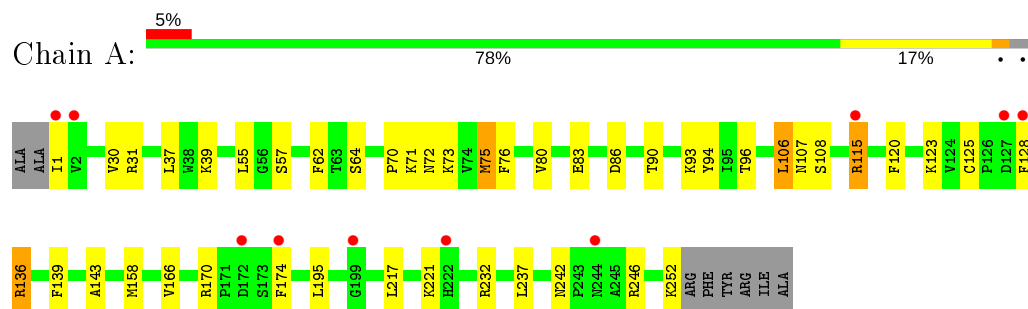
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total 36	O 36	0	0
3	B	84	Total 84	O 84	0	0
3	C	62	Total 62	O 62	0	0
3	D	56	Total 56	O 56	0	0
3	E	48	Total 48	O 48	0	0
3	F	16	Total 16	O 16	0	0
3	G	49	Total 49	O 49	0	0
3	H	22	Total 22	O 22	0	0

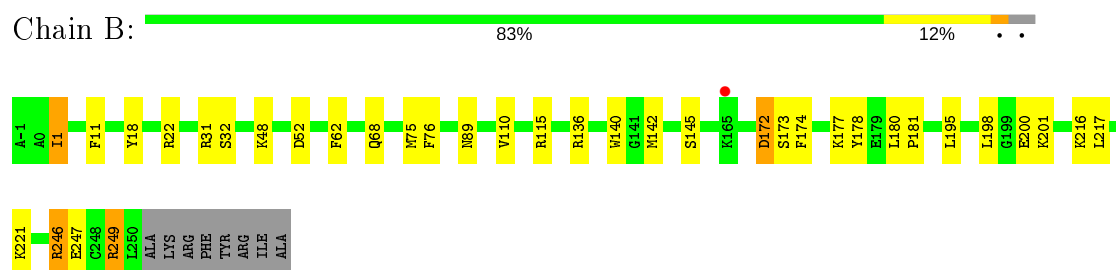
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: ADP-RIBOSYL CYCLASE

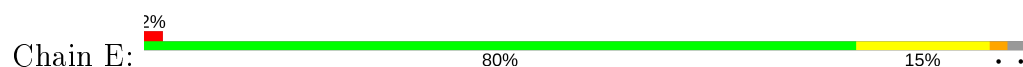


#### • Molecule 1: ADP-RIBOSYL CYCLASE

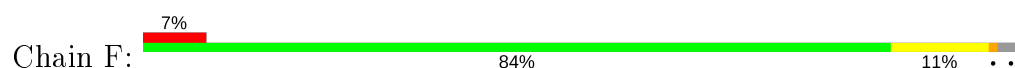




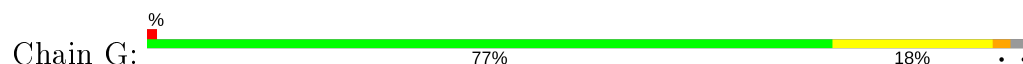
• Molecule 1: ADP-RIBOSYL CYCLASE



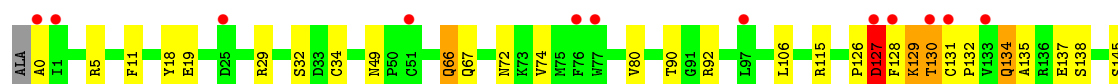
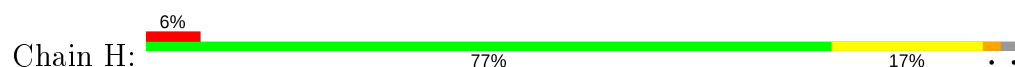
• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.96 Å 77.52 Å 140.50 Å 88.00° 89.16° 88.29°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.86-2.30) 71.4 (29.86-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.200 , 0.257 0.196 , 0.253	Depositor DCC
$R_{free}$ test set	4096 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l 0.026 for -h,k,-l 0.009 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.93	0/2069	0.88	2/2800 (0.1%)
1	B	1.09	3/2069 (0.1%)	0.91	1/2800 (0.0%)
1	C	1.05	4/2064 (0.2%)	0.91	1/2793 (0.0%)
1	D	0.98	2/2064 (0.1%)	0.90	2/2793 (0.1%)
1	E	1.04	4/2064 (0.2%)	0.92	5/2793 (0.2%)
1	F	0.80	0/2069	0.81	0/2800
1	G	1.02	5/2064 (0.2%)	0.92	3/2793 (0.1%)
1	H	0.82	1/2069 (0.0%)	0.80	1/2800 (0.0%)
All	All	0.97	19/16532 (0.1%)	0.88	15/22372 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	ASP	CB-CG	9.42	1.71	1.51
1	C	19	GLU	CG-CD	6.97	1.62	1.51
1	C	15	CYS	CB-SG	-6.73	1.70	1.82
1	E	174	PHE	CG-CD2	6.17	1.48	1.38
1	D	206	CYS	CB-SG	6.06	1.92	1.82
1	E	51	CYS	CB-SG	5.99	1.92	1.82
1	G	140	TRP	CB-CG	5.91	1.60	1.50
1	D	83	GLU	CG-CD	5.89	1.60	1.51
1	G	34	CYS	CB-SG	5.87	1.92	1.82
1	C	174	PHE	CG-CD2	5.73	1.47	1.38
1	B	140	TRP	CB-CG	5.64	1.60	1.50
1	G	174	PHE	CE1-CZ	5.50	1.47	1.37
1	H	34	CYS	CB-SG	5.41	1.91	1.82
1	G	98	GLU	CB-CG	5.27	1.62	1.52
1	C	174	PHE	CE1-CZ	5.20	1.47	1.37
1	G	174	PHE	CG-CD2	5.16	1.46	1.38
1	E	174	PHE	CE1-CZ	5.12	1.47	1.37
1	E	174	PHE	CD1-CE1	5.11	1.49	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	TYR	CD2-CE2	5.10	1.47	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	136	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	160	ASP	CB-CG-OD1	6.38	124.04	118.30
1	G	136	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	217	LEU	CA-CB-CG	5.78	128.60	115.30
1	E	160	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	G	136	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	25	ASP	CB-CG-OD1	5.61	123.35	118.30
1	E	25	ASP	CB-CG-OD1	5.59	123.33	118.30
1	E	22	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	106	LEU	CA-CB-CG	-5.38	102.92	115.30
1	E	170	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	G	22	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	H	235	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	E	249	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2017	0	1970	32	0
1	B	2017	0	1973	23	0
1	C	2012	0	1968	40	0
1	D	2012	0	1968	34	0
1	E	2012	0	1968	30	0
1	F	2017	0	1973	20	0
1	G	2012	0	1968	34	0
1	H	2017	0	1973	29	0
2	A	35	0	19	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	35	0	19	6	0
2	C	35	0	19	3	0
2	D	35	0	19	4	0
2	E	35	0	19	1	0
2	F	35	0	18	4	0
2	G	35	0	19	0	0
2	H	35	0	19	0	0
3	A	36	0	0	1	0
3	B	84	0	0	1	0
3	C	62	0	0	4	0
3	D	56	0	0	3	0
3	E	48	0	0	0	0
3	F	16	0	0	3	0
3	G	49	0	0	1	0
3	H	22	0	0	0	0
All	All	16769	0	15912	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:PRO:HA	3:F:2002:HOH:O	1.22	1.25
1:F:110:VAL:HB	3:F:2002:HOH:O	1.37	1.19
1:C:49:ASN:HB2	1:C:115:ARG:NH2	1.65	1.10
1:G:115:ARG:H	1:G:115:ARG:HD2	1.01	1.10
1:D:92:ARG:HE	1:D:93:LYS:HB2	1.20	1.06
1:H:129:LYS:H	1:H:129:LYS:HE2	1.26	1.01
1:B:246:ARG:HD2	1:B:249:ARG:HH21	1.29	0.96
1:G:115:ARG:H	1:G:115:ARG:CD	1.75	0.95
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.31	0.94
1:C:49:ASN:HB2	1:C:115:ARG:HH22	1.27	0.94
1:G:115:ARG:HD2	1:G:115:ARG:N	1.82	0.90
1:D:149:HIS:ND1	3:D:2038:HOH:O	2.08	0.85
1:C:249:ARG:HH11	1:C:249:ARG:HG3	1.39	0.84
1:G:127:ASP:O	1:G:130:THR:CG2	2.25	0.84
2:C:301:AVU:O5R	3:C:2061:HOH:O	1.99	0.81
1:C:127:ASP:OD2	1:C:129:LYS:HG2	1.82	0.80
1:H:126:PRO:HB2	1:H:130:THR:HG21	1.63	0.80
1:C:249:ARG:CG	1:C:249:ARG:HH11	1.95	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ARG:HG2	1:E:249:ARG:HH21	1.50	0.76
1:A:86:ASP:HB3	1:A:237:LEU:HD21	1.66	0.76
2:B:301:AVU:O5R	2:B:301:AVU:H5'A	1.86	0.75
1:H:214:LEU:O	1:H:218:VAL:HG23	1.86	0.75
1:C:49:ASN:HD22	1:C:115:ARG:HH12	1.33	0.75
1:B:174:PHE:CD2	2:B:301:AVU:H4'	2.23	0.74
1:E:140:TRP:HB3	1:E:174:PHE:HE2	1.51	0.74
1:G:127:ASP:O	1:G:130:THR:HG22	1.87	0.73
1:C:49:ASN:HB2	1:C:115:ARG:CZ	2.18	0.73
1:A:115:ARG:NH1	1:A:115:ARG:HG2	2.03	0.73
1:C:1:ILE:HA	3:C:2001:HOH:O	1.90	0.72
1:G:127:ASP:O	1:G:130:THR:HG23	1.90	0.72
1:H:180:LEU:HD21	1:H:217:LEU:HD13	1.72	0.72
1:E:246:ARG:CG	1:E:249:ARG:HH21	2.02	0.71
1:D:174:PHE:CD2	2:D:301:AVU:H2'	2.26	0.71
1:D:92:ARG:NE	1:D:93:LYS:HB2	2.01	0.71
1:E:77:TRP:CH2	1:E:81:TYR:HD2	2.09	0.70
1:D:89:ASN:OD1	1:D:92:ARG:NH1	2.24	0.69
1:D:1:ILE:HG22	1:D:125:CYS:O	1.92	0.69
1:E:15:CYS:HB2	1:E:105:MET:SD	2.33	0.69
1:E:128:PHE:O	1:E:136:ARG:HD2	1.92	0.68
3:C:2060:HOH:O	1:D:232:ARG:HD3	1.92	0.67
1:C:49:ASN:CB	1:C:115:ARG:HH22	2.04	0.67
1:D:92:ARG:HH21	1:D:93:LYS:HD2	1.59	0.67
1:E:127:ASP:O	1:E:130:THR:HG22	1.94	0.67
1:B:174:PHE:CD2	2:B:301:AVU:O1B	2.48	0.67
1:B:246:ARG:CD	1:B:249:ARG:HH21	2.06	0.66
1:C:5:ARG:NH1	3:C:2006:HOH:O	2.12	0.66
1:C:243:PRO:O	1:D:232:ARG:NH1	2.28	0.66
1:B:48:LYS:HE2	1:B:52:ASP:O	1.95	0.66
1:B:174:PHE:CE2	2:B:301:AVU:H4'	2.30	0.66
1:C:249:ARG:CG	1:C:249:ARG:NH1	2.55	0.65
1:F:174:PHE:CD2	2:F:301:AVU:O2'	2.49	0.64
1:A:86:ASP:CB	1:A:237:LEU:HD21	2.28	0.63
1:C:130:THR:HG22	1:G:217:LEU:HD22	1.80	0.63
1:E:218:VAL:HG13	1:E:223:PHE:HB2	1.81	0.63
1:H:134:GLN:NE2	1:H:134:GLN:H	1.98	0.61
1:D:174:PHE:CE2	2:D:301:AVU:H2'	2.35	0.61
1:F:174:PHE:CE2	2:F:301:AVU:O2'	2.54	0.61
1:E:49:ASN:HB2	1:E:115:ARG:HH11	1.64	0.61
1:H:129:LYS:HE2	1:H:129:LYS:N	2.08	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LYS:HG2	1:D:94:TYR:CD1	2.36	0.60
1:A:83:GLU:HG3	1:A:195:LEU:CD2	2.31	0.60
1:G:237:LEU:HD13	1:H:240:SER:OG	2.01	0.60
1:D:93:LYS:HG2	1:D:94:TYR:CE1	2.37	0.60
1:A:115:ARG:CG	1:A:115:ARG:HH11	2.12	0.60
1:A:174:PHE:CE2	2:A:301:AVU:O3'	2.53	0.59
1:A:131:CYS:HB3	1:A:132:PRO:HD2	1.84	0.59
1:G:50:PRO:CD	1:G:115:ARG:HH21	2.16	0.59
1:D:137:GLU:HG2	1:D:174:PHE:HE1	1.68	0.59
1:E:49:ASN:HB2	1:E:115:ARG:NH1	2.18	0.58
1:E:80:VAL:HG21	1:E:158:MET:HG2	1.86	0.58
1:H:66:GLN:HE21	1:H:67:GLN:H	1.51	0.58
1:H:127:ASP:O	1:H:129:LYS:HE2	2.03	0.58
1:A:106:LEU:HD13	1:A:139:PHE:CZ	2.39	0.58
1:E:126:PRO:HB2	1:E:130:THR:HG21	1.85	0.58
1:H:49:ASN:HD21	1:H:115:ARG:HH21	1.50	0.58
1:C:49:ASN:ND2	1:C:115:ARG:HH12	2.02	0.58
1:A:252:LYS:O	3:A:2036:HOH:O	2.17	0.57
1:C:174:PHE:HB2	2:C:301:AVU:PB	2.44	0.57
1:E:140:TRP:HB3	1:E:174:PHE:CE2	2.38	0.57
1:A:107:ASN:OD1	2:A:301:AVU:N6	2.37	0.57
2:B:301:AVU:C5R	2:B:301:AVU:H5'A	2.35	0.57
1:E:47:PHE:HE1	1:E:117:ASN:HD22	1.51	0.57
1:B:18:TYR:HA	1:B:22:ARG:HG2	1.86	0.56
1:E:180:LEU:HB3	1:E:181:PRO:HD3	1.86	0.56
1:C:49:ASN:HD22	1:C:115:ARG:NH1	2.02	0.56
1:E:173:SER:O	1:E:177:LYS:HD3	2.06	0.56
1:D:103:GLY:O	1:D:107:ASN:HB2	2.06	0.56
1:A:93:LYS:HD2	1:A:94:TYR:CE2	2.41	0.56
1:G:77:TRP:CH2	1:G:81:TYR:HD2	2.23	0.55
2:C:301:AVU:N3	2:C:301:AVU:H2'	2.22	0.55
1:G:1:ILE:HG12	1:G:110:VAL:HG11	1.89	0.55
1:A:128:PHE:C	1:A:130:THR:H	2.11	0.54
1:E:174:PHE:HB2	2:E:301:AVU:PB	2.47	0.54
1:A:158:MET:SD	1:A:195:LEU:HD13	2.47	0.54
1:B:246:ARG:HD2	1:B:249:ARG:NH2	2.12	0.54
1:C:170:ARG:HD2	1:C:172:ASP:OD2	2.07	0.54
1:H:0:ALA:N	1:H:127:ASP:OD1	2.41	0.54
1:H:154:GLU:HG2	1:H:189:ARG:HB3	1.89	0.53
1:A:1:ILE:HG22	1:A:125:CYS:O	2.07	0.53
1:H:66:GLN:NE2	1:H:67:GLN:H	2.06	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:LEU:N	1:F:102:PRO:HD2	2.24	0.53
1:C:129:LYS:HG3	1:G:217:LEU:HD21	1.90	0.53
1:A:71:LYS:O	1:A:72:ASN:HB2	2.07	0.53
1:A:108:SER:H	2:A:301:AVU:HN6	1.56	0.53
1:A:83:GLU:HG3	1:A:195:LEU:HD22	1.91	0.52
1:H:126:PRO:HB2	1:H:130:THR:CG2	2.37	0.52
1:A:80:VAL:HG21	1:A:158:MET:HG2	1.92	0.51
1:C:246:ARG:HE	1:C:249:ARG:HD2	1.74	0.51
1:H:80:VAL:HG11	1:H:195:LEU:HD22	1.91	0.51
1:G:50:PRO:HD3	1:G:115:ARG:NH2	2.26	0.51
1:D:249:ARG:HH11	1:D:249:ARG:HG2	1.77	0.50
1:D:140:TRP:CB	1:D:174:PHE:HE2	2.24	0.50
1:F:77:TRP:H	2:F:301:AVU:HO3R	1.57	0.50
1:B:75:MET:CG	1:B:76:PHE:N	2.73	0.50
2:D:301:AVU:N1	3:D:2031:HOH:O	2.34	0.50
1:B:173:SER:O	1:B:177:LYS:HG3	2.11	0.50
1:E:126:PRO:HB2	1:E:130:THR:CG2	2.42	0.49
1:B:180:LEU:HB3	1:B:181:PRO:HD3	1.94	0.49
1:F:54:ASP:CB	1:F:134:GLN:NE2	2.76	0.49
1:F:15:CYS:HB2	1:F:105:MET:SD	2.53	0.49
1:G:49:ASN:CG	1:G:50:PRO:HD2	2.33	0.49
1:H:127:ASP:O	1:H:129:LYS:CE	2.61	0.49
1:E:246:ARG:CG	1:E:249:ARG:NH2	2.76	0.48
1:F:77:TRP:CE2	2:F:301:AVU:H3R	2.48	0.48
1:D:80:VAL:HG11	1:D:195:LEU:HD22	1.93	0.48
1:C:117:ASN:H	1:C:117:ASN:HD22	1.61	0.48
1:C:49:ASN:HA	1:C:115:ARG:NH1	2.28	0.48
1:H:191:LYS:HG2	1:H:226:ASP:OD1	2.15	0.47
1:C:117:ASN:HD22	1:C:117:ASN:N	2.12	0.47
1:B:198:LEU:HD22	1:B:247:GLU:HB2	1.96	0.47
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.79	0.47
1:F:54:ASP:HB2	1:F:134:GLN:NE2	2.30	0.47
1:D:215:GLU:HG3	1:D:225:PHE:CD2	2.48	0.47
1:D:174:PHE:HB2	2:D:301:AVU:PB	2.55	0.47
1:G:115:ARG:CD	1:G:115:ARG:N	2.56	0.47
1:C:77:TRP:CH2	1:C:81:TYR:HD2	2.32	0.47
1:D:137:GLU:HG2	1:D:174:PHE:CE1	2.49	0.47
1:B:62:PHE:CD2	1:B:142:MET:HG3	2.49	0.46
1:C:189:ARG:HA	1:C:224:ALA:O	2.15	0.46
1:D:205:LYS:HE3	1:D:205:LYS:HB3	1.67	0.46
1:G:36:ALA:O	1:G:39:LYS:HG2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:PRO:HG3	1:G:121:ASN:O	2.15	0.46
1:B:68:GLN:NE2	3:B:2038:HOH:O	2.48	0.46
1:C:128:PHE:O	1:C:136:ARG:HD2	2.16	0.46
1:G:103:GLY:O	1:G:107:ASN:HB2	2.15	0.46
1:E:133:VAL:HA	1:E:136:ARG:HG2	1.97	0.46
1:G:50:PRO:HD2	1:G:115:ARG:HH21	1.80	0.46
1:B:249:ARG:HG2	1:B:249:ARG:NH1	2.30	0.46
1:C:49:ASN:CG	1:C:50:PRO:HD2	2.36	0.45
1:E:246:ARG:HG2	1:E:249:ARG:NH2	2.27	0.45
1:F:103:GLY:O	1:F:107:ASN:HB2	2.16	0.45
1:D:126:PRO:HD2	1:D:128:PHE:CE1	2.51	0.45
1:A:70:PRO:HG2	1:A:73:LYS:HB2	1.99	0.45
1:A:106:LEU:O	1:A:107:ASN:C	2.54	0.45
1:C:133:VAL:HA	1:C:136:ARG:HG2	1.97	0.45
1:G:52:ASP:O	1:G:53:LEU:HD23	2.17	0.45
1:G:128:PHE:O	1:G:136:ARG:HD2	2.17	0.45
1:B:75:MET:HG2	1:B:76:PHE:N	2.31	0.45
1:C:71:LYS:O	1:C:72:ASN:HB2	2.16	0.45
1:G:218:VAL:HG13	1:G:223:PHE:HB2	1.99	0.45
1:G:47:PHE:HA	1:G:114:GLN:O	2.15	0.45
1:G:75:MET:CE	1:G:156:THR:HG22	2.47	0.45
1:H:18:TYR:O	1:H:19:GLU:C	2.56	0.45
1:F:128:PHE:C	1:F:130:THR:H	2.21	0.44
1:G:251:ALA:HB2	1:H:249:ARG:HG3	1.99	0.44
1:G:72:ASN:HA	1:G:154:GLU:O	2.17	0.44
1:H:129:LYS:CE	1:H:129:LYS:H	2.11	0.44
1:B:62:PHE:CD2	1:B:142:MET:CG	3.00	0.44
1:D:140:TRP:HB3	1:D:174:PHE:HE2	1.82	0.44
1:F:88:ALA:HB1	1:F:94:TYR:HB2	1.99	0.44
1:C:49:ASN:ND2	1:C:50:PRO:HD2	2.33	0.44
1:E:181:PRO:HA	1:E:221:LYS:HE3	1.98	0.44
1:C:75:MET:HG2	1:C:96:THR:HG22	1.99	0.44
1:E:49:ASN:CG	1:E:50:PRO:HD2	2.37	0.44
1:G:127:ASP:OD2	1:G:129:LYS:HG2	2.18	0.44
1:D:80:VAL:O	1:D:81:TYR:C	2.56	0.44
1:E:75:MET:HG2	1:E:96:THR:HG22	1.98	0.44
1:G:36:ALA:HA	1:G:39:LYS:HE3	2.00	0.44
1:F:127:ASP:HB2	1:F:130:THR:OG1	2.18	0.44
1:B:1:ILE:HD11	1:B:110:VAL:HG11	2.00	0.44
1:C:103:GLY:O	1:C:107:ASN:HB2	2.18	0.44
1:C:198:LEU:HD22	1:C:247:GLU:HB2	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:HD11	1:E:129:LYS:HB3	2.00	0.44
1:A:62:PHE:CZ	1:A:143:ALA:HB2	2.52	0.43
1:E:80:VAL:O	1:E:80:VAL:HG23	2.18	0.43
1:F:31:ARG:HD2	3:F:2007:HOH:O	2.17	0.43
1:D:72:ASN:HA	1:D:154:GLU:O	2.18	0.43
1:D:106:LEU:HD23	1:D:139:PHE:HZ	1.84	0.43
1:B:246:ARG:HE	1:B:246:ARG:HB3	1.60	0.43
1:F:137:GLU:HG2	1:F:174:PHE:CZ	2.53	0.43
1:A:128:PHE:HB3	1:A:136:ARG:HG2	2.00	0.43
1:A:166:VAL:HG13	1:A:170:ARG:HD3	2.01	0.43
1:A:174:PHE:CD2	2:A:301:AVU:O3'	2.62	0.43
1:D:186:LYS:HB2	1:D:186:LYS:HE2	1.82	0.43
1:B:177:LYS:HD2	1:E:133:VAL:HG21	2.01	0.43
1:A:55:LEU:HG	1:A:55:LEU:H	1.73	0.43
1:F:88:ALA:CB	1:F:94:TYR:HB2	2.48	0.43
1:E:91:GLY:HA2	1:E:94:TYR:O	2.18	0.43
1:C:40:ASP:HA	1:C:43:LYS:HE3	2.01	0.42
1:D:16:LYS:HE2	1:D:16:LYS:HB2	1.87	0.42
1:D:52:ASP:HB2	3:D:2014:HOH:O	2.19	0.42
1:D:127:ASP:C	1:D:129:LYS:H	2.21	0.42
1:A:75:MET:HG2	1:A:96:THR:HG22	2.02	0.42
1:H:137:GLU:HG2	1:H:174:PHE:CZ	2.55	0.42
3:G:2010:HOH:O	1:H:5:ARG:NH2	2.52	0.42
1:G:50:PRO:HD3	1:G:115:ARG:HH21	1.80	0.42
1:H:229:GLU:O	1:H:230:ASN:C	2.58	0.42
1:C:129:LYS:HG3	1:G:217:LEU:HD11	2.00	0.42
1:H:131:CYS:HA	1:H:132:PRO:HD2	1.85	0.42
1:E:170:ARG:HD2	1:E:170:ARG:HH11	1.65	0.42
1:C:217:LEU:HD21	1:G:129:LYS:HG3	2.01	0.42
1:D:89:ASN:OD1	1:D:92:ARG:HG2	2.19	0.41
1:G:180:LEU:HB3	1:G:181:PRO:HD3	2.02	0.41
1:A:75:MET:HG3	1:A:76:PHE:N	2.35	0.41
1:C:49:ASN:HB2	1:C:115:ARG:NH1	2.35	0.41
1:D:28:PRO:HG2	1:D:67:GLN:HB3	2.03	0.41
1:A:80:VAL:HB	1:A:83:GLU:HG2	2.03	0.41
2:B:301:AVU:O5R	2:B:301:AVU:C5'	2.63	0.41
1:C:73:LYS:HD3	1:C:73:LYS:HA	1.77	0.41
1:D:92:ARG:HH21	1:D:93:LYS:CD	2.31	0.41
1:F:129:LYS:HB2	1:F:129:LYS:HE2	1.87	0.41
1:F:77:TRP:HA	1:F:158:MET:O	2.20	0.41
1:G:251:ALA:HA	1:H:251:ALA:HA	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASN:HA	1:C:154:GLU:O	2.21	0.41
1:F:117:ASN:OD1	1:F:118:PRO:HA	2.20	0.41
1:H:72:ASN:OD1	1:H:153:GLY:HA3	2.21	0.41
1:E:128:PHE:CZ	1:E:129:LYS:NZ	2.89	0.40
1:G:75:MET:HG3	1:G:76:PHE:N	2.35	0.40
1:H:197:ARG:NH1	1:H:197:ARG:HG2	2.35	0.40
1:A:37:LEU:HD23	1:A:64:SER:HB3	2.03	0.40
1:C:49:ASN:CB	1:C:115:ARG:NH1	2.84	0.40
1:C:240:SER:OG	1:D:237:LEU:HG	2.21	0.40
1:H:135:ALA:O	1:H:138:SER:HB3	2.21	0.40
1:A:71:LYS:O	1:A:72:ASN:CB	2.69	0.40
1:B:11:PHE:CD1	1:B:11:PHE:C	2.95	0.40
1:H:11:PHE:C	1:H:11:PHE:CD1	2.95	0.40
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.81	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	250/260 (96%)	239 (96%)	10 (4%)	1 (0%)	34	42
1	B	250/260 (96%)	242 (97%)	8 (3%)	0	100	100
1	C	249/260 (96%)	240 (96%)	8 (3%)	1 (0%)	34	42
1	D	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
1	E	249/260 (96%)	240 (96%)	9 (4%)	0	100	100
1	F	250/260 (96%)	234 (94%)	15 (6%)	1 (0%)	34	42
1	G	249/260 (96%)	244 (98%)	5 (2%)	0	100	100
1	H	250/260 (96%)	238 (95%)	10 (4%)	2 (1%)	19	23
All	All	1996/2080 (96%)	1918 (96%)	73 (4%)	5 (0%)	41	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	F	129	LYS
1	H	127	ASP
1	C	222	HIS
1	H	128	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	220/226 (97%)	205 (93%)	15 (7%)	16	21
1	B	220/226 (97%)	205 (93%)	15 (7%)	16	21
1	C	220/226 (97%)	207 (94%)	13 (6%)	19	27
1	D	220/226 (97%)	202 (92%)	18 (8%)	11	14
1	E	220/226 (97%)	210 (96%)	10 (4%)	27	39
1	F	220/226 (97%)	206 (94%)	14 (6%)	17	23
1	G	220/226 (97%)	204 (93%)	16 (7%)	14	18
1	H	220/226 (97%)	203 (92%)	17 (8%)	13	16
All	All	1760/1808 (97%)	1642 (93%)	118 (7%)	16	21

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	31	ARG
1	A	39	LYS
1	A	57	SER
1	A	75	MET
1	A	90	THR
1	A	115	ARG
1	A	120	PHE
1	A	123	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	129	LYS
1	A	136	ARG
1	A	221	LYS
1	A	232	ARG
1	A	242	ASN
1	A	246	ARG
1	B	1	ILE
1	B	31	ARG
1	B	32	SER
1	B	89	ASN
1	B	115	ARG
1	B	136	ARG
1	B	145	SER
1	B	172	ASP
1	B	195	LEU
1	B	200	GLU
1	B	201	LYS
1	B	216	LYS
1	B	221	LYS
1	B	246	ARG
1	B	249	ARG
1	C	1	ILE
1	C	43	LYS
1	C	71	LYS
1	C	75	MET
1	C	89	ASN
1	C	123	LYS
1	C	172	ASP
1	C	200	GLU
1	C	204	GLU
1	C	237	LEU
1	C	242	ASN
1	C	246	ARG
1	C	249	ARG
1	D	1	ILE
1	D	19	GLU
1	D	25	ASP
1	D	39	LYS
1	D	64	SER
1	D	75	MET
1	D	92	ARG
1	D	93	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	106	LEU
1	D	124	VAL
1	D	127	ASP
1	D	130	THR
1	D	134	GLN
1	D	142	MET
1	D	174	PHE
1	D	205	LYS
1	D	212	LEU
1	D	249	ARG
1	E	31	ARG
1	E	35	SER
1	E	75	MET
1	E	106	LEU
1	E	115	ARG
1	E	130	THR
1	E	174	PHE
1	E	195	LEU
1	E	237	LEU
1	E	242	ASN
1	F	1	ILE
1	F	31	ARG
1	F	90	THR
1	F	98	GLU
1	F	115	ARG
1	F	121	ASN
1	F	124	VAL
1	F	127	ASP
1	F	129	LYS
1	F	130	THR
1	F	145	SER
1	F	216	LYS
1	F	232	ARG
1	F	242	ASN
1	G	30	VAL
1	G	33	ASP
1	G	35	SER
1	G	43	LYS
1	G	71	LYS
1	G	75	MET
1	G	115	ARG
1	G	130	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	145	SER
1	G	162	SER
1	G	186	LYS
1	G	195	LEU
1	G	228	VAL
1	G	237	LEU
1	G	242	ASN
1	G	246	ARG
1	H	29	ARG
1	H	32	SER
1	H	66	GLN
1	H	74	VAL
1	H	90	THR
1	H	92	ARG
1	H	106	LEU
1	H	127	ASP
1	H	129	LYS
1	H	130	THR
1	H	134	GLN
1	H	145	SER
1	H	189	ARG
1	H	195	LEU
1	H	212	LEU
1	H	215	GLU
1	H	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	117	ASN
1	A	222	HIS
1	A	242	ASN
1	B	89	ASN
1	B	242	ASN
1	C	49	ASN
1	C	89	ASN
1	C	117	ASN
1	C	242	ASN
1	D	117	ASN
1	D	134	GLN
1	D	242	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	89	ASN
1	E	117	ASN
1	E	242	ASN
1	F	89	ASN
1	F	134	GLN
1	F	242	ASN
1	G	242	ASN
1	H	49	ASN
1	H	66	GLN
1	H	89	ASN
1	H	134	GLN
1	H	182	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](#)

8 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	F	301	1	33,38,38	1.03	2 (6%)	37,58,58	1.43	4 (10%)

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	1.29	3 (9%)	37,58,58	1.45	4 (10%)
2	AVU	C	301	1	33,38,38	0.94	2 (6%)	37,58,58	1.67	7 (18%)
2	AVU	H	301	1	33,38,38	0.96	1 (3%)	37,58,58	1.71	7 (18%)
2	AVU	E	301	1	33,38,38	1.03	2 (6%)	37,58,58	1.63	6 (16%)
2	AVU	G	301	1	33,38,38	1.06	2 (6%)	37,58,58	1.66	7 (18%)
2	AVU	A	301	1	33,38,38	1.01	2 (6%)	37,58,58	1.90	8 (21%)
2	AVU	D	301	1	33,38,38	0.96	1 (3%)	37,58,58	1.93	11 (29%)

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	F	301	1	-	4/18/51/51	0/4/4/4
2	AVU	B	301	1	-	3/18/51/51	0/4/4/4
2	AVU	C	301	1	-	9/18/51/51	0/4/4/4
2	AVU	H	301	1	-	6/18/51/51	0/4/4/4
2	AVU	E	301	1	-	4/18/51/51	0/4/4/4
2	AVU	G	301	1	-	5/18/51/51	0/4/4/4
2	AVU	A	301	1	-	8/18/51/51	0/4/4/4
2	AVU	D	301	1	-	3/18/51/51	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	AVU	O4'-C1'	3.83	1.46	1.41
2	A	301	AVU	O4'-C1'	3.74	1.46	1.41
2	G	301	AVU	O4'-C1'	3.50	1.46	1.41
2	B	301	AVU	C2-N3	3.22	1.37	1.32
2	E	301	AVU	O4'-C1'	3.14	1.45	1.41
2	H	301	AVU	O4'-C1'	3.07	1.45	1.41
2	F	301	AVU	F2R-C2R	-2.68	1.34	1.40
2	F	301	AVU	O4'-C1'	2.63	1.44	1.41
2	B	301	AVU	C4-N3	2.59	1.39	1.35
2	D	301	AVU	O4'-C1'	2.34	1.44	1.41
2	C	301	AVU	O4'-C1'	2.11	1.44	1.41
2	G	301	AVU	C2-N3	2.08	1.35	1.32
2	E	301	AVU	F2R-C2R	-2.08	1.35	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AVU	C2-N3	2.07	1.35	1.32
2	C	301	AVU	C2-N3	2.00	1.35	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	AVU	N3-C2-N1	-6.09	119.16	128.68
2	C	301	AVU	N3-C2-N1	-5.73	119.73	128.68
2	A	301	AVU	N3-C2-N1	-5.38	120.26	128.68
2	G	301	AVU	N3-C2-N1	-5.31	120.39	128.68
2	B	301	AVU	N3-C2-N1	-5.28	120.43	128.68
2	E	301	AVU	N3-C2-N1	-5.15	120.63	128.68
2	D	301	AVU	N3-C2-N1	-5.04	120.80	128.68
2	F	301	AVU	N3-C2-N1	-4.97	120.92	128.68
2	D	301	AVU	C3'-C2'-C1'	4.10	107.15	100.98
2	A	301	AVU	O4'-C1'-C2'	-4.00	101.08	106.93
2	D	301	AVU	C1'-N9-C4	-3.91	119.78	126.64
2	A	301	AVU	O4'-C4'-C5'	3.86	122.08	109.37
2	A	301	AVU	C2R-C3R-C4R	3.76	107.27	102.34
2	D	301	AVU	C2R-C3R-C4R	3.71	107.21	102.34
2	E	301	AVU	C2R-C3R-C4R	3.64	107.11	102.34
2	A	301	AVU	O3'-C3'-C4'	-3.54	100.80	111.05
2	C	301	AVU	PB-O3A-PA	-3.51	120.77	132.83
2	H	301	AVU	C2R-C3R-C4R	3.44	106.85	102.34
2	H	301	AVU	C3'-C2'-C1'	3.31	105.96	100.98
2	D	301	AVU	O3R-C3R-C2R	-3.09	100.25	111.44
2	F	301	AVU	PB-O3A-PA	-3.05	122.34	132.83
2	B	301	AVU	C3'-C2'-C1'	3.04	105.55	100.98
2	C	301	AVU	C3'-C2'-C1'	3.01	105.51	100.98
2	G	301	AVU	F2R-C2R-C3R	-2.96	105.90	108.57
2	G	301	AVU	PB-O3A-PA	-2.90	122.87	132.83
2	C	301	AVU	O5'-C5'-C4'	2.86	118.83	108.99
2	A	301	AVU	O4R-C4R-C3R	2.84	107.22	104.70
2	H	301	AVU	O3R-C3R-C2R	-2.80	101.30	111.44
2	A	301	AVU	O4R-C1R-C2R	2.78	109.18	104.88
2	H	301	AVU	O4R-C1R-C2R	2.74	109.11	104.88
2	H	301	AVU	O4R-C4R-C3R	2.67	107.06	104.70
2	G	301	AVU	C2R-C3R-C4R	2.66	105.83	102.34
2	B	301	AVU	O5R-C5R-C4R	2.65	118.11	108.99
2	C	301	AVU	C2R-C3R-C4R	2.65	105.81	102.34
2	E	301	AVU	PB-O3A-PA	-2.50	124.24	132.83
2	D	301	AVU	PB-O3A-PA	-2.49	124.27	132.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	AVU	O5'-C5'-C4'	2.47	117.50	108.99
2	F	301	AVU	C3'-C2'-C1'	2.46	104.68	100.98
2	D	301	AVU	O5'-C5'-C4'	-2.41	100.70	108.99
2	D	301	AVU	C4-C5-N7	-2.30	107.00	109.40
2	E	301	AVU	C1R-O4R-C4R	2.28	113.48	108.16
2	A	301	AVU	C5'-C4'-C3'	-2.24	106.78	115.18
2	G	301	AVU	O2A-PA-O1A	2.23	123.27	112.24
2	D	301	AVU	O2A-PA-O1A	2.17	122.98	112.24
2	D	301	AVU	O3R-C3R-C4R	2.14	117.24	111.05
2	D	301	AVU	O4R-C1R-C2R	2.11	108.14	104.88
2	E	301	AVU	O2A-PA-O1A	2.09	122.58	112.24
2	F	301	AVU	C1'-N9-C4	-2.09	122.98	126.64
2	C	301	AVU	C2'-C3'-C4'	2.08	106.69	102.64
2	C	301	AVU	C1R-O4R-C4R	2.07	113.00	108.16
2	G	301	AVU	O5'-C5'-C4'	-2.07	101.87	108.99
2	G	301	AVU	O4'-C4'-C3'	2.06	109.20	105.11
2	E	301	AVU	O5'-C5'-C4'	-2.04	101.98	108.99
2	H	301	AVU	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	AVU	C5'-O5'-PA-O2A
2	C	301	AVU	C3'-C4'-C5'-O5'
2	C	301	AVU	O4'-C4'-C5'-O5'
2	H	301	AVU	C5'-O5'-PA-O2A
2	G	301	AVU	C5'-O5'-PA-O2A
2	A	301	AVU	C5'-O5'-PA-O2A
2	D	301	AVU	PB-O3A-PA-O5'
2	E	301	AVU	C3'-C4'-C5'-O5'
2	E	301	AVU	O4'-C4'-C5'-O5'
2	H	301	AVU	C4R-C5R-O5R-PB
2	E	301	AVU	C4R-C5R-O5R-PB
2	F	301	AVU	C3'-C4'-C5'-O5'
2	B	301	AVU	C4R-C5R-O5R-PB
2	F	301	AVU	O4'-C4'-C5'-O5'
2	D	301	AVU	C4R-C5R-O5R-PB
2	F	301	AVU	C4R-C5R-O5R-PB
2	C	301	AVU	C4R-C5R-O5R-PB
2	G	301	AVU	C4R-C5R-O5R-PB
2	F	301	AVU	PB-O3A-PA-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	H	301	AVU	PB-O3A-PA-O5'
2	A	301	AVU	PB-O3A-PA-O5'
2	C	301	AVU	C5'-O5'-PA-O3A
2	H	301	AVU	C5'-O5'-PA-O3A
2	G	301	AVU	C5'-O5'-PA-O3A
2	A	301	AVU	C5'-O5'-PA-O3A
2	D	301	AVU	O4'-C4'-C5'-O5'
2	A	301	AVU	PA-O3A-PB-O1B
2	H	301	AVU	C5'-O5'-PA-O1A
2	G	301	AVU	C5'-O5'-PA-O1A
2	A	301	AVU	C5'-O5'-PA-O1A
2	B	301	AVU	C3'-C4'-C5'-O5'
2	A	301	AVU	C4R-C5R-O5R-PB
2	G	301	AVU	O4'-C4'-C5'-O5'
2	C	301	AVU	C4'-C5'-O5'-PA
2	A	301	AVU	O4'-C4'-C5'-O5'
2	B	301	AVU	PB-O3A-PA-O5'
2	C	301	AVU	PA-O3A-PB-O1B
2	C	301	AVU	PA-O3A-PB-O2B
2	E	301	AVU	PA-O3A-PB-O1B
2	A	301	AVU	PA-O3A-PB-O2B
2	C	301	AVU	C5'-O5'-PA-O1A
2	H	301	AVU	O4'-C4'-C5'-O5'

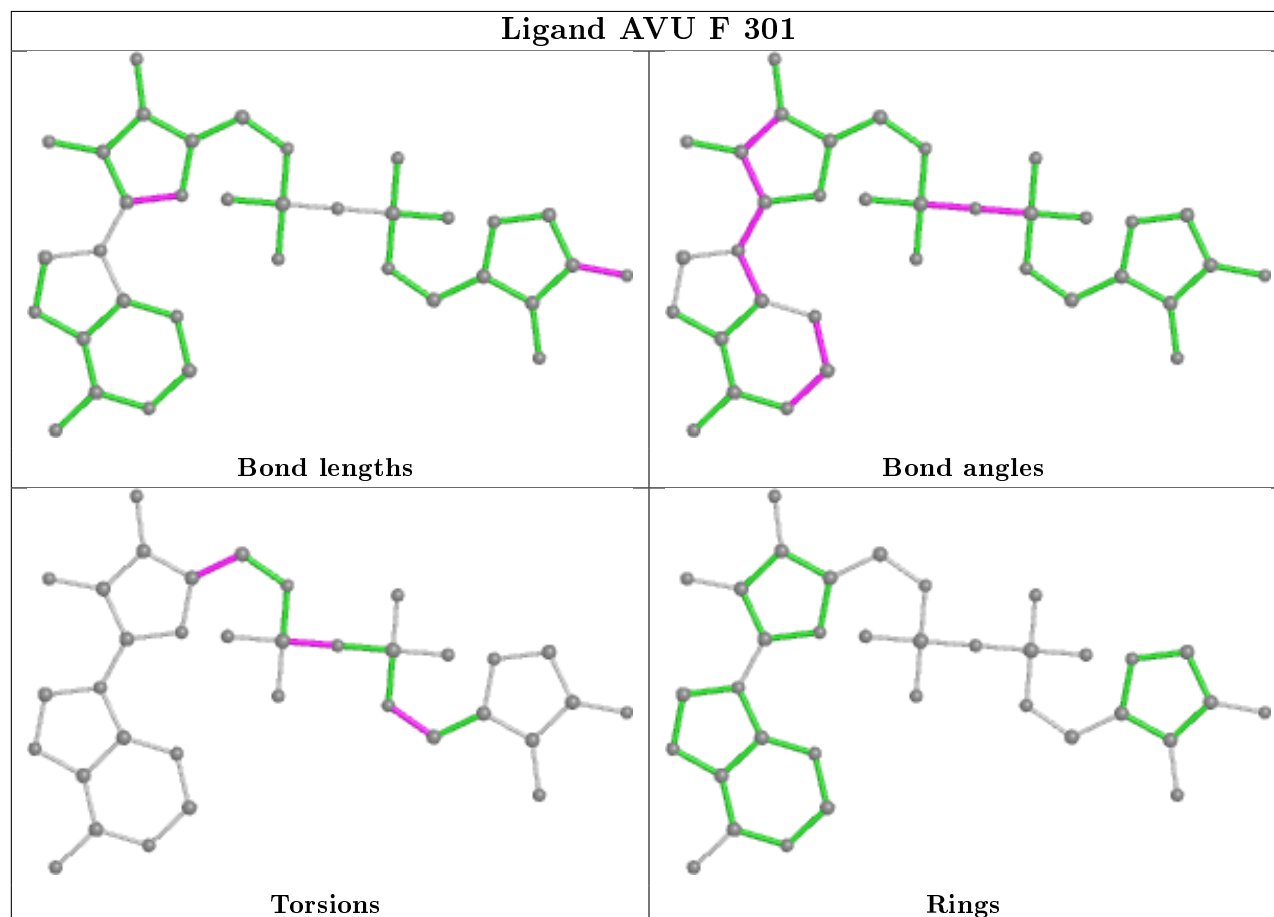
There are no ring outliers.

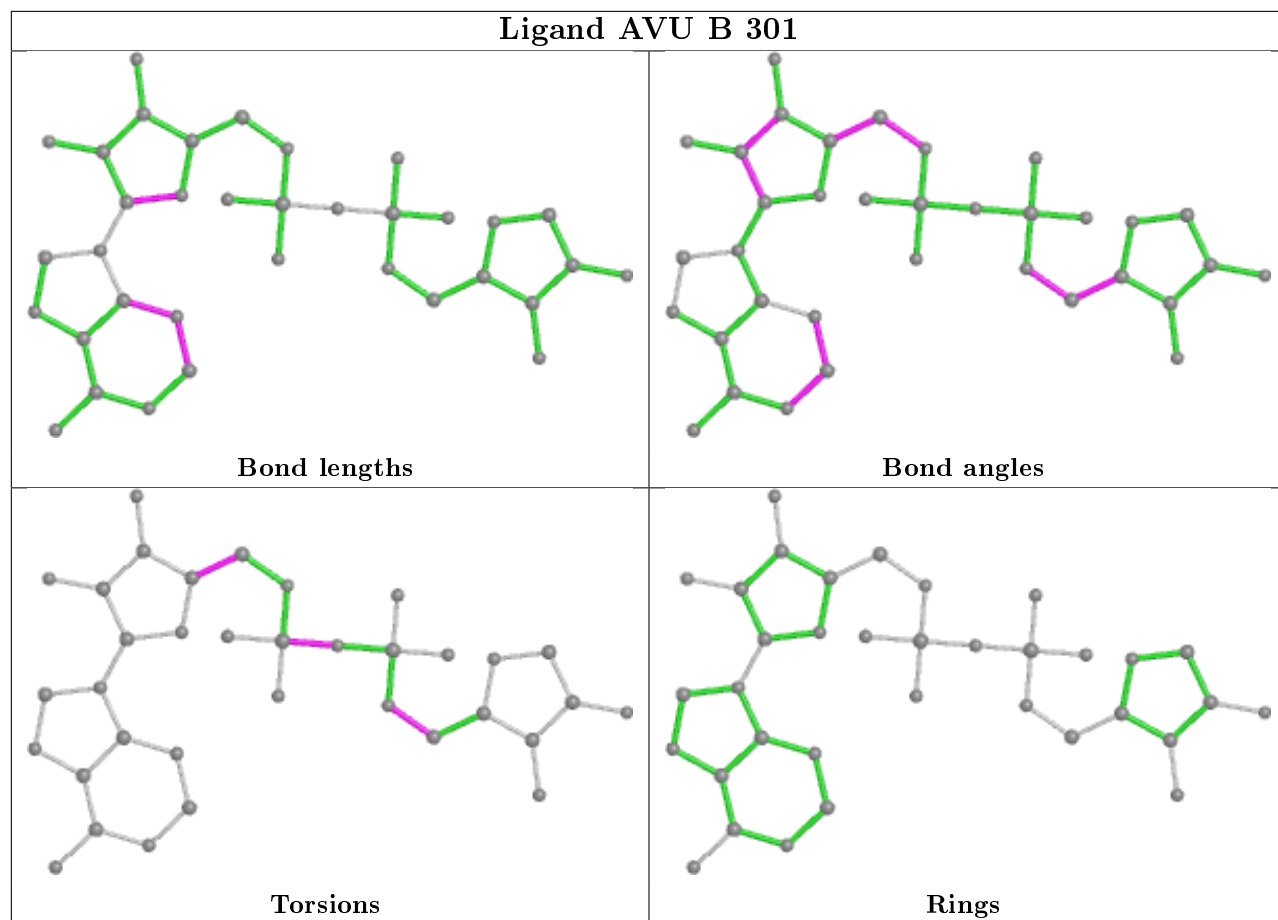
6 monomers are involved in 22 short contacts:

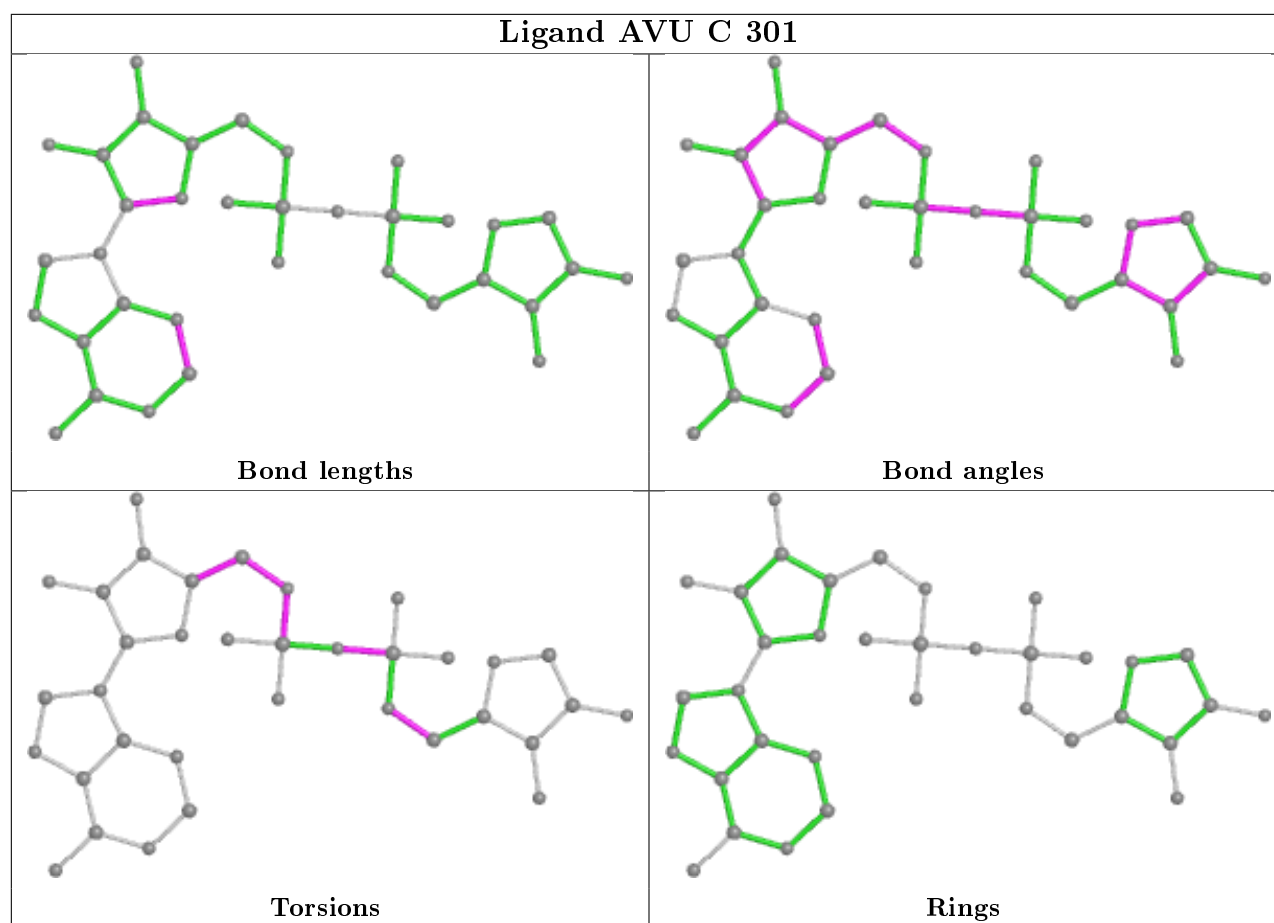
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	AVU	4	0
2	B	301	AVU	6	0
2	C	301	AVU	3	0
2	E	301	AVU	1	0
2	A	301	AVU	4	0
2	D	301	AVU	4	0

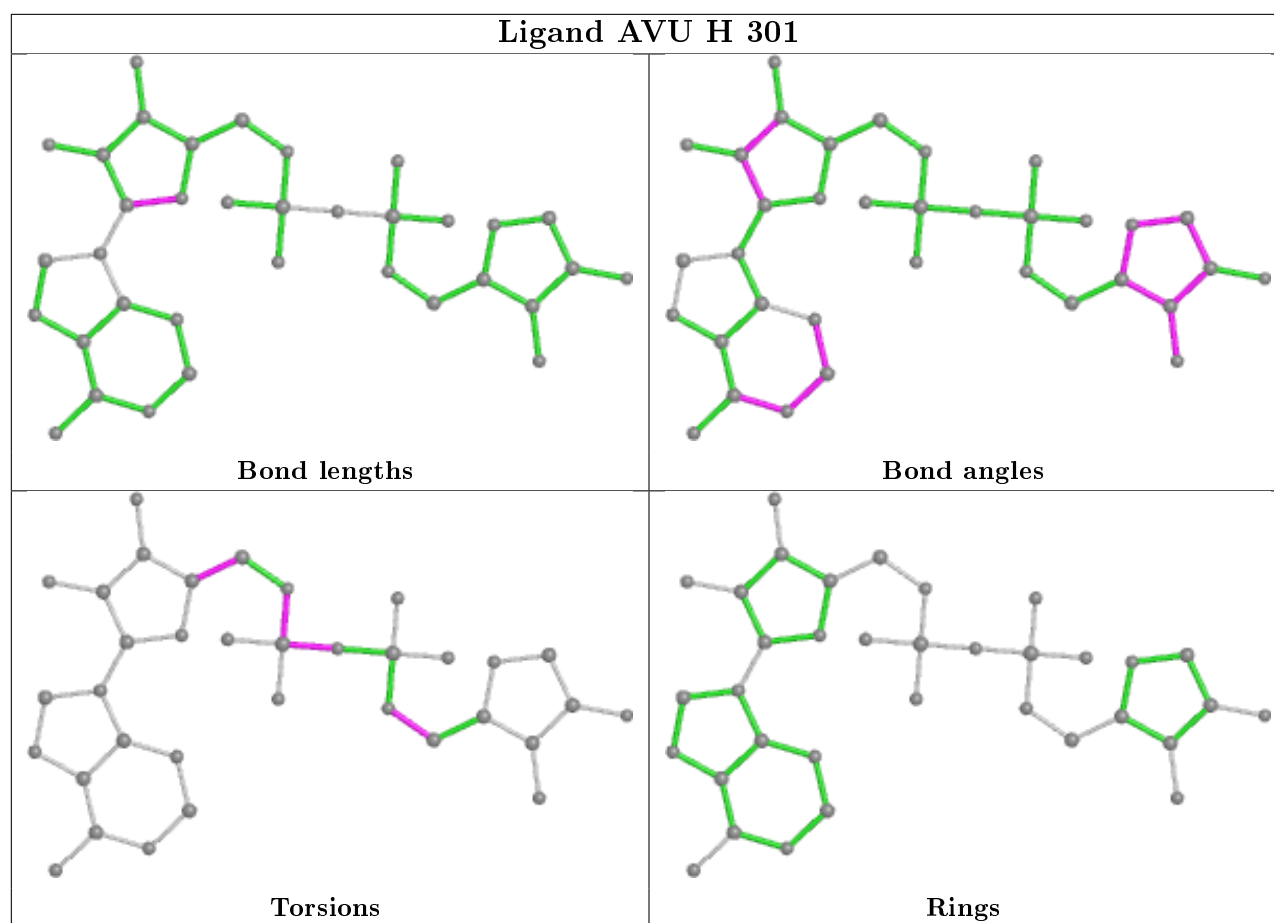
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

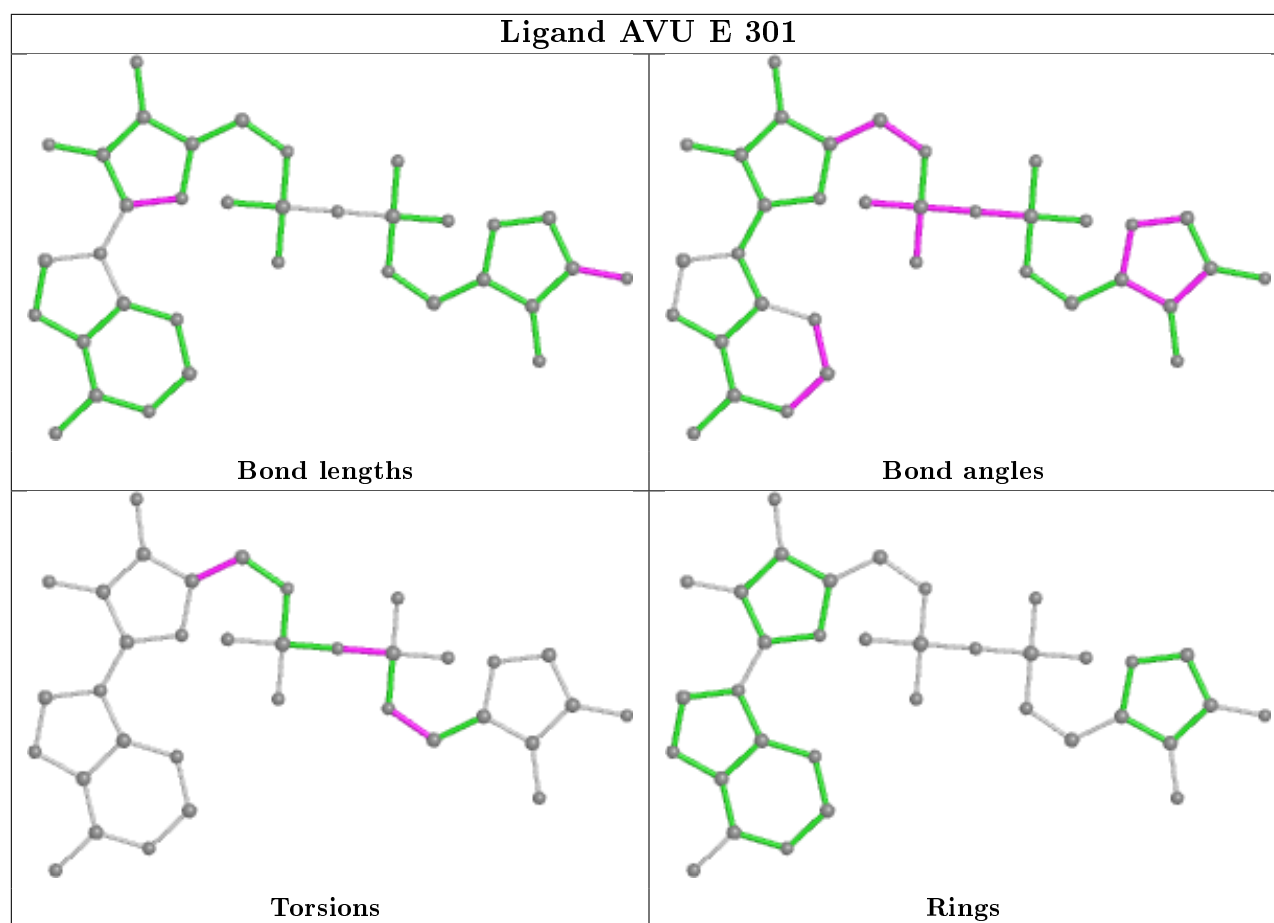
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



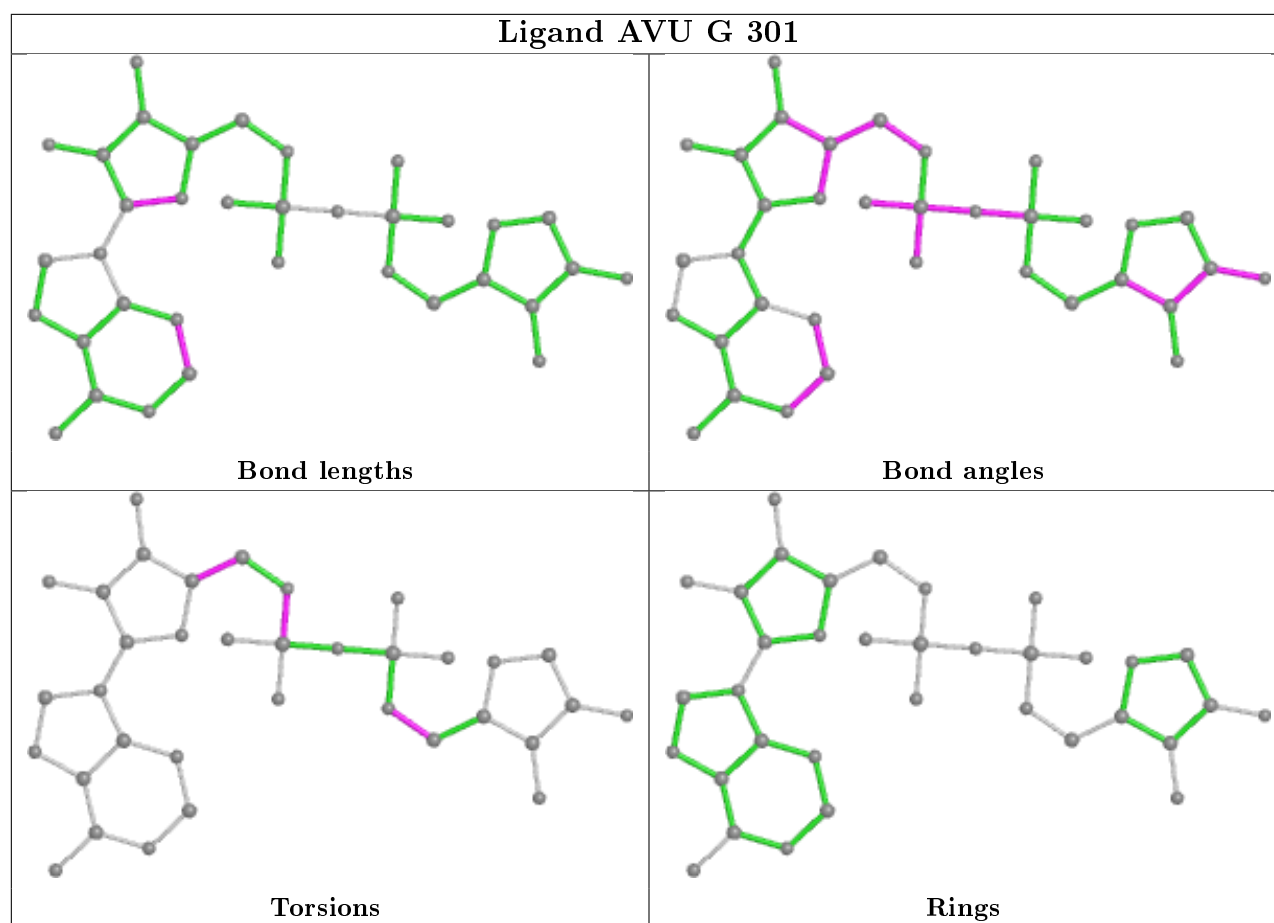


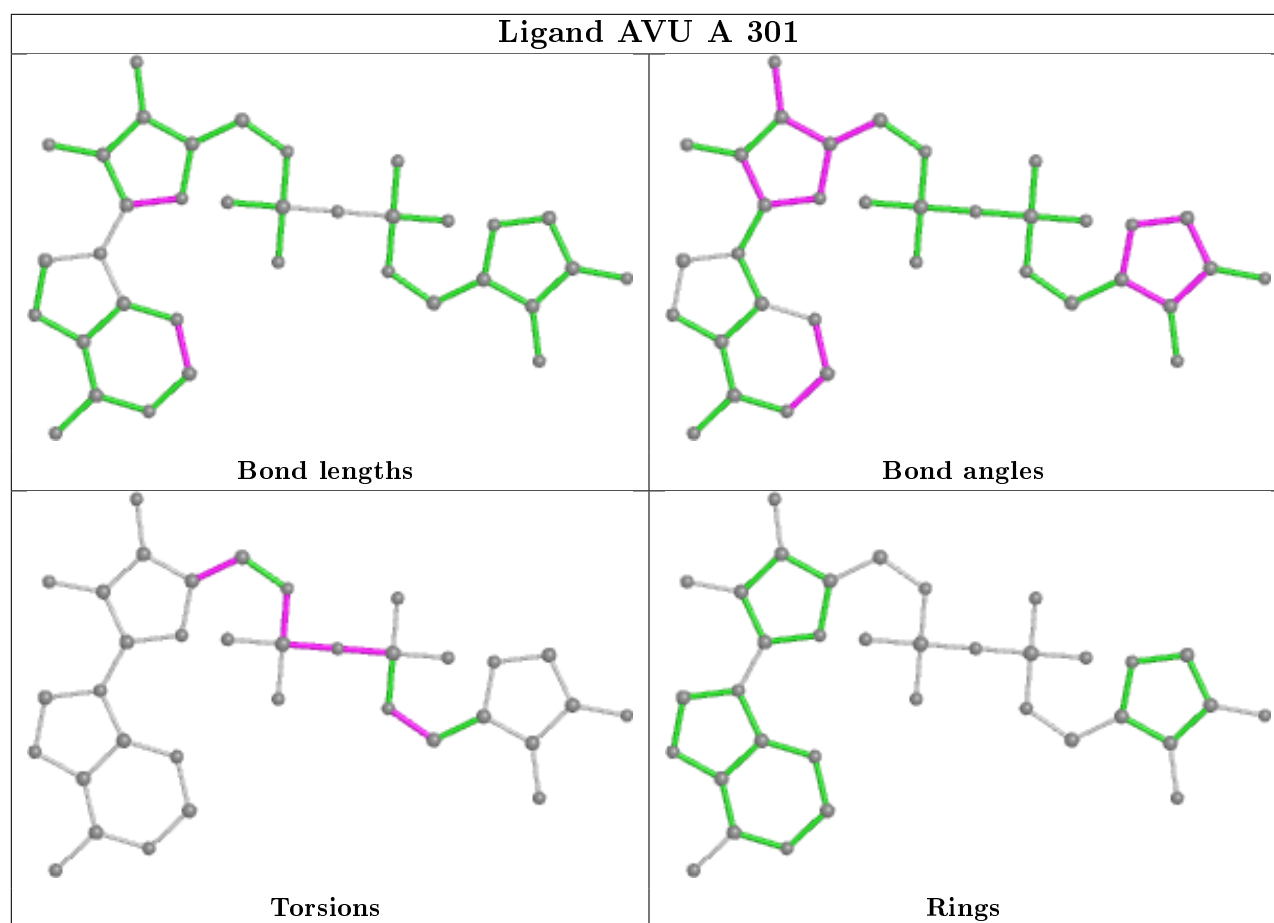


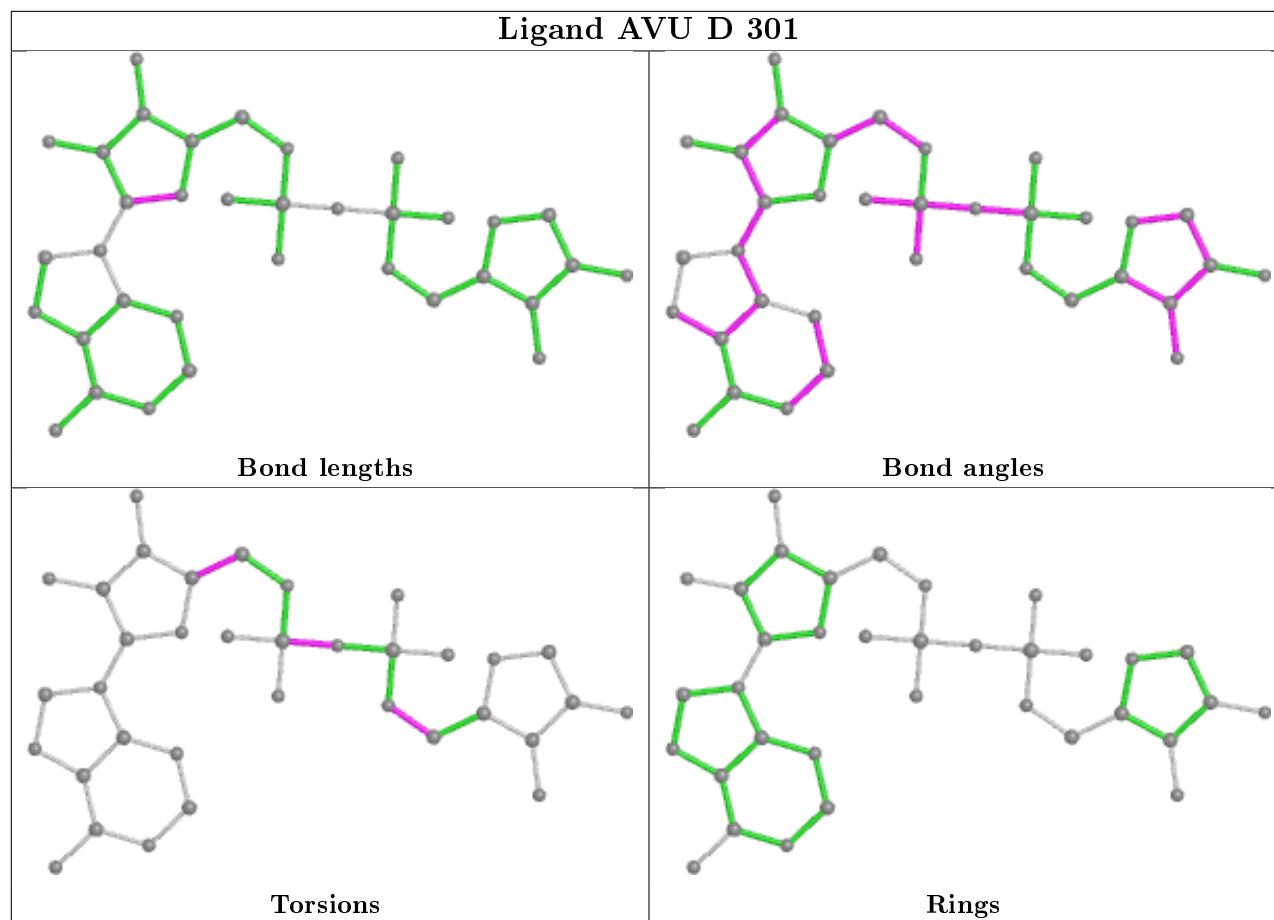












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	252/260 (96%)	0.04	13 (5%) 27 34	24, 46, 74, 95	0
1	B	252/260 (96%)	-0.23	1 (0%) 92 95	19, 34, 54, 63	0
1	C	251/260 (96%)	-0.21	2 (0%) 86 89	20, 38, 59, 70	0
1	D	251/260 (96%)	0.02	12 (4%) 30 37	25, 38, 75, 86	0
1	E	251/260 (96%)	-0.20	4 (1%) 72 77	22, 38, 58, 72	0
1	F	252/260 (96%)	0.34	19 (7%) 14 19	37, 61, 88, 98	0
1	G	251/260 (96%)	-0.20	3 (1%) 79 83	23, 39, 59, 74	0
1	H	252/260 (96%)	0.25	15 (5%) 21 28	35, 52, 77, 91	0
All	All	2012/2080 (96%)	-0.02	69 (3%) 45 52	19, 42, 74, 98	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	PHE	6.9
1	F	133	VAL	5.9
1	D	128	PHE	4.4
1	F	43	LYS	4.3
1	H	0	ALA	4.3
1	F	127	ASP	4.1
1	A	130	THR	4.0
1	H	131	CYS	3.8
1	F	128	PHE	3.7
1	C	251	ALA	3.6
1	D	166	VAL	3.5
1	G	47	PHE	3.4
1	H	127	ASP	3.3
1	D	51	CYS	3.3
1	F	134	GLN	3.1
1	D	124	VAL	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	25	ASP	3.1
1	D	1	ILE	3.0
1	A	199	GLY	3.0
1	H	133	VAL	2.9
1	D	116	ALA	2.9
1	C	115	ARG	2.9
1	A	127	ASP	2.9
1	A	1	ILE	2.9
1	H	128	PHE	2.8
1	H	174	PHE	2.8
1	F	188	THR	2.8
1	F	174	PHE	2.8
1	H	77	TRP	2.8
1	A	222	HIS	2.8
1	F	55	LEU	2.7
1	D	174	PHE	2.7
1	A	131	CYS	2.6
1	F	132	PRO	2.6
1	F	222	HIS	2.6
1	B	165	LYS	2.6
1	H	1	ILE	2.5
1	F	51	CYS	2.5
1	F	49	ASN	2.5
1	A	129	LYS	2.4
1	F	116	ALA	2.4
1	H	130	THR	2.4
1	F	131	CYS	2.4
1	D	131	CYS	2.4
1	F	136	ARG	2.3
1	D	130	THR	2.3
1	A	115	ARG	2.3
1	F	115	ARG	2.3
1	E	115	ARG	2.3
1	A	2	VAL	2.3
1	F	39	LYS	2.3
1	H	51	CYS	2.2
1	H	157	TYR	2.2
1	F	47	PHE	2.2
1	A	244	ASN	2.2
1	D	249	ARG	2.2
1	H	212	LEU	2.2
1	A	172	ASP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	251	ALA	2.1
1	E	157	TYR	2.1
1	F	0	ALA	2.1
1	E	159	VAL	2.1
1	G	157	TYR	2.1
1	D	50	PRO	2.1
1	A	174	PHE	2.1
1	D	53	LEU	2.1
1	H	76	PHE	2.1
1	G	115	ARG	2.0
1	H	97	LEU	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](#)

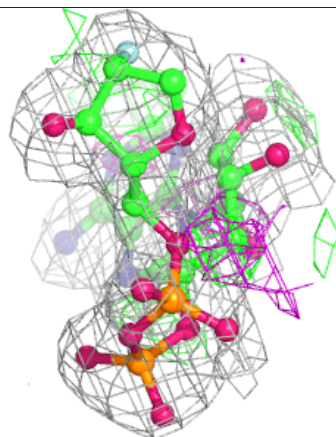
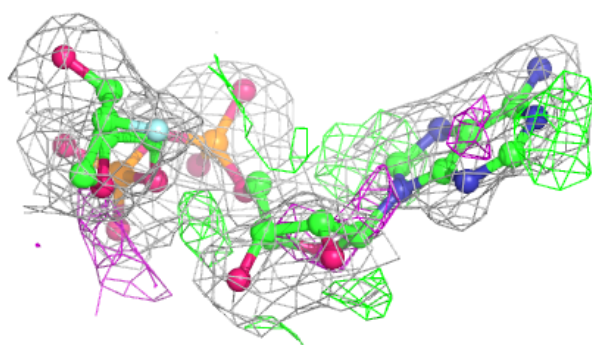
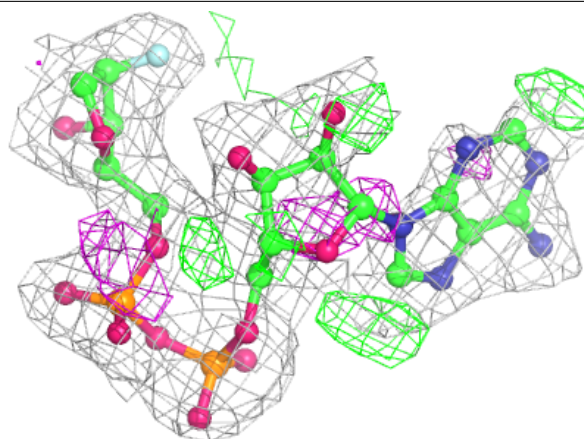
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AVU	B	301	35/35	0.88	0.17	30,63,85,85	0
2	AVU	E	301	35/35	0.89	0.17	36,63,93,93	0
2	AVU	A	301	35/35	0.91	0.15	50,70,97,98	0
2	AVU	C	301	35/35	0.93	0.14	38,71,94,94	0
2	AVU	G	301	35/35	0.94	0.14	36,62,92,93	0
2	AVU	H	301	35/35	0.94	0.18	52,62,80,82	0
2	AVU	D	301	35/35	0.94	0.14	42,61,88,89	0
2	AVU	F	301	35/35	0.95	0.20	62,70,94,96	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.

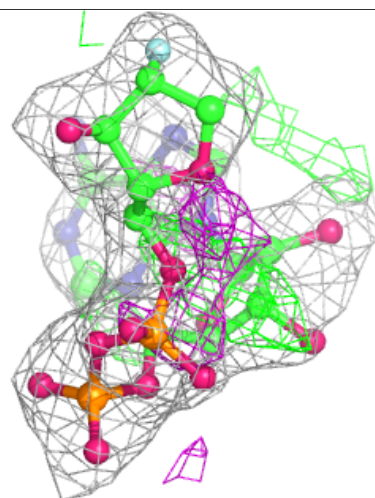
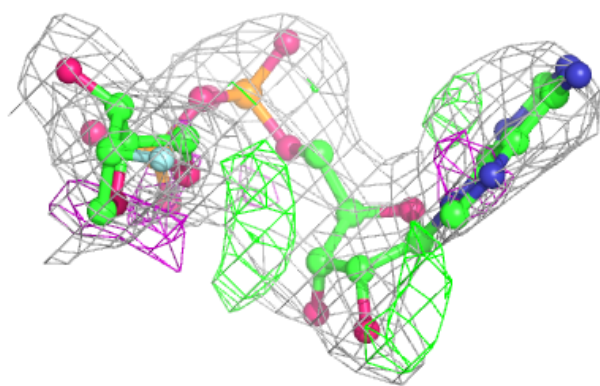
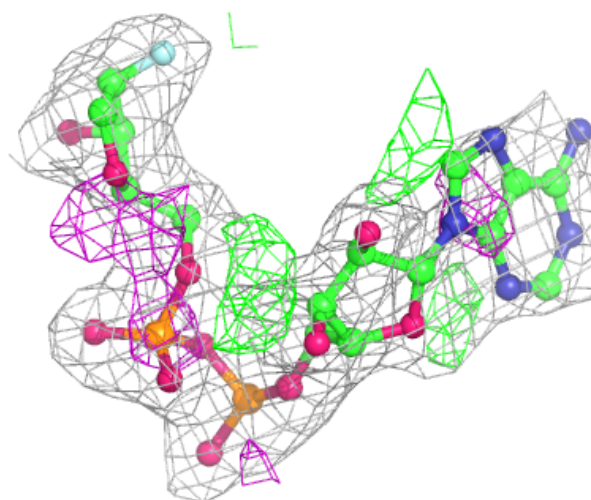
**Electron density around AVU B 301:**

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



**Electron density around AVU E 301:**

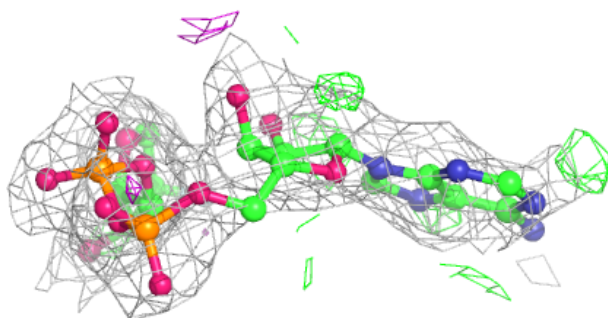
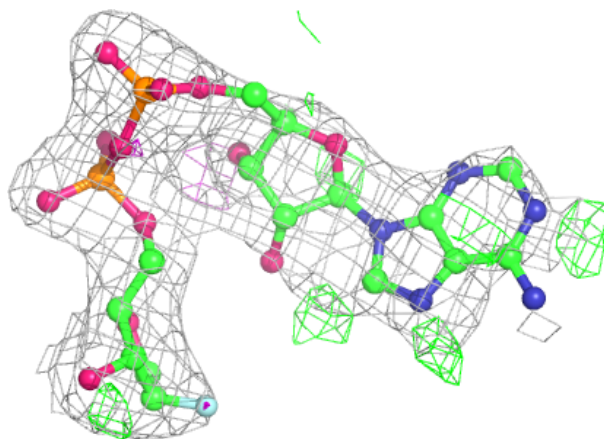
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





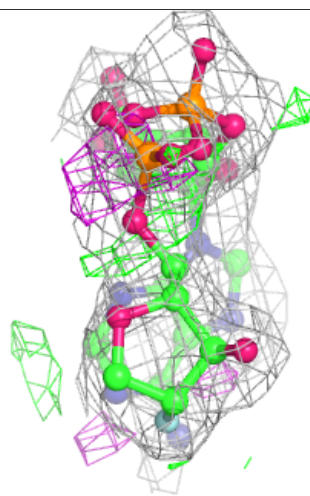
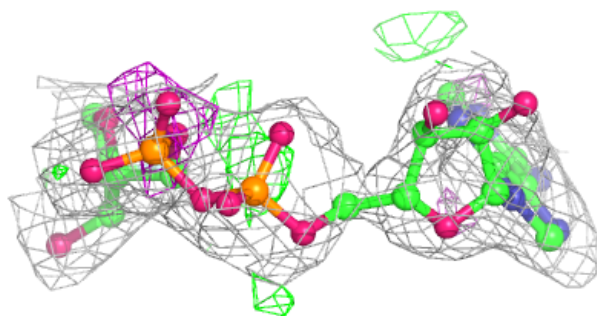
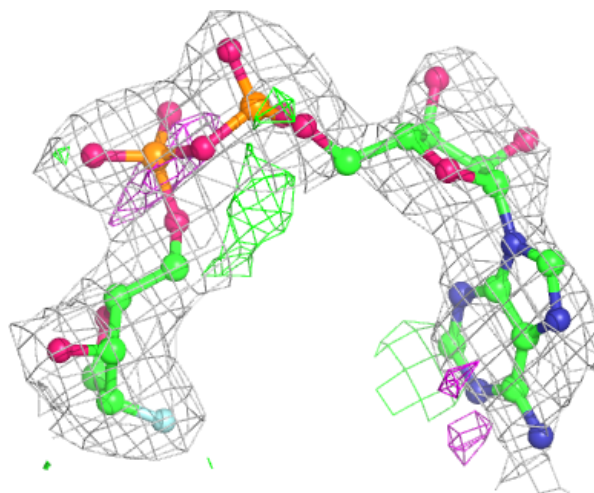
**Electron density around AVU A 301:**

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



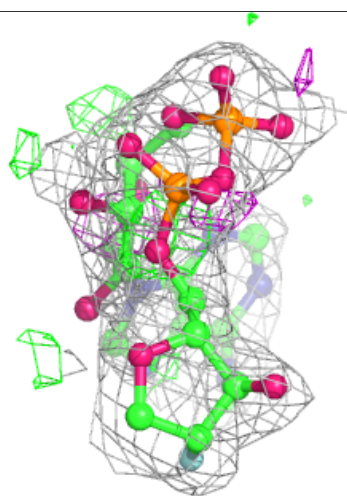
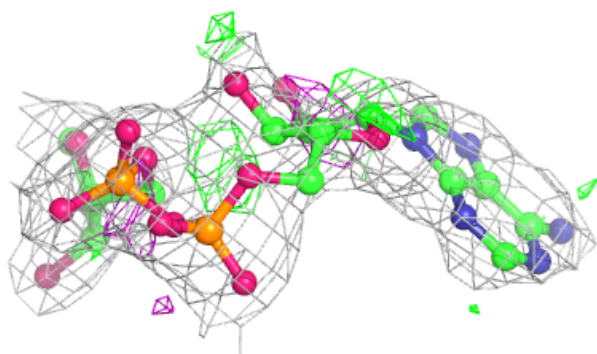
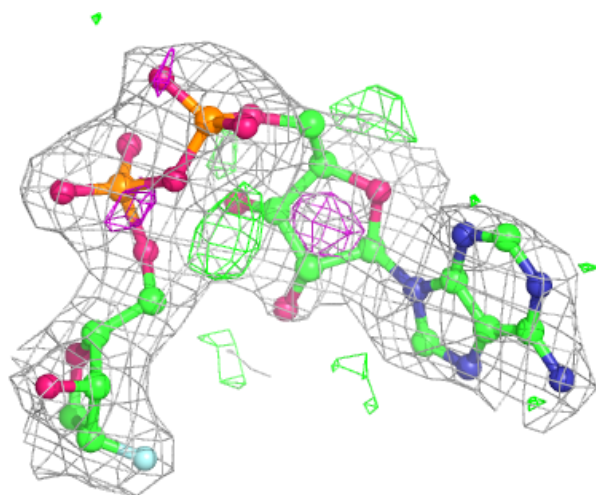
**Electron density around AVU C 301:**

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



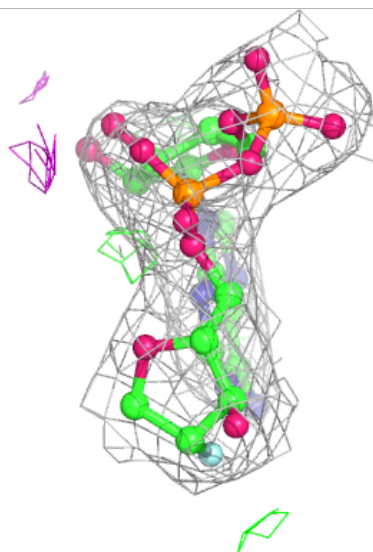
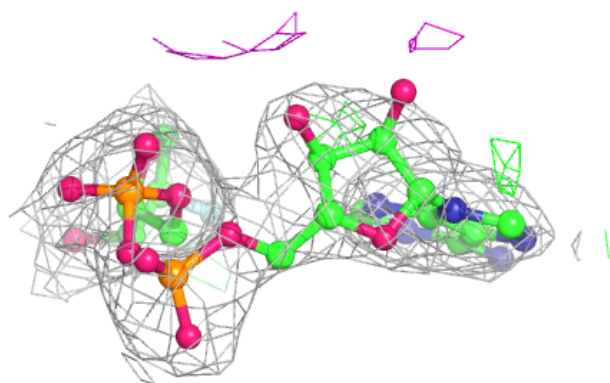
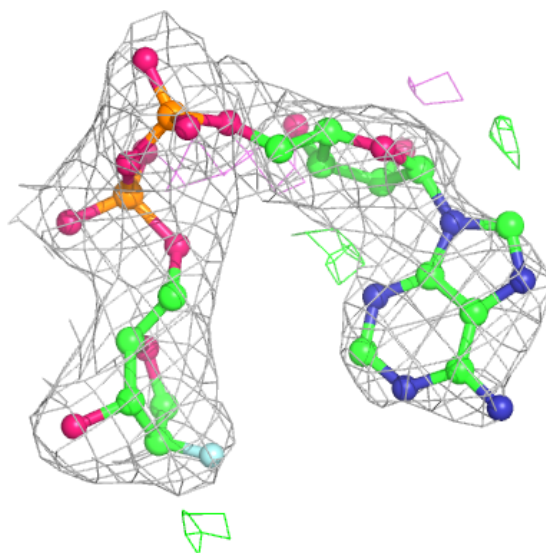
**Electron density around AVU G 301:**

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



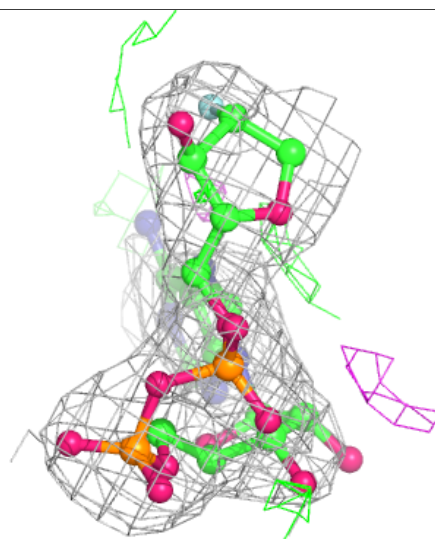
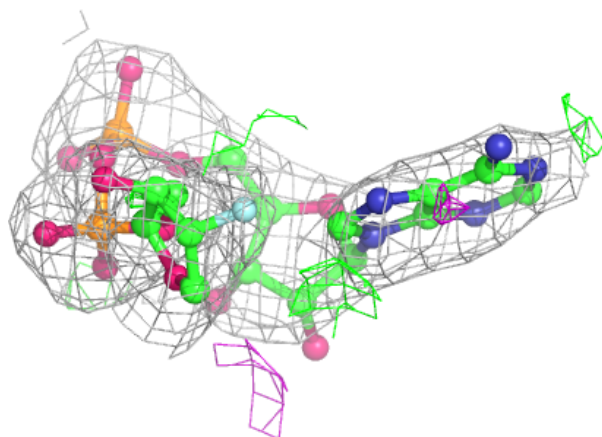
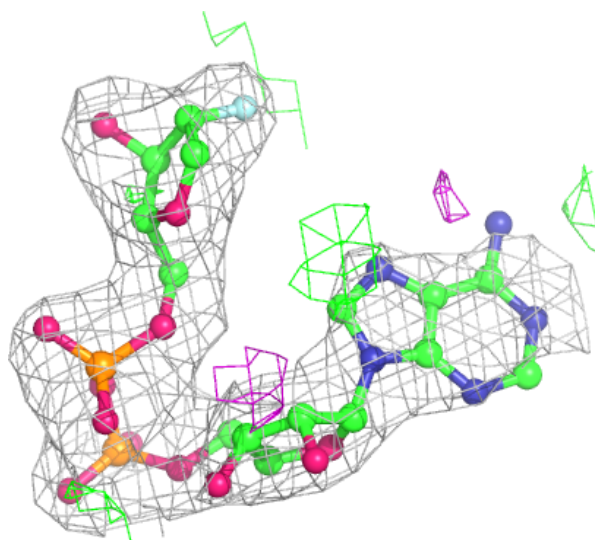
**Electron density around AVU H 301:**

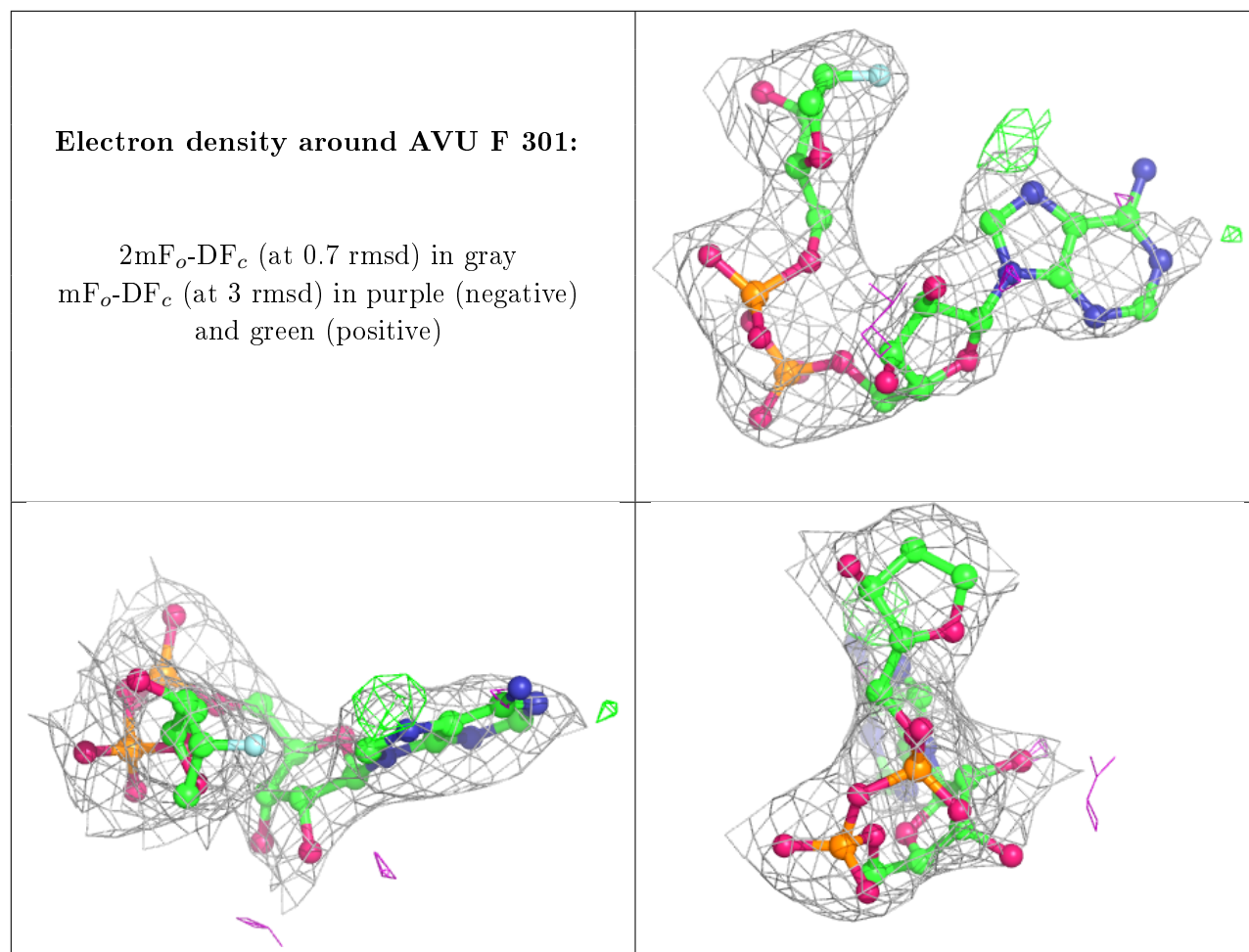
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AVU 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.