



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 3ZWV / pdb_00003zwv
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

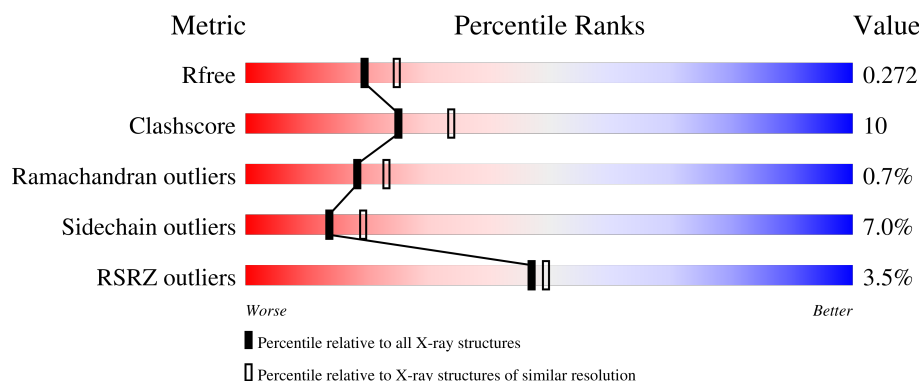
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	3% 71% 23% ..
1	B	260	2% 77% 18% ..
1	C	260	5% 72% 24% ..
1	D	260	% 75% 20% ..
1	E	260	3% 77% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	260	8% 64% 27% 5%
1	G	260	2% 73% 20%
1	H	260	5% 68% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16687 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	253	Total	C	N	O	S	0	0	1
			2018	1291	344	369	14			
1	B	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			
1	C	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			
1	D	252	Total	C	N	O	S	0	0	0
			2017	1291	343	369	14			
1	E	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			
1	F	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			
1	G	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			
1	H	252	Total	C	N	O	S	0	0	1
			2013	1288	343	368	14			

There are 16 discrepancies between the modelled and reference sequences:

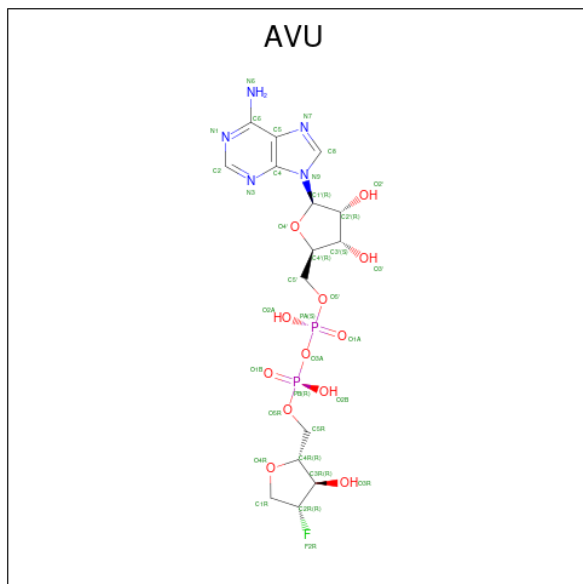
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P29241
A	0	ALA	-	expression tag	UNP P29241
B	-1	ALA	-	expression tag	UNP P29241
B	0	ALA	-	expression tag	UNP P29241
C	-1	ALA	-	expression tag	UNP P29241
C	0	ALA	-	expression tag	UNP P29241
D	-1	ALA	-	expression tag	UNP P29241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

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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 (CCD ID: AVU) (formula: C₁₅H₂₂FN₅O₁₂P₂).

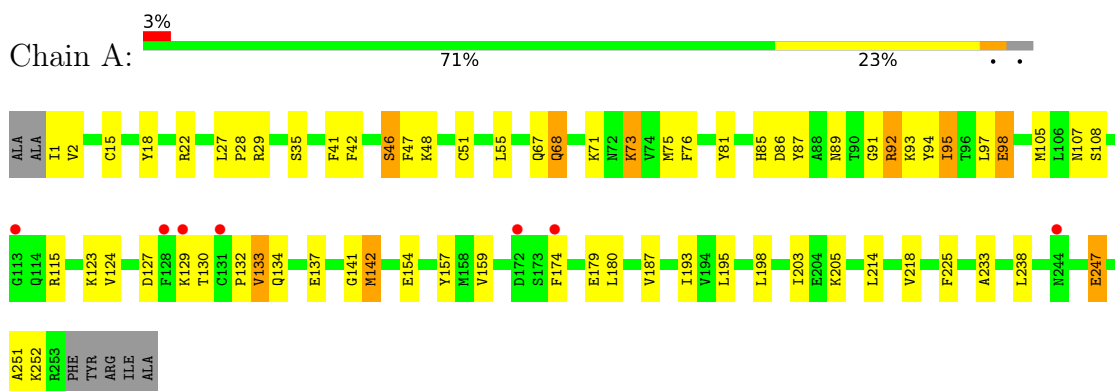


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	47	Total 47	O 47	0	0
3	C	32	Total 32	O 32	0	0
3	D	49	Total 49	O 49	0	0
3	E	40	Total 40	O 40	0	0
3	F	19	Total 19	O 19	0	0
3	G	42	Total 42	O 42	0	0
3	H	30	Total 30	O 30	0	0

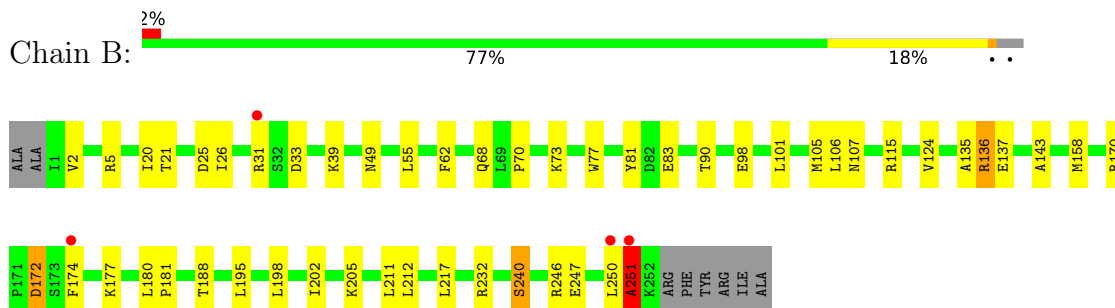
3 Residue-property plots [i](#)

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.

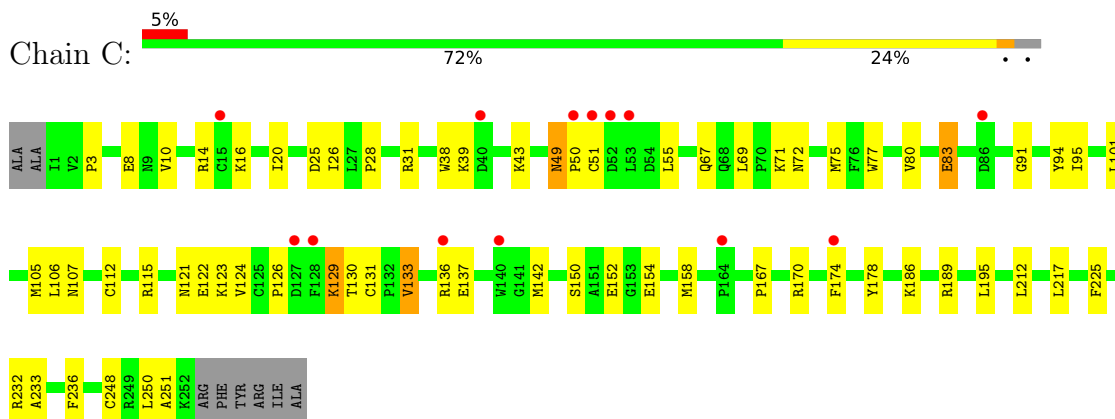
• Molecule 1: ADP-RIBOSYL CYCLASE



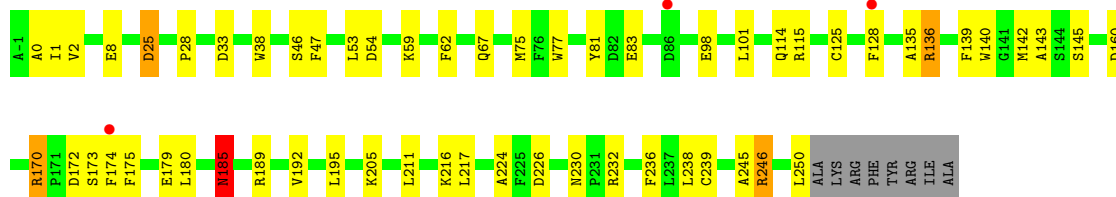
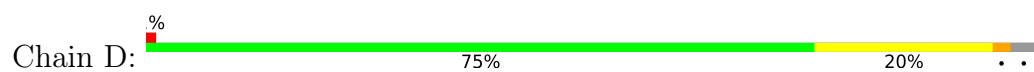
• Molecule 1: ADP-RIBOSYL CYCLASE



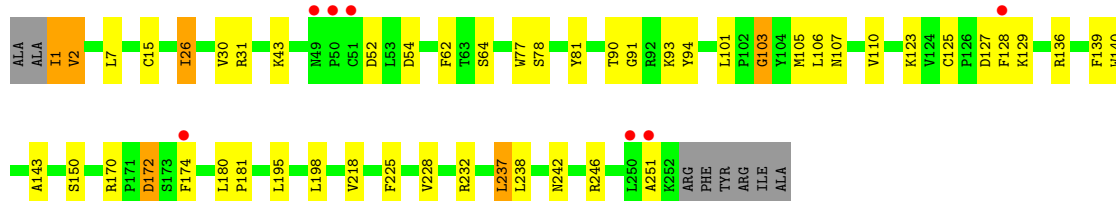
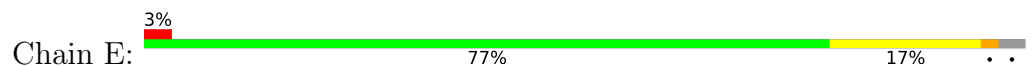
• Molecule 1: ADP-RIBOSYL CYCLASE



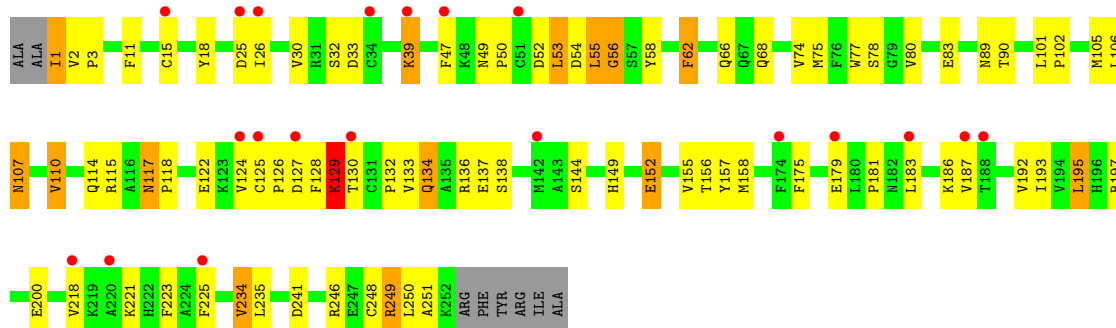
• Molecule 1: ADP-RIBOSYL CYCLASE



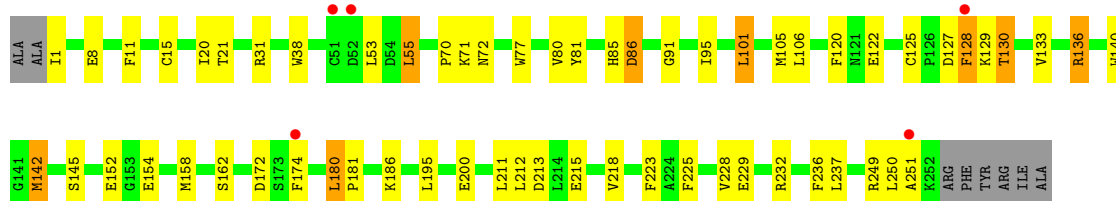
• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE

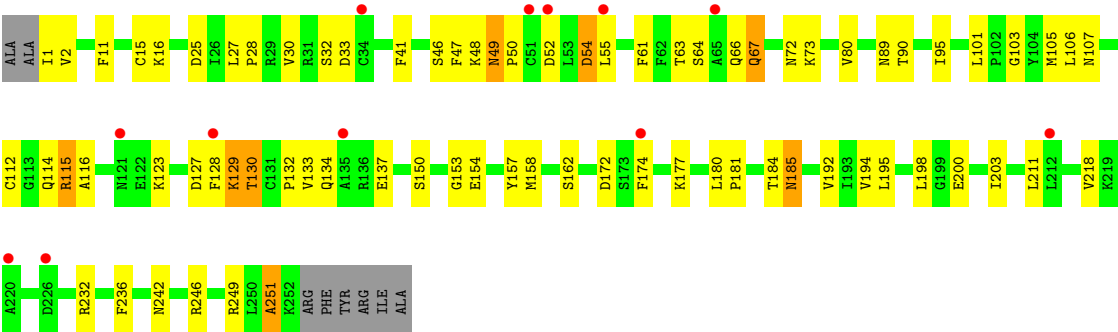


• Molecule 1: ADP-RIBOSYL CYCLASE



• Molecule 1: ADP-RIBOSYL CYCLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.15Å 76.48Å 141.37Å 88.09° 90.88° 91.02°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.5 (30.00-2.30) 68.5 (30.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.277 (Not available) , 0.272	Depositor DCC
R_{free} test set	3933 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l 0.022 for -h,k,-l 0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.06	2/2070 (0.1%)	1.18	6/2802 (0.2%)
1	B	1.15	3/2065 (0.1%)	1.18	3/2795 (0.1%)
1	C	0.98	1/2065 (0.0%)	1.12	3/2795 (0.1%)
1	D	1.17	2/2069 (0.1%)	1.21	12/2800 (0.4%)
1	E	1.16	3/2065 (0.1%)	1.19	5/2795 (0.2%)
1	F	0.95	1/2065 (0.0%)	1.14	5/2795 (0.2%)
1	G	1.16	4/2065 (0.2%)	1.23	11/2795 (0.4%)
1	H	0.94	1/2065 (0.0%)	1.10	2/2795 (0.1%)
All	All	1.08	17/16529 (0.1%)	1.17	47/22372 (0.2%)

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	E	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	251	ALA	C-N	-8.18	1.21	1.33
1	F	251	ALA	C-N	-7.72	1.22	1.33
1	G	251	ALA	C-N	-6.42	1.24	1.33
1	A	252	LYS	C-N	-5.98	1.25	1.33
1	E	7	LEU	C-O	-5.72	1.17	1.24
1	C	251	ALA	C-N	-5.71	1.25	1.33
1	G	70	PRO	C-O	5.70	1.30	1.23
1	D	145	SER	N-CA	5.62	1.53	1.46
1	B	251	ALA	C-N	-5.58	1.25	1.33
1	E	78	SER	C-O	-5.55	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	172	ASP	CA-C	5.51	1.60	1.52
1	B	135	ALA	C-O	-5.38	1.17	1.24
1	E	90	THR	CA-CB	5.38	1.62	1.53
1	B	124	VAL	CA-CB	5.34	1.61	1.54
1	D	160	ASP	CA-C	-5.28	1.46	1.52
1	G	180	LEU	C-O	-5.27	1.19	1.24
1	A	187	VAL	CA-CB	5.15	1.60	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2	VAL	CA-C-N	-10.14	109.60	120.66
1	H	2	VAL	C-N-CA	-10.14	109.60	120.66
1	A	27	LEU	CA-C-N	9.99	129.94	119.85
1	A	27	LEU	C-N-CA	9.99	129.94	119.85
1	A	2	VAL	N-CA-C	8.13	114.96	107.56
1	G	101	LEU	CA-C-N	-7.73	110.18	119.84
1	G	101	LEU	C-N-CA	-7.73	110.18	119.84
1	G	20	ILE	N-CA-C	7.66	118.46	110.72
1	B	2	VAL	N-CA-C	7.61	116.41	107.73
1	D	0	ALA	N-CA-C	7.33	123.25	113.72
1	F	62	PHE	N-CA-C	7.25	118.82	111.07
1	F	110	VAL	CB-CA-C	-6.93	100.22	110.33
1	F	234	VAL	N-CA-C	-6.88	104.14	110.82
1	B	107	ASN	N-CA-C	6.74	120.61	110.64
1	E	2	VAL	CB-CA-C	-6.74	103.50	110.71
1	D	101	LEU	CA-C-N	-6.64	111.54	119.84
1	D	101	LEU	C-N-CA	-6.64	111.54	119.84
1	F	2	VAL	N-CA-C	6.61	114.43	107.76
1	D	139	PHE	N-CA-C	6.55	118.30	111.03
1	D	192	VAL	N-CA-C	6.31	117.38	108.36
1	E	139	PHE	N-CA-C	5.97	117.66	111.03
1	D	180	LEU	CA-C-N	-5.97	113.67	119.87
1	D	180	LEU	C-N-CA	-5.97	113.67	119.87
1	A	76	PHE	N-CA-C	-5.84	100.61	109.85
1	G	172	ASP	N-CA-C	5.80	120.22	113.20
1	G	21	THR	CA-C-N	-5.69	114.96	122.99
1	G	21	THR	C-N-CA	-5.69	114.96	122.99
1	D	170	ARG	CB-CA-C	-5.68	102.60	110.16
1	D	2	VAL	N-CA-C	5.63	113.63	107.60
1	C	49	ASN	CA-C-N	5.54	125.22	119.56
1	C	49	ASN	C-N-CA	5.54	125.22	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ALA	N-CA-C	-5.54	105.32	111.36
1	E	103	GLY	N-CA-C	-5.51	105.59	113.86
1	G	20	ILE	CB-CA-C	-5.37	104.81	112.22
1	G	86	ASP	N-CA-C	5.36	116.81	110.97
1	D	173	SER	N-CA-C	-5.33	102.86	110.59
1	G	11	PHE	N-CA-C	-5.27	105.44	111.14
1	E	26	ILE	N-CA-C	-5.26	107.64	111.90
1	G	145	SER	CB-CA-C	-5.25	102.63	110.88
1	A	41	PHE	N-CA-C	-5.23	105.02	111.40
1	D	230	ASN	CA-C-N	-5.20	114.36	119.92
1	D	230	ASN	C-N-CA	-5.20	114.36	119.92
1	E	251	ALA	CA-C-N	5.17	126.53	116.20
1	F	149	HIS	N-CA-C	-5.13	106.85	113.01
1	A	203	ILE	N-CA-C	-5.13	107.15	111.56
1	B	212	LEU	N-CA-C	-5.13	105.39	111.69
1	G	53	LEU	N-CA-C	5.07	117.07	110.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	123	LYS	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	2018	0	1970	38	0
1	B	2013	0	1968	25	0
1	C	2013	0	1968	44	0
1	D	2017	0	1973	35	0
1	E	2013	0	1968	38	0
1	F	2013	0	1968	63	0
1	G	2013	0	1968	28	0
1	H	2013	0	1968	48	0
2	A	35	0	19	2	0
2	B	35	0	19	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	35	0	19	2	0
2	D	35	0	19	5	0
2	E	35	0	19	3	0
2	F	35	0	19	5	0
2	G	35	0	19	0	0
2	H	35	0	19	0	0
3	A	35	0	0	0	0
3	B	47	0	0	4	0
3	C	32	0	0	1	0
3	D	49	0	0	2	0
3	E	40	0	0	3	0
3	F	19	0	0	2	0
3	G	42	0	0	1	0
3	H	30	0	0	1	0
All	All	16687	0	15903	313	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 10.

All (313) 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:A:28:PRO:HG3	1:A:68:GLN:NE2	1.56	1.19
1:D:128:PHE:O	1:D:136:ARG:HD2	1.43	1.17
1:H:115:ARG:HG3	1:H:115:ARG:HH11	1.11	1.10
2:B:301:AVU:C2	3:B:2035:HOH:O	1.98	1.09
1:A:28:PRO:CG	1:A:68:GLN:HE22	1.66	1.07
1:A:28:PRO:HG3	1:A:68:GLN:HE22	0.87	0.99
2:B:301:AVU:H2	3:B:2035:HOH:O	1.60	0.95
1:H:30:VAL:HG21	1:H:64:SER:O	1.66	0.95
1:A:68:GLN:H	1:A:68:GLN:CD	1.75	0.94
1:A:89:ASN:O	1:A:92:ARG:HD3	1.68	0.94
1:C:137:GLU:HG2	1:C:174:PHE:CZ	2.03	0.94
1:E:1:ILE:HG23	1:E:110:VAL:HG11	1.47	0.93
1:H:115:ARG:HG3	1:H:115:ARG:NH1	1.86	0.89
1:C:136:ARG:HG3	1:C:137:GLU:HG3	1.59	0.84
1:F:129:LYS:HD3	1:F:129:LYS:H	1.43	0.83
1:C:133:VAL:O	1:C:136:ARG:HG2	1.80	0.81
1:E:180:LEU:HB3	1:E:181:PRO:HD3	1.60	0.81
1:H:101:LEU:HG	1:H:105:MET:HE2	1.63	0.80
1:F:49:ASN:HB2	1:F:52:ASP:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLU:OE2	2:B:301:AVU:N6	2.16	0.79
1:C:137:GLU:HG2	1:C:174:PHE:HZ	1.45	0.78
1:F:127:ASP:HB3	1:F:130:THR:OG1	1.84	0.77
1:D:128:PHE:O	1:D:136:ARG:CD	2.30	0.77
2:B:301:AVU:N1	3:B:2035:HOH:O	2.12	0.75
1:H:246:ARG:HG3	1:H:249:ARG:HH21	1.50	0.75
1:F:74:VAL:HG22	3:F:2008:HOH:O	1.85	0.74
1:F:117:ASN:HD22	1:F:118:PRO:HA	1.50	0.74
1:H:137:GLU:HG2	1:H:174:PHE:CZ	2.22	0.74
1:B:101:LEU:HG	1:B:105:MET:HE2	1.69	0.74
1:F:15:CYS:HB2	1:F:105:MET:SD	2.29	0.73
1:E:1:ILE:HG22	1:E:125:CYS:HB2	1.69	0.73
1:C:49:ASN:HD22	1:C:115:ARG:HH21	1.34	0.73
1:C:55:LEU:O	1:C:142:MET:HE2	1.89	0.72
1:G:101:LEU:HG	1:G:105:MET:HE2	1.72	0.71
1:C:174:PHE:CD2	2:C:301:AVU:O2'	2.43	0.70
1:D:54:ASP:HB2	3:D:2017:HOH:O	1.91	0.70
1:E:172:ASP:OD2	3:E:2034:HOH:O	2.11	0.69
1:D:195:LEU:HD11	1:D:238:LEU:HD11	1.76	0.68
1:A:68:GLN:CD	1:A:68:GLN:N	2.51	0.68
1:F:74:VAL:HG23	1:F:155:VAL:HG12	1.76	0.68
1:F:80:VAL:HG21	1:F:158:MET:HG2	1.75	0.67
1:H:30:VAL:HG22	1:H:32:SER:H	1.59	0.67
1:F:133:VAL:O	1:F:137:GLU:HG3	1.95	0.66
1:G:127:ASP:HB3	1:G:130:THR:HG22	1.76	0.66
1:A:107:ASN:O	1:A:108:SER:HB2	1.96	0.66
1:G:128:PHE:N	1:G:128:PHE:CD1	2.63	0.66
1:C:25:ASP:OD2	3:C:2008:HOH:O	2.14	0.65
1:C:250:LEU:HD11	1:D:236:PHE:CZ	2.30	0.65
1:F:74:VAL:CG2	1:F:155:VAL:HG12	2.26	0.65
1:G:127:ASP:O	1:G:130:THR:HG23	1.96	0.65
1:E:140:TRP:CB	1:E:174:PHE:HE2	2.10	0.65
1:C:250:LEU:HD13	1:D:232:ARG:CZ	2.26	0.65
1:F:129:LYS:HD3	1:F:129:LYS:N	2.11	0.64
1:E:1:ILE:CG2	1:E:110:VAL:HG11	2.25	0.64
1:D:128:PHE:HB3	1:D:136:ARG:HG3	1.79	0.64
1:E:170:ARG:HD2	1:E:172:ASP:OD2	1.97	0.63
1:G:140:TRP:HB3	1:G:174:PHE:HE2	1.62	0.63
1:H:80:VAL:HG21	1:H:158:MET:HG2	1.81	0.63
1:C:49:ASN:ND2	1:C:115:ARG:HH21	1.97	0.63
1:B:205:LYS:O	1:B:211:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:GLU:OE2	1:F:186:LYS:HE3	2.00	0.62
1:F:246:ARG:O	1:F:249:ARG:HG3	1.99	0.62
1:E:128:PHE:O	1:E:136:ARG:HD2	1.99	0.62
1:F:3:PRO:HA	1:F:110:VAL:HB	1.81	0.62
1:H:137:GLU:HG2	1:H:174:PHE:HZ	1.63	0.61
1:E:91:GLY:HA2	1:E:94:TYR:O	2.01	0.61
1:C:232:ARG:HG3	1:C:232:ARG:HH11	1.65	0.61
1:A:15:CYS:HB2	1:A:105:MET:SD	2.41	0.60
1:E:127:ASP:OD2	1:E:129:LYS:HG2	2.01	0.60
1:E:140:TRP:HB2	1:E:174:PHE:HE2	1.65	0.60
1:G:77:TRP:CH2	1:G:81:TYR:HD2	2.20	0.60
1:H:128:PHE:H	1:H:130:THR:HG22	1.67	0.60
1:B:83:GLU:HG2	1:B:195:LEU:HD11	1.83	0.59
1:B:49:ASN:HD21	1:B:115:ARG:HH21	1.49	0.59
1:E:140:TRP:CH2	2:E:301:AVU:N6	2.70	0.59
1:A:133:VAL:HG13	1:A:134:GLN:H	1.67	0.58
1:F:49:ASN:HB2	1:F:52:ASP:CB	2.34	0.57
1:E:174:PHE:HB2	2:E:301:AVU:PB	2.45	0.57
1:F:80:VAL:HG12	1:F:197:ARG:NH2	2.19	0.57
1:F:181:PRO:HA	1:F:221:LYS:NZ	2.20	0.57
1:B:55:LEU:HG	1:B:55:LEU:O	2.06	0.56
1:D:59:LYS:HA	1:D:142:MET:HE2	1.86	0.56
1:H:198:LEU:HD12	1:H:242:ASN:HB3	1.87	0.56
1:A:87:TYR:CE1	1:A:93:LYS:HE2	2.41	0.56
1:B:136:ARG:HG2	1:B:137:GLU:HG3	1.88	0.56
1:H:174:PHE:HD1	1:H:174:PHE:N	2.03	0.56
1:G:15:CYS:HB2	1:G:105:MET:SD	2.46	0.56
1:G:55:LEU:HD12	1:G:142:MET:HG3	1.87	0.56
1:G:215:GLU:HG3	1:G:225:PHE:CD2	2.41	0.56
1:C:80:VAL:HB	1:C:83:GLU:HG2	1.85	0.56
1:H:41:PHE:HB2	1:H:61:PHE:CD1	2.41	0.56
1:H:72:ASN:OD1	1:H:153:GLY:HA3	2.05	0.55
1:A:85:HIS:NE2	1:A:98:GLU:HG2	2.21	0.55
1:E:198:LEU:HD12	1:E:242:ASN:HB3	1.88	0.55
1:E:15:CYS:HB2	1:E:105:MET:SD	2.47	0.55
1:F:54:ASP:O	1:F:56:GLY:N	2.37	0.55
1:H:174:PHE:N	1:H:174:PHE:CD1	2.73	0.55
1:D:170:ARG:HD2	1:D:172:ASP:OD1	2.07	0.54
1:E:30:VAL:HG21	1:E:64:SER:O	2.06	0.54
1:A:127:ASP:O	1:A:130:THR:HG22	2.07	0.54
1:A:28:PRO:HG2	1:A:67:GLN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PRO:HD2	1:C:170:ARG:HD3	1.91	0.54
1:F:33:ASP:C	1:F:33:ASP:OD1	2.51	0.54
1:F:128:PHE:C	1:F:130:THR:H	2.15	0.53
1:H:47:PHE:HA	1:H:114:GLN:O	2.09	0.53
1:H:103:GLY:O	1:H:107:ASN:HB2	2.08	0.53
1:H:128:PHE:C	1:H:130:THR:N	2.63	0.53
1:E:77:TRP:CH2	1:E:81:TYR:HD2	2.27	0.53
1:D:28:PRO:HG2	1:D:67:GLN:HB2	1.91	0.53
1:D:83:GLU:HG2	1:D:195:LEU:HD21	1.90	0.52
1:F:128:PHE:C	1:F:130:THR:N	2.67	0.52
1:G:133:VAL:HA	1:G:136:ARG:HG3	1.90	0.52
1:A:198:LEU:HD22	1:A:247:GLU:CG	2.40	0.52
1:F:144:SER:OG	2:F:301:AVU:H1RA	2.10	0.52
1:H:246:ARG:HG3	1:H:249:ARG:NH2	2.21	0.52
1:D:77:TRP:CH2	1:D:81:TYR:HD2	2.28	0.52
1:E:1:ILE:HG23	1:E:110:VAL:CG1	2.31	0.52
1:G:77:TRP:HA	1:G:158:MET:O	2.10	0.51
1:H:180:LEU:N	1:H:181:PRO:HD2	2.25	0.51
1:C:121:ASN:HD21	1:C:124:VAL:HG12	1.76	0.51
1:F:75:MET:HE3	1:F:156:THR:CG2	2.41	0.51
1:G:180:LEU:HB3	1:G:181:PRO:HD3	1.91	0.51
1:B:205:LYS:C	1:B:211:LEU:HD12	2.36	0.51
1:B:26:ILE:HD11	3:B:2032:HOH:O	2.11	0.50
1:B:77:TRP:CH2	1:B:81:TYR:HD2	2.29	0.50
1:H:115:ARG:HH11	1:H:115:ARG:CG	1.99	0.50
1:F:58:TYR:O	1:F:62:PHE:HD2	1.95	0.50
1:H:66:GLN:HB3	3:H:2008:HOH:O	2.11	0.50
1:C:16:LYS:HD3	1:C:20:ILE:HD12	1.94	0.50
1:H:128:PHE:N	1:H:130:THR:HG22	2.25	0.50
1:C:152:GLU:HG2	1:C:186:LYS:HB3	1.92	0.50
1:C:137:GLU:OE2	1:C:174:PHE:CE1	2.64	0.49
1:E:101:LEU:HG	1:E:105:MET:HE2	1.93	0.49
1:C:3:PRO:HG2	1:C:122:GLU:O	2.12	0.49
1:B:90:THR:HG22	1:B:90:THR:O	2.12	0.49
1:G:152:GLU:HG2	1:G:186:LYS:HB3	1.95	0.49
1:G:91:GLY:HA2	1:G:95:ILE:HD13	1.94	0.49
1:A:174:PHE:CD2	2:A:301:AVU:H2'	2.47	0.49
1:A:42:PHE:O	1:A:46:SER:HB2	2.13	0.48
1:B:25:ASP:OD1	1:B:25:ASP:N	2.44	0.48
1:A:91:GLY:HA2	1:A:95:ILE:HD13	1.95	0.48
1:F:101:LEU:HG	1:F:105:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:VAL:O	1:G:81:TYR:C	2.56	0.48
2:D:301:AVU:H5'	3:D:2048:HOH:O	2.13	0.48
1:C:154:GLU:HG2	1:C:189:ARG:HB3	1.96	0.48
1:E:1:ILE:CG2	1:E:110:VAL:CG1	2.92	0.48
1:E:103:GLY:O	1:E:107:ASN:HB2	2.14	0.48
1:B:70:PRO:HB2	1:B:73:LYS:HD3	1.95	0.47
1:C:137:GLU:CG	1:C:174:PHE:CZ	2.88	0.47
1:E:140:TRP:HB2	1:E:174:PHE:CE2	2.48	0.47
1:F:129:LYS:HG3	1:F:136:ARG:HD3	1.95	0.47
1:H:11:PHE:CD1	1:H:11:PHE:C	2.92	0.47
1:A:137:GLU:O	1:A:141:GLY:HA3	2.14	0.47
1:F:181:PRO:HA	1:F:221:LYS:HZ1	1.79	0.47
1:H:49:ASN:OD1	1:H:50:PRO:HD2	2.15	0.47
1:F:1:ILE:HG22	1:F:125:CYS:O	2.15	0.47
1:C:49:ASN:HD22	1:C:115:ARG:NH2	2.09	0.47
1:F:39:LYS:HA	1:F:39:LYS:NZ	2.29	0.47
1:B:174:PHE:HB2	2:B:301:AVU:PB	2.54	0.47
1:C:236:PHE:CD2	1:D:239:CYS:HB3	2.49	0.47
1:F:101:LEU:N	1:F:102:PRO:HD2	2.30	0.47
1:B:170:ARG:NH1	1:B:172:ASP:OD2	2.47	0.47
1:D:189:ARG:HB2	1:D:224:ALA:HB3	1.97	0.47
1:E:218:VAL:HG11	1:E:225:PHE:HB2	1.95	0.47
1:G:72:ASN:HA	1:G:154:GLU:O	2.15	0.47
1:G:229:GLU:OE2	3:G:2036:HOH:O	2.20	0.47
1:H:72:ASN:HA	1:H:154:GLU:O	2.14	0.47
1:H:127:ASP:HB2	1:H:130:THR:HG22	1.97	0.47
1:C:137:GLU:OE1	1:C:178:TYR:OH	2.31	0.47
2:F:301:AVU:O1B	2:F:301:AVU:O3'	2.27	0.47
1:H:129:LYS:H	1:H:129:LYS:HG2	1.52	0.47
1:A:133:VAL:HG13	1:A:134:GLN:N	2.30	0.47
1:A:233:ALA:O	1:B:240:SER:HB3	2.14	0.46
1:A:198:LEU:HD22	1:A:247:GLU:HG2	1.97	0.46
1:C:106:LEU:O	1:C:107:ASN:C	2.58	0.46
1:F:218:VAL:HG11	1:F:225:PHE:HB2	1.97	0.46
1:A:174:PHE:HB2	2:A:301:AVU:PB	2.56	0.46
1:A:214:LEU:O	1:A:218:VAL:HG23	2.15	0.46
1:C:71:LYS:O	1:C:72:ASN:HB2	2.16	0.46
1:D:174:PHE:HB2	2:D:301:AVU:PB	2.55	0.46
1:E:128:PHE:O	1:E:136:ARG:CD	2.62	0.46
3:E:2024:HOH:O	1:F:241:ASP:HA	2.16	0.46
1:F:39:LYS:HA	1:F:39:LYS:HZ3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:VAL:HG13	1:H:134:GLN:N	2.30	0.46
1:G:127:ASP:O	1:G:130:THR:CG2	2.61	0.46
1:B:62:PHE:CZ	1:B:143:ALA:HB2	2.51	0.46
1:F:234:VAL:O	1:F:235:LEU:C	2.58	0.46
1:A:179:GLU:O	1:A:180:LEU:C	2.59	0.46
1:G:218:VAL:HG13	1:G:223:PHE:HB2	1.98	0.46
1:A:28:PRO:CB	1:A:68:GLN:HE22	2.26	0.46
1:C:248:CYS:O	1:C:250:LEU:HD12	2.16	0.46
1:F:83:GLU:HG2	1:F:195:LEU:HD21	1.97	0.46
1:E:93:LYS:HG2	1:E:94:TYR:CE1	2.51	0.45
1:D:8:GLU:HG3	1:D:38:TRP:CE2	2.52	0.45
1:D:62:PHE:CZ	1:D:143:ALA:HB2	2.52	0.45
1:F:175:PHE:HA	1:F:179:GLU:HB2	1.99	0.45
1:D:1:ILE:HB	1:D:125:CYS:O	2.16	0.45
1:F:55:LEU:O	1:F:55:LEU:CD2	2.65	0.45
1:F:249:ARG:NH2	3:F:2017:HOH:O	2.49	0.45
1:H:48:LYS:HE2	1:H:52:ASP:O	2.16	0.45
1:F:183:LEU:HD22	1:F:187:VAL:HG21	1.99	0.45
1:E:180:LEU:HB3	1:E:181:PRO:CD	2.39	0.45
1:A:51:CYS:HB3	1:A:132:PRO:HD2	1.99	0.45
1:A:93:LYS:HG2	1:A:94:TYR:CE1	2.51	0.45
1:D:216:LYS:HB2	1:D:216:LYS:NZ	2.31	0.45
1:G:212:LEU:O	1:G:213:ASP:C	2.59	0.45
1:H:128:PHE:H	1:H:130:THR:CG2	2.30	0.44
1:D:47:PHE:HA	1:D:114:GLN:O	2.17	0.44
1:B:77:TRP:HA	1:B:158:MET:O	2.18	0.44
1:B:198:LEU:HD22	1:B:247:GLU:HB2	1.99	0.44
1:D:140:TRP:CZ3	2:D:301:AVU:N6	2.85	0.44
1:F:106:LEU:O	1:F:107:ASN:C	2.60	0.44
1:E:140:TRP:HB3	1:E:174:PHE:HE2	1.80	0.44
1:H:15:CYS:HB2	1:H:105:MET:SD	2.58	0.44
1:B:180:LEU:HB3	1:B:181:PRO:HD3	1.98	0.44
1:D:98:GLU:OE2	2:D:301:AVU:N1	2.51	0.44
1:H:194:VAL:HG21	1:H:211:LEU:HD11	2.00	0.44
1:C:77:TRP:HA	1:C:158:MET:O	2.17	0.44
1:D:53:LEU:HB2	1:D:135:ALA:HA	1.99	0.44
1:D:189:ARG:HD3	1:D:226:ASP:OD2	2.17	0.44
1:D:170:ARG:NH1	1:D:172:ASP:OD1	2.50	0.43
1:G:250:LEU:O	1:H:251:ALA:HB2	2.18	0.43
1:D:174:PHE:CE2	2:D:301:AVU:O2'	2.71	0.43
1:F:78:SER:OG	2:F:301:AVU:O2B	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:O	1:A:130:THR:N	2.43	0.43
1:C:51:CYS:HB3	1:C:131:CYS:HB3	1.93	0.43
1:F:53:LEU:N	1:F:53:LEU:HD12	2.33	0.43
1:D:195:LEU:HA	1:D:195:LEU:HD12	1.64	0.43
1:F:11:PHE:CD1	1:F:11:PHE:C	2.97	0.43
1:D:217:LEU:HD11	1:E:129:LYS:HG3	1.99	0.43
1:F:75:MET:HE3	1:F:156:THR:HG22	2.00	0.43
1:H:114:GLN:HG3	1:H:116:ALA:O	2.18	0.43
1:C:39:LYS:O	1:C:43:LYS:HG2	2.19	0.43
1:G:120:PHE:HE2	1:G:122:GLU:CD	2.26	0.43
1:E:62:PHE:CZ	1:E:143:ALA:HB2	2.54	0.43
1:F:75:MET:CE	1:F:156:THR:HG22	2.48	0.43
1:C:8:GLU:OE1	1:C:38:TRP:NE1	2.52	0.43
1:F:246:ARG:HA	1:F:246:ARG:NE	2.34	0.43
1:C:50:PRO:CB	1:C:126:PRO:HG2	2.49	0.42
1:A:71:LYS:HB3	1:A:71:LYS:HE3	1.88	0.42
1:B:217:LEU:HD23	1:B:217:LEU:HA	1.90	0.42
1:B:250:LEU:O	1:B:251:ALA:HB3	2.20	0.42
1:C:236:PHE:O	1:D:236:PHE:HB3	2.20	0.42
1:F:47:PHE:O	1:F:115:ARG:HD3	2.19	0.42
1:F:144:SER:OG	2:F:301:AVU:C1R	2.67	0.42
1:H:50:PRO:HB3	1:H:112:CYS:HB2	2.01	0.42
1:C:10:VAL:O	1:C:14:ARG:HG3	2.19	0.42
1:C:28:PRO:HG2	1:C:67:GLN:HB3	2.02	0.42
1:F:18:TYR:CD1	1:F:18:TYR:C	2.97	0.42
1:F:47:PHE:HA	1:F:114:GLN:O	2.19	0.42
1:F:187:VAL:O	1:F:223:PHE:CD1	2.72	0.42
1:B:172:ASP:O	1:B:177:LYS:HE2	2.19	0.42
1:C:112:CYS:SG	1:C:126:PRO:HD2	2.59	0.42
1:E:195:LEU:CD1	1:E:238:LEU:HD11	2.50	0.42
1:H:46:SER:C	1:H:48:LYS:H	2.27	0.42
1:H:162:SER:HA	1:H:203:ILE:HG12	2.00	0.42
1:A:18:TYR:HA	1:A:22:ARG:CG	2.50	0.42
1:E:232:ARG:NH2	1:F:248:CYS:O	2.53	0.42
1:H:157:TYR:O	1:H:192:VAL:HA	2.20	0.42
1:G:8:GLU:HG3	1:G:38:TRP:CE2	2.55	0.42
1:C:174:PHE:CE2	2:C:301:AVU:O2'	2.72	0.42
1:E:180:LEU:CB	1:E:181:PRO:HD3	2.40	0.42
1:A:87:TYR:CZ	1:A:93:LYS:HE2	2.55	0.42
1:E:54:ASP:HB2	3:E:2015:HOH:O	2.20	0.42
1:E:174:PHE:HB2	2:E:301:AVU:O1B	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LEU:C	1:H:251:ALA:HB2	2.45	0.42
1:H:137:GLU:OE2	1:H:174:PHE:CE1	2.73	0.42
1:F:187:VAL:O	1:F:223:PHE:HD1	2.03	0.42
1:G:140:TRP:CB	1:G:174:PHE:HE2	2.29	0.41
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.85	0.41
1:C:69:LEU:HG	1:C:150:SER:HB3	2.02	0.41
1:E:237:LEU:HD12	1:E:237:LEU:HA	1.76	0.41
1:F:54:ASP:HB2	1:F:134:GLN:HG3	2.02	0.41
1:G:236:PHE:HB3	1:H:236:PHE:O	2.20	0.41
1:H:54:ASP:OD1	1:H:54:ASP:N	2.51	0.41
1:C:133:VAL:O	1:C:136:ARG:CG	2.60	0.41
1:E:30:VAL:CG2	1:E:64:SER:O	2.68	0.41
1:E:128:PHE:HE1	1:E:129:LYS:HD3	1.85	0.41
1:F:197:ARG:HD2	1:F:200:GLU:OE1	2.20	0.41
1:A:47:PHE:C	1:A:48:LYS:HG3	2.45	0.41
1:A:195:LEU:HD11	1:A:238:LEU:HD21	2.02	0.41
1:B:174:PHE:HB2	2:B:301:AVU:O5R	2.21	0.41
1:C:91:GLY:HA2	1:C:94:TYR:O	2.21	0.41
1:D:185:ASN:C	1:D:185:ASN:HD22	2.29	0.41
1:F:157:TYR:O	1:F:192:VAL:HA	2.21	0.41
1:H:115:ARG:NH1	1:H:115:ARG:CG	2.66	0.41
1:A:81:TYR:CD1	1:A:81:TYR:C	2.99	0.41
1:A:225:PHE:CD1	1:A:225:PHE:C	2.98	0.41
1:B:174:PHE:CE2	2:B:301:AVU:O2'	2.71	0.41
1:C:75:MET:HB3	1:C:95:ILE:O	2.21	0.41
1:D:25:ASP:OD1	1:D:25:ASP:N	2.49	0.41
1:D:46:SER:O	1:D:47:PHE:HB2	2.20	0.41
1:D:245:ALA:O	1:D:246:ARG:C	2.63	0.41
1:F:49:ASN:CB	1:F:52:ASP:HB2	2.43	0.41
1:H:177:LYS:O	1:H:181:PRO:HG3	2.22	0.41
1:H:184:THR:O	1:H:185:ASN:C	2.64	0.41
1:A:157:TYR:CE2	1:A:159:VAL:CG1	3.04	0.40
1:E:232:ARG:NH1	1:F:250:LEU:HD12	2.36	0.40
1:F:77:TRP:O	2:F:301:AVU:H5RA	2.21	0.40
1:F:83:GLU:H	1:F:83:GLU:CD	2.30	0.40
1:C:50:PRO:HB2	1:C:126:PRO:HG2	2.02	0.40
1:D:205:LYS:O	1:D:211:LEU:HD12	2.21	0.40
1:F:50:PRO:HB2	1:F:126:PRO:HG3	2.03	0.40
1:H:16:LYS:HB2	1:H:16:LYS:HE2	1.76	0.40
1:C:225:PHE:CD1	1:C:225:PHE:C	2.99	0.40
1:G:1:ILE:CG2	1:G:125:CYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:TYR:CE2	1:G:85:HIS:CE1	3.10	0.40
1:H:28:PRO:HG2	1:H:67:GLN:HB3	2.03	0.40
1:A:55:LEU:O	1:A:142:MET:HG2	2.21	0.40
1:C:101:LEU:O	1:C:105:MET:HG3	2.21	0.40
1:D:175:PHE:HA	1:D:179:GLU:HB2	2.03	0.40
1:F:89:ASN:O	1:F:90:THR:C	2.64	0.40
1:F:192:VAL:O	1:F:193:ILE:HD13	2.22	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	251/260 (96%)	238 (95%)	11 (4%)	2 (1%)	16	20
1	B	250/260 (96%)	236 (94%)	13 (5%)	1 (0%)	30	38
1	C	250/260 (96%)	234 (94%)	15 (6%)	1 (0%)	30	38
1	D	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	38
1	E	250/260 (96%)	237 (95%)	13 (5%)	0	100	100
1	F	250/260 (96%)	230 (92%)	14 (6%)	6 (2%)	4	4
1	G	250/260 (96%)	245 (98%)	4 (2%)	1 (0%)	30	38
1	H	250/260 (96%)	233 (93%)	14 (6%)	3 (1%)	10	12
All	All	2001/2080 (96%)	1890 (94%)	96 (5%)	15 (1%)	18	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	ALA
1	F	55	LEU
1	A	251	ALA

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Mol	Chain	Res	Type
1	C	129	LYS
1	F	129	LYS
1	G	129	LYS
1	H	185	ASN
1	A	133	VAL
1	D	185	ASN
1	F	56	GLY
1	F	107	ASN
1	F	132	PRO
1	H	132	PRO
1	F	26	ILE
1	H	218	VAL

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%)	199 (90%)	21 (10%)	8	10
1	B	220/226 (97%)	205 (93%)	15 (7%)	14	20
1	C	220/226 (97%)	210 (96%)	10 (4%)	24	37
1	D	220/226 (97%)	212 (96%)	8 (4%)	31	47
1	E	220/226 (97%)	208 (94%)	12 (6%)	19	28
1	F	220/226 (97%)	203 (92%)	17 (8%)	12	16
1	G	220/226 (97%)	203 (92%)	17 (8%)	12	16
1	H	220/226 (97%)	197 (90%)	23 (10%)	6	8
All	All	1760/1808 (97%)	1637 (93%)	123 (7%)	14	19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	29	ARG
1	A	35	SER

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Mol	Chain	Res	Type
1	A	46	SER
1	A	68	GLN
1	A	73	LYS
1	A	75	MET
1	A	86	ASP
1	A	92	ARG
1	A	95	ILE
1	A	97	LEU
1	A	98	GLU
1	A	115	ARG
1	A	123	LYS
1	A	124	VAL
1	A	129	LYS
1	A	142	MET
1	A	154	GLU
1	A	193	ILE
1	A	205	LYS
1	A	247	GLU
1	B	5	ARG
1	B	20	ILE
1	B	21	THR
1	B	31	ARG
1	B	33	ASP
1	B	39	LYS
1	B	68	GLN
1	B	106	LEU
1	B	136	ARG
1	B	172	ASP
1	B	188	THR
1	B	202	ILE
1	B	232	ARG
1	B	240	SER
1	B	246	ARG
1	C	26	ILE
1	C	31	ARG
1	C	83	GLU
1	C	123	LYS
1	C	129	LYS
1	C	130	THR
1	C	133	VAL
1	C	195	LEU
1	C	212	LEU

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Mol	Chain	Res	Type
1	C	217	LEU
1	D	25	ASP
1	D	33	ASP
1	D	75	MET
1	D	115	ARG
1	D	136	ARG
1	D	185	ASN
1	D	246	ARG
1	D	250	LEU
1	E	1	ILE
1	E	2	VAL
1	E	26	ILE
1	E	31	ARG
1	E	43	LYS
1	E	52	ASP
1	E	106	LEU
1	E	150	SER
1	E	172	ASP
1	E	228	VAL
1	E	237	LEU
1	E	246	ARG
1	F	1	ILE
1	F	25	ASP
1	F	30	VAL
1	F	32	SER
1	F	39	LYS
1	F	53	LEU
1	F	66	GLN
1	F	68	GLN
1	F	117	ASN
1	F	122	GLU
1	F	124	VAL
1	F	129	LYS
1	F	134	GLN
1	F	138	SER
1	F	152	GLU
1	F	195	LEU
1	F	249	ARG
1	G	31	ARG
1	G	55	LEU
1	G	71	LYS
1	G	86	ASP

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Mol	Chain	Res	Type
1	G	106	LEU
1	G	128	PHE
1	G	130	THR
1	G	136	ARG
1	G	142	MET
1	G	162	SER
1	G	195	LEU
1	G	200	GLU
1	G	211	LEU
1	G	228	VAL
1	G	232	ARG
1	G	237	LEU
1	G	249	ARG
1	H	1	ILE
1	H	25	ASP
1	H	27	LEU
1	H	33	ASP
1	H	49	ASN
1	H	54	ASP
1	H	55	LEU
1	H	63	THR
1	H	67	GLN
1	H	73	LYS
1	H	89	ASN
1	H	90	THR
1	H	95	ILE
1	H	106	LEU
1	H	115	ARG
1	H	123	LYS
1	H	129	LYS
1	H	130	THR
1	H	150	SER
1	H	172	ASP
1	H	195	LEU
1	H	200	GLU
1	H	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	107	ASN

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Mol	Chain	Res	Type
1	A	114	GLN
1	B	68	GLN
1	B	89	ASN
1	B	117	ASN
1	B	242	ASN
1	C	49	ASN
1	C	89	ASN
1	C	149	HIS
1	D	49	ASN
1	D	89	ASN
1	D	107	ASN
1	D	185	ASN
1	D	242	ASN
1	E	89	ASN
1	E	107	ASN
1	E	242	ASN
1	F	89	ASN
1	F	114	GLN
1	F	117	ASN
1	F	134	GLN
1	G	89	ASN
1	G	242	ASN
1	H	68	GLN
1	H	89	ASN
1	H	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	E	301	1	38,38,38	1.05	3 (7%)	54,58,58	2.30	14 (25%)
2	AVU	C	301	1	38,38,38	1.19	3 (7%)	54,58,58	1.76	12 (22%)
2	AVU	A	301	1	38,38,38	1.07	4 (10%)	54,58,58	1.97	14 (25%)
2	AVU	B	301	1	38,38,38	1.32	4 (10%)	54,58,58	1.90	15 (27%)
2	AVU	D	301	1	38,38,38	1.21	3 (7%)	54,58,58	2.00	15 (27%)
2	AVU	H	301	1	38,38,38	1.08	2 (5%)	54,58,58	1.95	16 (29%)
2	AVU	F	301	1	38,38,38	1.05	3 (7%)	54,58,58	2.00	17 (31%)
2	AVU	G	301	1	38,38,38	1.05	2 (5%)	54,58,58	2.04	16 (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	E	301	1	-	6/22/51/51	0/4/4/4
2	AVU	C	301	1	-	9/22/51/51	0/4/4/4
2	AVU	A	301	1	-	5/22/51/51	0/4/4/4
2	AVU	B	301	1	-	9/22/51/51	0/4/4/4
2	AVU	D	301	1	-	6/22/51/51	0/4/4/4
2	AVU	H	301	1	-	5/22/51/51	0/4/4/4
2	AVU	F	301	1	-	5/22/51/51	0/4/4/4
2	AVU	G	301	1	-	4/22/51/51	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	AVU	PB-O3A	4.65	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	AVU	PB-O3A	4.59	1.64	1.59
2	C	301	AVU	PA-O3A	3.72	1.63	1.59
2	C	301	AVU	PB-O3A	3.34	1.63	1.59
2	H	301	AVU	C8-N7	2.77	1.37	1.31
2	B	301	AVU	PB-O5R	2.73	1.70	1.59
2	E	301	AVU	C8-N7	2.56	1.36	1.31
2	A	301	AVU	PA-O3A	2.52	1.62	1.59
2	B	301	AVU	C8-N7	2.44	1.36	1.31
2	F	301	AVU	C8-N7	2.32	1.36	1.31
2	F	301	AVU	F2R-C2R	-2.31	1.35	1.40
2	D	301	AVU	C8-N7	2.30	1.36	1.31
2	A	301	AVU	C8-N7	2.27	1.36	1.31
2	E	301	AVU	C1'-N9	2.24	1.52	1.46
2	G	301	AVU	O4R-C4R	-2.22	1.40	1.44
2	D	301	AVU	C5-N7	-2.21	1.35	1.39
2	B	301	AVU	C4-N9	-2.20	1.33	1.37
2	E	301	AVU	PB-O3A	2.18	1.61	1.59
2	G	301	AVU	C8-N7	2.12	1.35	1.31
2	F	301	AVU	C1R-C2R	-2.08	1.49	1.53
2	H	301	AVU	F2R-C2R	-2.05	1.36	1.40
2	A	301	AVU	PB-O3A	2.04	1.61	1.59
2	C	301	AVU	C8-N7	2.04	1.35	1.31
2	A	301	AVU	F2R-C2R	-2.02	1.36	1.40

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	AVU	F2R-C2R-C1R	-9.75	97.39	109.75
2	E	301	AVU	N3-C2-N1	-5.66	120.01	128.58
2	H	301	AVU	O4'-C1'-N9	5.66	118.96	108.09
2	D	301	AVU	F2R-C2R-C1R	-5.64	102.60	109.75
2	E	301	AVU	C5-C4-N3	-5.56	119.06	126.72
2	D	301	AVU	N3-C2-N1	-5.55	120.19	128.58
2	G	301	AVU	C5-C4-N3	-5.20	119.55	126.72
2	F	301	AVU	N3-C2-N1	-5.08	120.90	128.58
2	G	301	AVU	N3-C2-N1	-5.06	120.93	128.58
2	C	301	AVU	N3-C2-N1	-5.04	120.95	128.58
2	D	301	AVU	C5-C4-N3	-5.04	119.78	126.72
2	B	301	AVU	N3-C2-N1	-4.84	121.25	128.58
2	F	301	AVU	F2R-C2R-C1R	-4.60	103.91	109.75
2	H	301	AVU	C5-C4-N3	-4.52	120.49	126.72
2	C	301	AVU	C5-C4-N3	-4.46	120.57	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	AVU	N3-C2-N1	-4.45	121.85	128.58
2	A	301	AVU	N9-C8-N7	-4.44	107.64	113.94
2	F	301	AVU	C5-C4-N3	-4.44	120.60	126.72
2	A	301	AVU	C2R-C3R-C4R	4.43	108.29	102.38
2	F	301	AVU	F2R-C2R-C3R	-4.43	104.62	108.56
2	A	301	AVU	C5-C4-N3	-4.39	120.67	126.72
2	F	301	AVU	N9-C8-N7	-4.36	107.75	113.94
2	A	301	AVU	N3-C2-N1	-4.32	122.05	128.58
2	B	301	AVU	C5-C4-N3	-4.11	121.05	126.72
2	E	301	AVU	C2-N3-C4	4.11	121.86	111.83
2	A	301	AVU	C4-C5-N7	-4.04	105.97	110.58
2	E	301	AVU	F2R-C2R-C3R	-4.00	105.01	108.56
2	A	301	AVU	C4-N9-C8	3.99	109.93	105.74
2	C	301	AVU	C2R-C3R-C4R	3.93	107.62	102.38
2	B	301	AVU	F2R-C2R-C1R	-3.83	104.89	109.75
2	G	301	AVU	N3-C4-N9	3.81	133.65	127.17
2	G	301	AVU	C2R-C3R-C4R	3.80	107.44	102.38
2	G	301	AVU	F2R-C2R-C1R	-3.79	104.95	109.75
2	G	301	AVU	O3A-PA-O1A	-3.60	99.86	110.70
2	B	301	AVU	C2R-C3R-C4R	3.56	107.12	102.38
2	D	301	AVU	N3-C4-N9	3.55	133.21	127.17
2	D	301	AVU	C2-N3-C4	3.53	120.45	111.83
2	B	301	AVU	N9-C8-N7	-3.50	108.98	113.94
2	G	301	AVU	N9-C8-N7	-3.49	108.98	113.94
2	F	301	AVU	C2-N3-C4	3.47	120.30	111.83
2	H	301	AVU	O3R-C3R-C2R	-3.45	99.25	111.63
2	G	301	AVU	C2-N3-C4	3.45	120.27	111.83
2	C	301	AVU	N9-C8-N7	-3.45	109.04	113.94
2	H	301	AVU	N9-C8-N7	-3.45	109.05	113.94
2	B	301	AVU	C4-C5-N7	-3.42	106.68	110.58
2	B	301	AVU	O5R-C5R-C4R	3.36	120.43	108.99
2	B	301	AVU	O4'-C1'-N9	3.34	114.50	108.09
2	E	301	AVU	C2R-C3R-C4R	3.32	106.81	102.38
2	A	301	AVU	C5-N7-C8	3.30	108.64	103.45
2	H	301	AVU	C2-N3-C4	3.26	119.78	111.83
2	E	301	AVU	N3-C4-N9	3.25	132.70	127.17
2	A	301	AVU	C2-N3-C4	3.25	119.77	111.83
2	C	301	AVU	C2-N3-C4	3.25	119.77	111.83
2	H	301	AVU	C4-C5-N7	-3.24	106.88	110.58
2	B	301	AVU	C2-N3-C4	3.23	119.72	111.83
2	C	301	AVU	N3-C4-N9	3.22	132.63	127.17
2	D	301	AVU	F2R-C2R-C3R	-3.19	105.72	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	AVU	C4-N9-C8	3.17	109.06	105.74
2	H	301	AVU	C2R-C3R-C4R	3.16	106.59	102.38
2	C	301	AVU	C4-N9-C8	3.04	108.93	105.74
2	D	301	AVU	C2R-C3R-C4R	3.01	106.40	102.38
2	F	301	AVU	C5-N7-C8	3.00	108.17	103.45
2	E	301	AVU	N9-C8-N7	-2.98	109.70	113.94
2	D	301	AVU	N9-C8-N7	-2.97	109.73	113.94
2	D	301	AVU	O2A-PA-O3A	-2.96	99.28	107.27
2	B	301	AVU	C5-C4-N9	2.84	108.91	105.81
2	A	301	AVU	C4-N9-C1'	-2.84	119.99	126.63
2	E	301	AVU	C4-C5-N7	-2.82	107.36	110.58
2	A	301	AVU	C3'-C2'-C1'	2.78	106.73	101.46
2	G	301	AVU	C1R-O4R-C4R	2.75	114.14	108.06
2	F	301	AVU	N3-C4-N9	2.74	131.83	127.17
2	C	301	AVU	O4'-C1'-N9	2.74	113.34	108.09
2	F	301	AVU	C4-C5-N7	-2.73	107.46	110.58
2	G	301	AVU	C5-N7-C8	2.67	107.64	103.45
2	B	301	AVU	C5-N7-C8	2.65	107.62	103.45
2	G	301	AVU	C4-N9-C8	2.62	108.49	105.74
2	H	301	AVU	C5-C4-N9	2.58	108.62	105.81
2	G	301	AVU	C2'-C1'-N9	-2.58	106.89	113.30
2	C	301	AVU	O3R-C3R-C2R	-2.58	102.39	111.63
2	A	301	AVU	F2R-C2R-C3R	2.56	110.84	108.56
2	A	301	AVU	O3R-C3R-C2R	-2.56	102.44	111.63
2	F	301	AVU	O5'-C5'-C4'	-2.56	100.28	108.99
2	E	301	AVU	C5-N7-C8	2.55	107.46	103.45
2	A	301	AVU	N3-C4-N9	2.55	131.50	127.17
2	D	301	AVU	O2A-PA-O1A	2.54	124.25	112.44
2	H	301	AVU	C5-N7-C8	2.54	107.44	103.45
2	H	301	AVU	F2R-C2R-C3R	2.49	110.77	108.56
2	G	301	AVU	O2A-PA-O1A	2.49	124.02	112.44
2	F	301	AVU	O4'-C4'-C5'	2.45	117.19	109.33
2	G	301	AVU	O5R-C5R-C4R	2.39	117.12	108.99
2	F	301	AVU	O2A-PA-O3A	2.38	113.71	107.27
2	C	301	AVU	C5-N7-C8	2.36	107.15	103.45
2	E	301	AVU	C1R-O4R-C4R	2.35	113.26	108.06
2	B	301	AVU	C1R-O4R-C4R	2.34	113.22	108.06
2	F	301	AVU	C4-N9-C1'	-2.31	121.23	126.63
2	E	301	AVU	C2'-C3'-C4'	2.30	107.06	102.61
2	E	301	AVU	C5-C4-N9	2.23	108.25	105.81
2	D	301	AVU	C5-N7-C8	2.21	106.92	103.45
2	D	301	AVU	C4-N9-C8	2.21	108.06	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	AVU	O3A-PA-O1A	-2.19	104.11	110.70
2	G	301	AVU	C4-C5-N7	-2.19	108.08	110.58
2	C	301	AVU	C4-C5-N7	-2.18	108.08	110.58
2	H	301	AVU	N3-C4-N9	2.18	130.87	127.17
2	A	301	AVU	C6-C5-N7	2.17	136.28	132.09
2	B	301	AVU	O4R-C1R-C2R	2.16	108.21	104.88
2	H	301	AVU	C4-N9-C8	2.15	108.00	105.74
2	F	301	AVU	C1R-C2R-C3R	-2.13	101.70	104.26
2	F	301	AVU	C5'-C4'-C3'	-2.12	107.56	115.21
2	D	301	AVU	C3'-C2'-C1'	2.12	105.47	101.46
2	B	301	AVU	C2'-C3'-C4'	2.09	106.64	102.61
2	H	301	AVU	O2A-PA-O1A	2.07	122.09	112.44
2	F	301	AVU	O2'-C2'-C3'	-2.06	105.20	111.82
2	E	301	AVU	C3'-C2'-C1'	2.06	105.36	101.46
2	B	301	AVU	O2B-PB-O3A	2.06	112.84	107.27
2	G	301	AVU	O5'-C5'-C4'	2.04	115.94	108.99
2	H	301	AVU	C4-N9-C1'	-2.03	121.89	126.63
2	D	301	AVU	O5R-C5R-C4R	2.02	115.88	108.99
2	C	301	AVU	O3A-PA-O1A	-2.01	104.65	110.70
2	D	301	AVU	C4-C5-N7	-2.01	108.28	110.58

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	AVU	PB-O3A-PA-O5'
2	B	301	AVU	C5'-O5'-PA-O1A
2	B	301	AVU	C5'-O5'-PA-O2A
2	B	301	AVU	C5'-O5'-PA-O3A
2	C	301	AVU	C2'-C1'-N9-C8
2	C	301	AVU	C5'-O5'-PA-O1A
2	C	301	AVU	C5'-O5'-PA-O3A
2	E	301	AVU	PB-O3A-PA-O5'
2	G	301	AVU	C4R-C5R-O5R-PB
2	G	301	AVU	C3'-C4'-C5'-O5'
2	G	301	AVU	O4'-C4'-C5'-O5'
2	B	301	AVU	C3'-C4'-C5'-O5'
2	B	301	AVU	O4'-C4'-C5'-O5'
2	C	301	AVU	C2'-C1'-N9-C4
2	F	301	AVU	C2'-C1'-N9-C4
2	B	301	AVU	C4R-C5R-O5R-PB
2	C	301	AVU	C4R-C5R-O5R-PB

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Mol	Chain	Res	Type	Atoms
2	H	301	AVU	C4R-C5R-O5R-PB
2	F	301	AVU	C2'-C1'-N9-C8
2	D	301	AVU	O4'-C4'-C5'-O5'
2	E	301	AVU	O4'-C4'-C5'-O5'
2	A	301	AVU	PB-O3A-PA-O1A
2	A	301	AVU	C4R-C5R-O5R-PB
2	E	301	AVU	C4R-C5R-O5R-PB
2	D	301	AVU	C4R-C5R-O5R-PB
2	A	301	AVU	PB-O3A-PA-O5'
2	C	301	AVU	PB-O3A-PA-O5'
2	D	301	AVU	PB-O3A-PA-O5'
2	H	301	AVU	PB-O3A-PA-O5'
2	A	301	AVU	C2'-C1'-N9-C8
2	B	301	AVU	C2'-C1'-N9-C8
2	C	301	AVU	C5'-O5'-PA-O2A
2	H	301	AVU	C5'-O5'-PA-O1A
2	F	301	AVU	C4R-C5R-O5R-PB
2	H	301	AVU	C3'-C4'-C5'-O5'
2	E	301	AVU	PA-O3A-PB-O1B
2	H	301	AVU	PB-O3A-PA-O1A
2	B	301	AVU	O4'-C1'-N9-C8
2	E	301	AVU	C3'-C4'-C5'-O5'
2	A	301	AVU	O4'-C1'-N9-C8
2	C	301	AVU	O4'-C4'-C5'-O5'
2	D	301	AVU	PA-O3A-PB-O1B
2	E	301	AVU	PA-O3A-PB-O2B
2	F	301	AVU	PA-O3A-PB-O1B
2	D	301	AVU	C3'-C4'-C5'-O5'
2	F	301	AVU	O4'-C1'-N9-C8
2	C	301	AVU	PB-O3A-PA-O1A
2	D	301	AVU	PA-O3A-PB-O2B
2	G	301	AVU	PA-O3A-PB-O2B

There are no ring outliers.

6 monomers are involved in 24 short contacts:

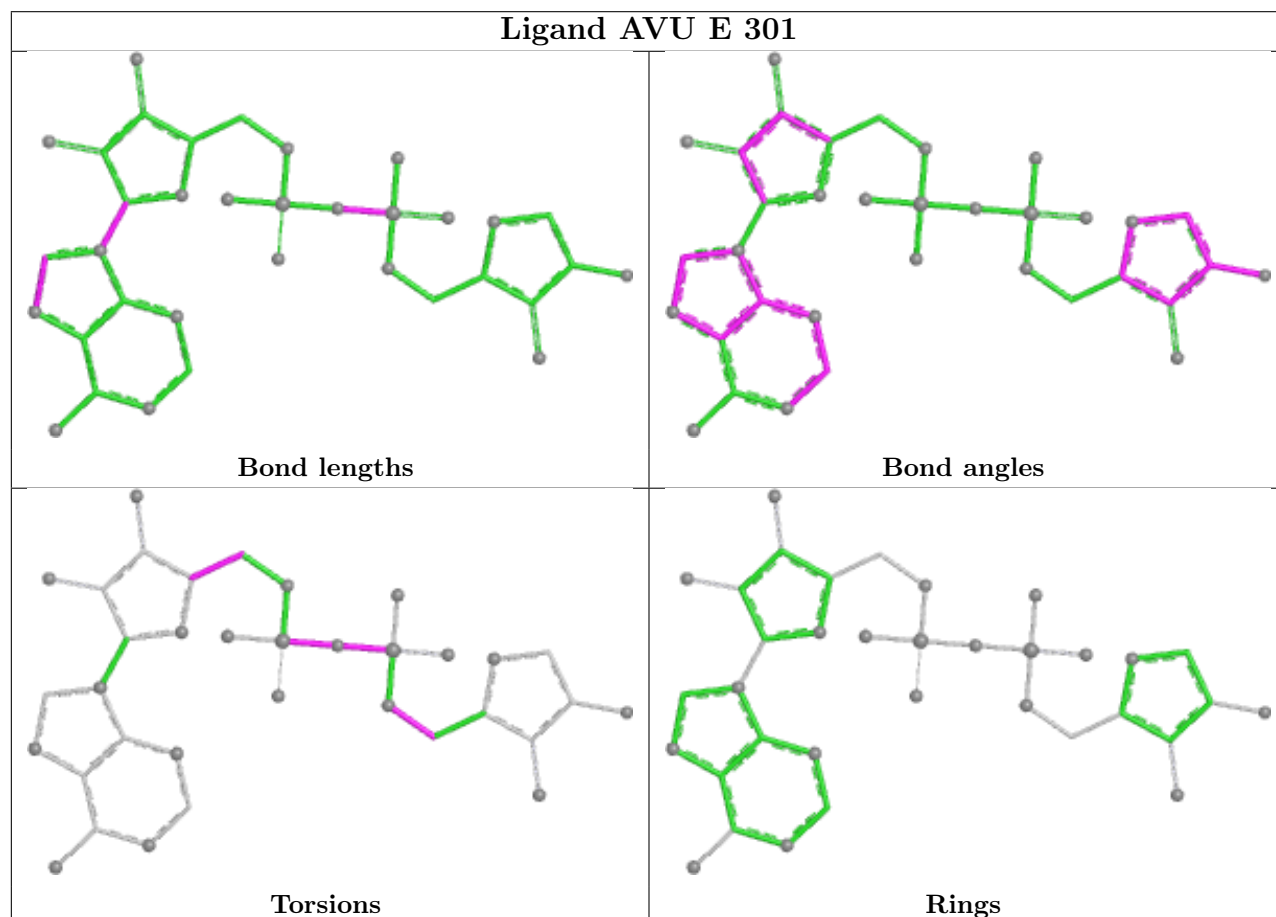
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	AVU	3	0
2	C	301	AVU	2	0
2	A	301	AVU	2	0
2	B	301	AVU	7	0
2	D	301	AVU	5	0

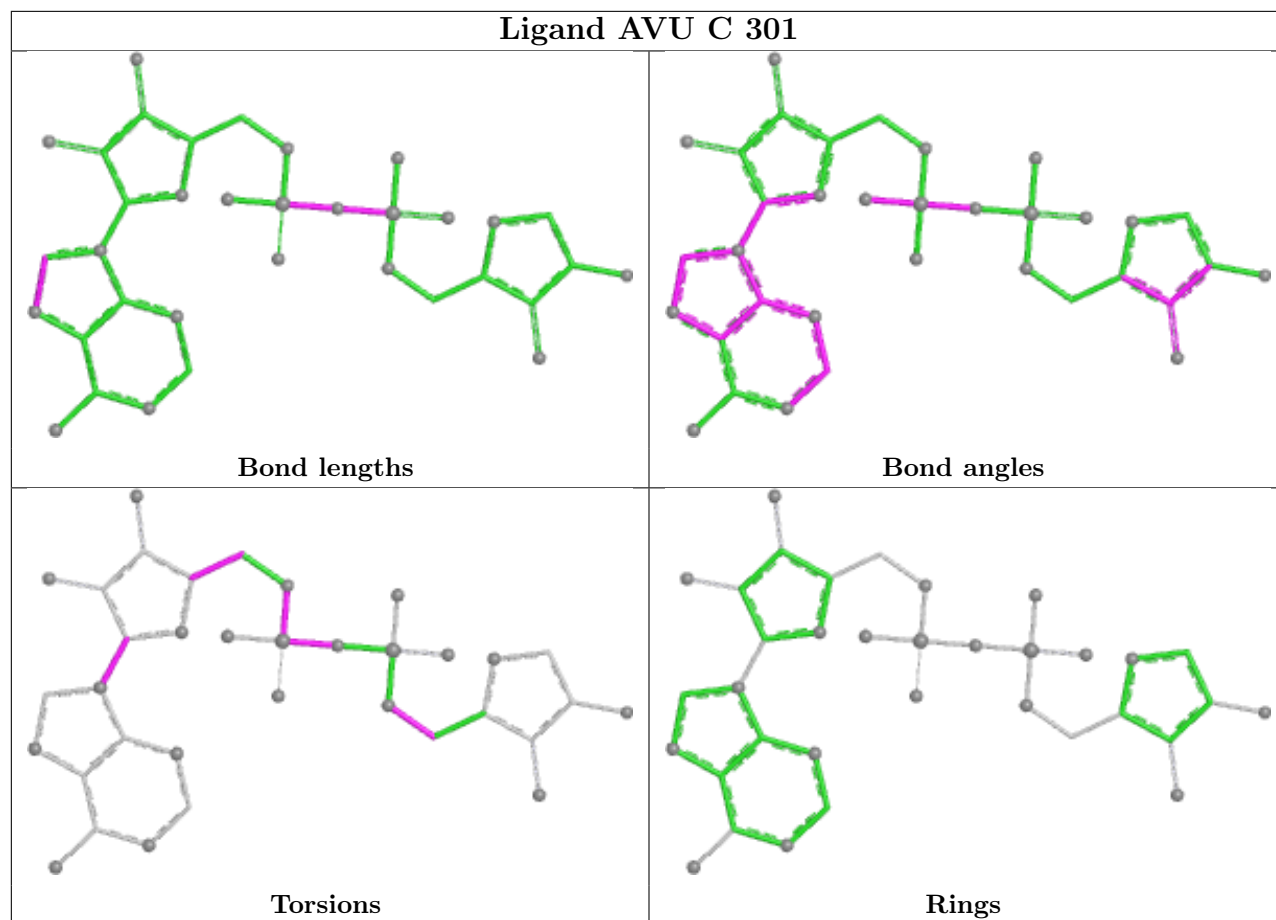
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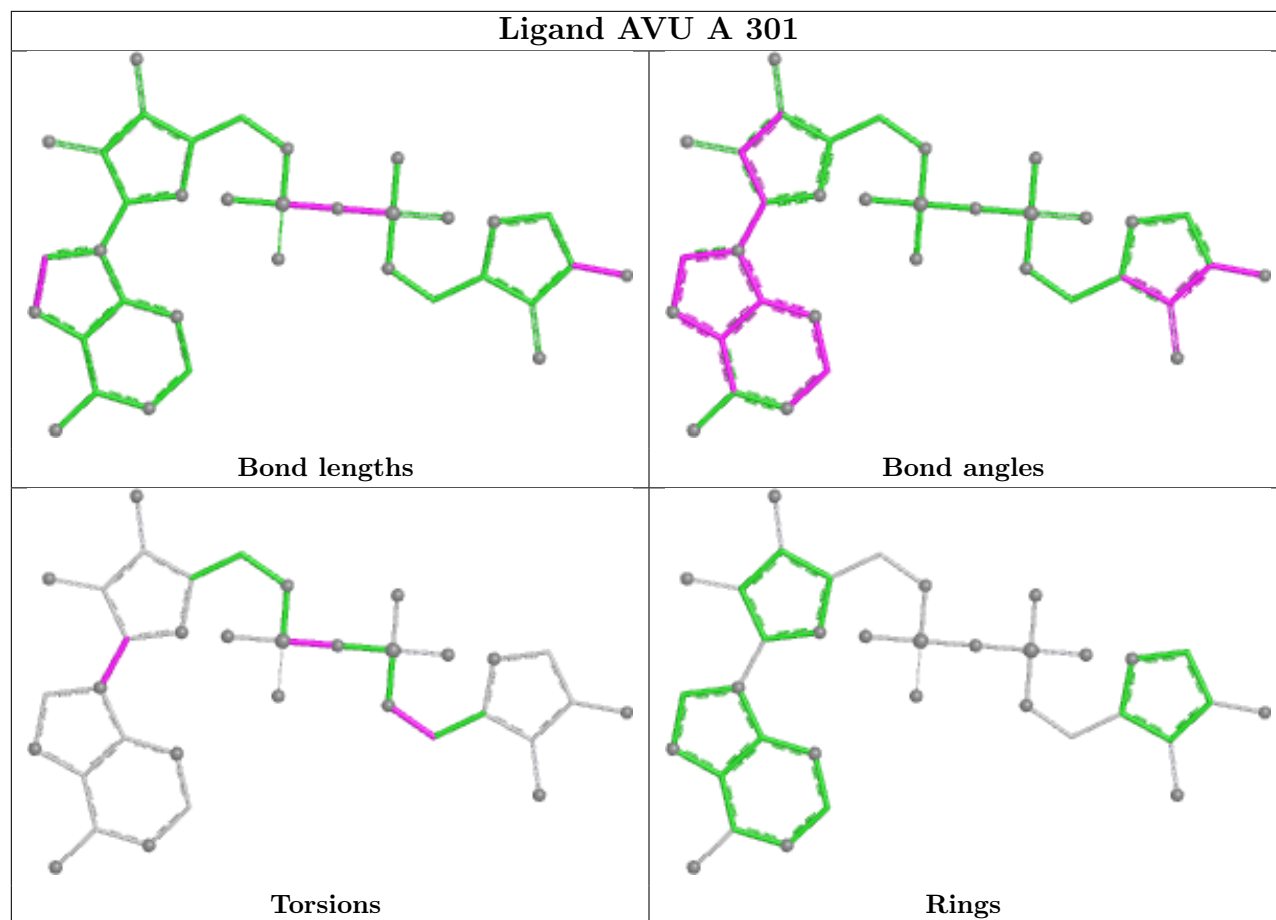
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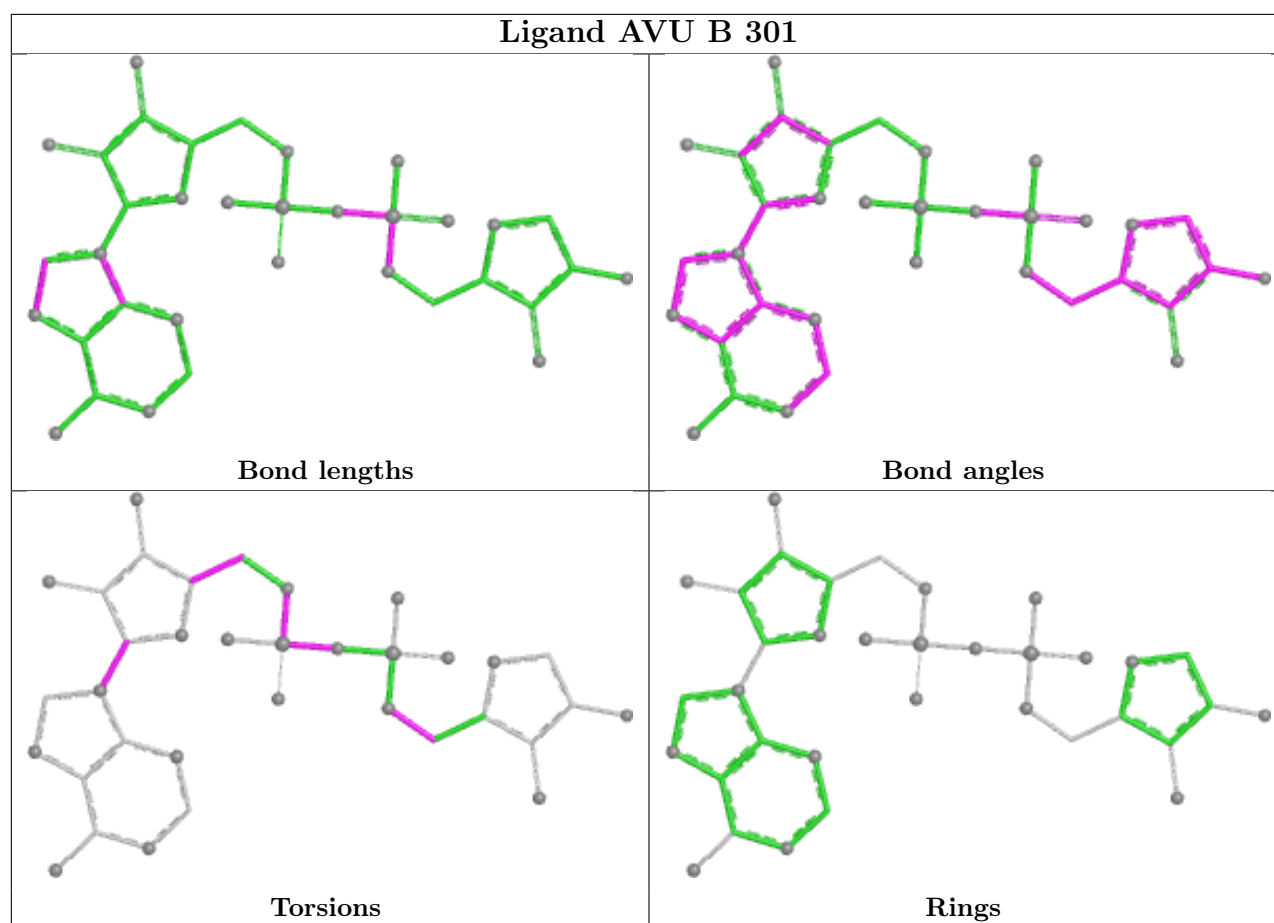
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	AVU	5	0

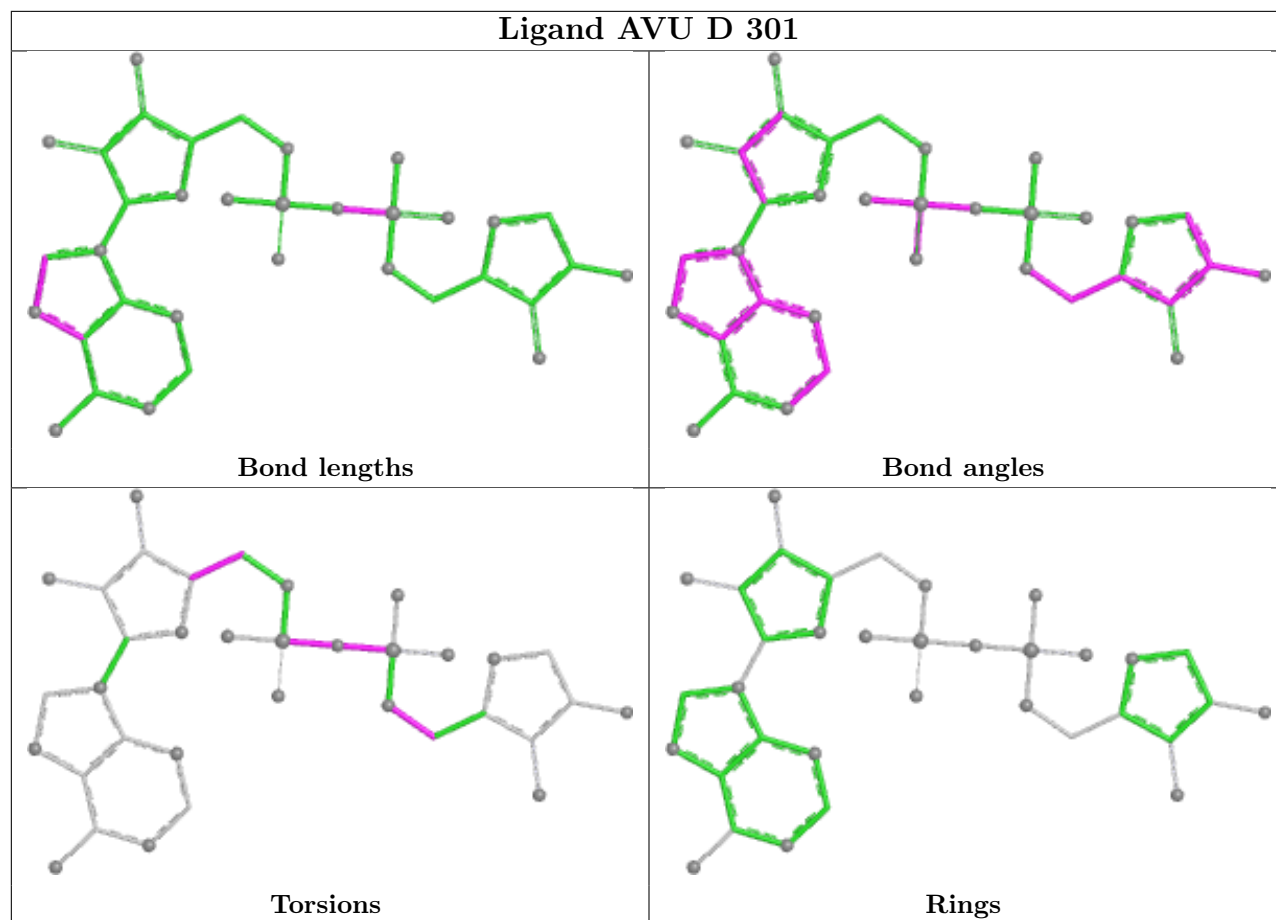
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

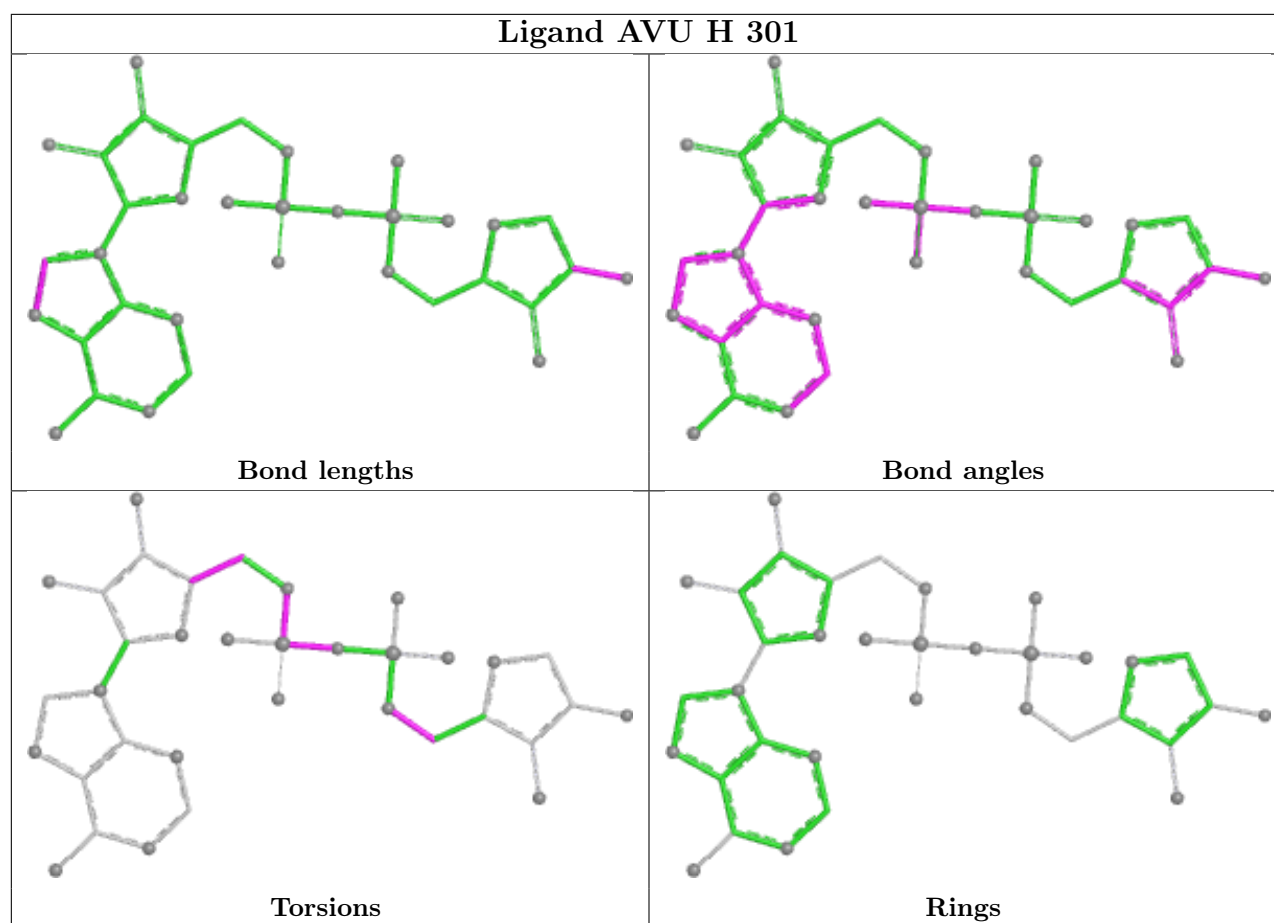


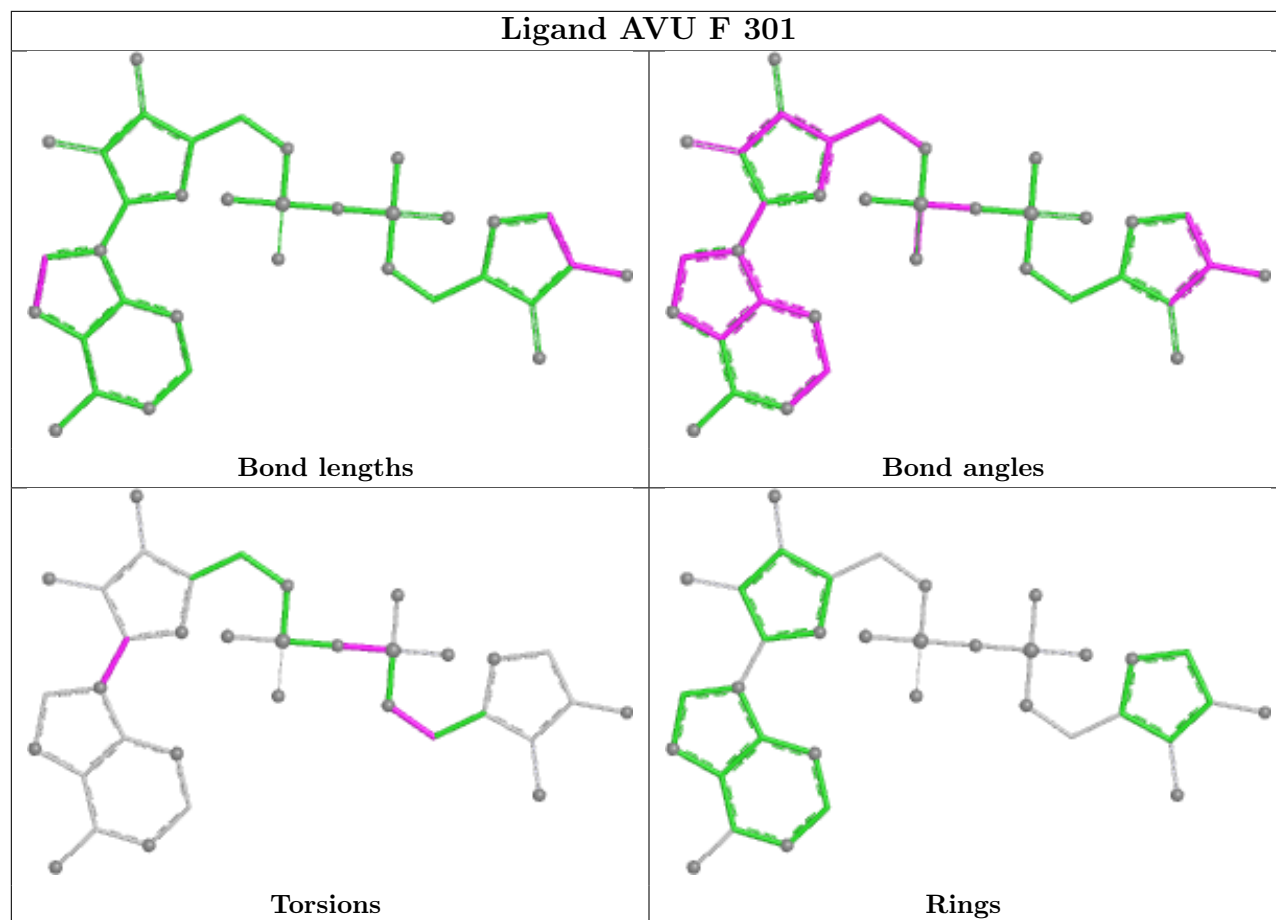


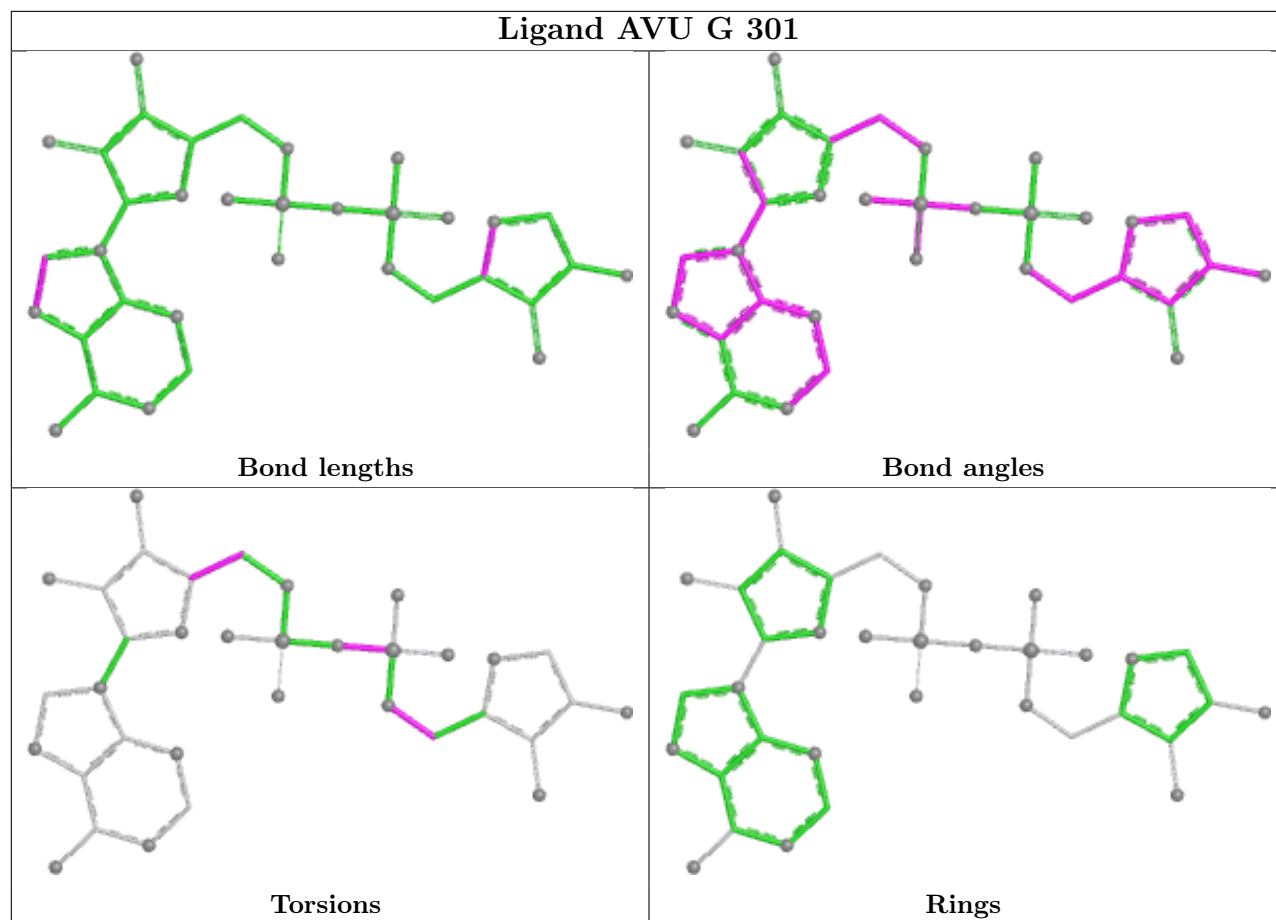












5.7 Other polymers [i](#)

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, 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	253/260 (97%)	0.32	7 (2%) 55 57	29, 47, 80, 95	0
1	B	252/260 (96%)	0.10	4 (1%) 70 72	27, 41, 61, 76	0
1	C	252/260 (96%)	0.35	13 (5%) 33 34	33, 51, 80, 96	0
1	D	252/260 (96%)	0.10	3 (1%) 76 77	27, 41, 59, 67	0
1	E	252/260 (96%)	0.18	7 (2%) 55 57	28, 42, 64, 73	0
1	F	252/260 (96%)	0.71	20 (7%) 18 20	42, 67, 98, 107	0
1	G	252/260 (96%)	0.17	5 (1%) 65 66	28, 44, 65, 75	0
1	H	252/260 (96%)	0.49	12 (4%) 35 37	36, 57, 82, 93	0
All	All	2017/2080 (96%)	0.30	71 (3%) 47 49	27, 48, 81, 107	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	174	PHE	4.9
1	H	174	PHE	4.4
1	F	51	CYS	4.0
1	D	174	PHE	3.7
1	E	51	CYS	3.6
1	H	128	PHE	3.6
1	F	15	CYS	3.5
1	F	34	CYS	3.4
1	A	128	PHE	3.4
1	G	128	PHE	3.3
1	A	131	CYS	3.2
1	C	140	TRP	3.2
1	F	127	ASP	3.1
1	G	174	PHE	3.1
1	E	49	ASN	3.1
1	F	218	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	25	ASP	3.0
1	C	174	PHE	2.9
1	F	187	VAL	2.9
1	F	220	ALA	2.7
1	A	174	PHE	2.7
1	C	51	CYS	2.7
1	B	250	LEU	2.7
1	B	174	PHE	2.6
1	D	86	ASP	2.6
1	H	135	ALA	2.6
1	H	55	LEU	2.6
1	F	179	GLU	2.5
1	C	127	ASP	2.5
1	G	251	ALA	2.5
1	H	34	CYS	2.5
1	E	251	ALA	2.5
1	H	52	ASP	2.4
1	F	142	MET	2.4
1	A	113	GLY	2.4
1	H	51	CYS	2.4
1	D	128	PHE	2.4
1	H	220	ALA	2.3
1	C	15	CYS	2.3
1	C	128	PHE	2.3
1	F	125	CYS	2.3
1	H	65	ALA	2.3
1	H	212	LEU	2.3
1	C	50	PRO	2.3
1	F	47	PHE	2.2
1	G	52	ASP	2.2
1	B	31	ARG	2.2
1	C	136	ARG	2.2
1	C	53	LEU	2.2
1	G	51	CYS	2.2
1	C	40	ASP	2.2
1	B	251	ALA	2.2
1	F	183	LEU	2.1
1	E	50	PRO	2.1
1	A	129	LYS	2.1
1	E	250	LEU	2.1
1	F	124	VAL	2.1
1	F	39	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	172	ASP	2.1
1	C	52	ASP	2.1
1	F	26	ILE	2.1
1	E	128	PHE	2.1
1	E	174	PHE	2.1
1	C	86	ASP	2.0
1	H	226	ASP	2.0
1	C	164	PRO	2.0
1	F	225	PHE	2.0
1	F	130	THR	2.0
1	F	188	THR	2.0
1	A	244	ASN	2.0
1	H	121	ASN	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 oligosaccharides 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.

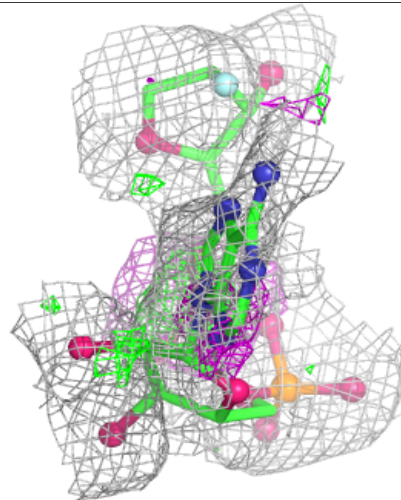
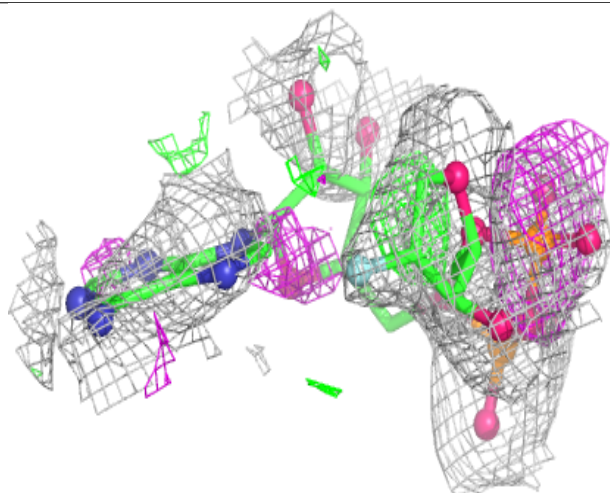
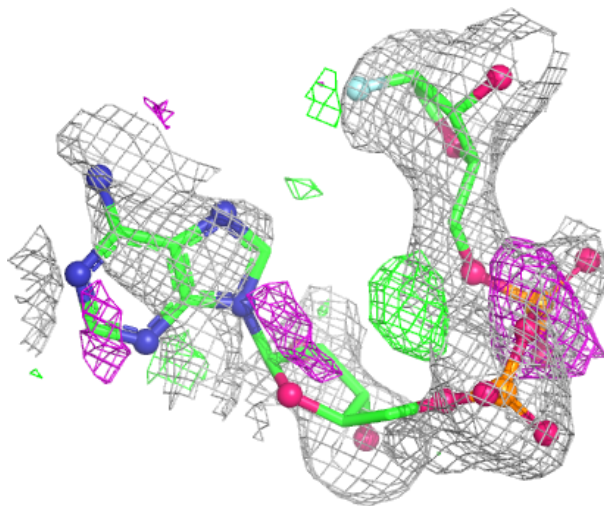
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AVU	B	301	35/35	0.84	0.17	34,63,102,103	0
2	AVU	A	301	35/35	0.87	0.12	50,74,83,85	0
2	AVU	D	301	35/35	0.87	0.14	38,66,101,101	0
2	AVU	C	301	35/35	0.88	0.13	54,77,95,96	0
2	AVU	G	301	35/35	0.88	0.16	39,64,102,102	0
2	AVU	E	301	35/35	0.90	0.13	36,66,109,110	0
2	AVU	F	301	35/35	0.93	0.10	58,70,85,87	0
2	AVU	H	301	35/35	0.93	0.10	55,64,77,79	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.

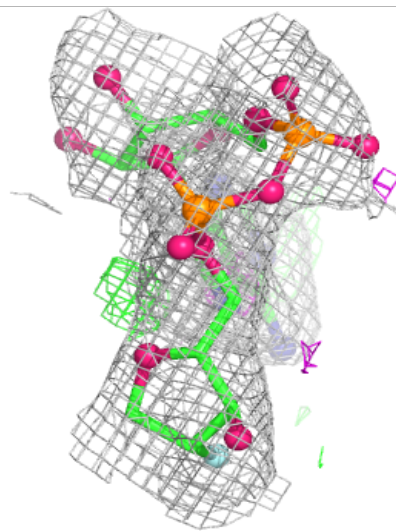
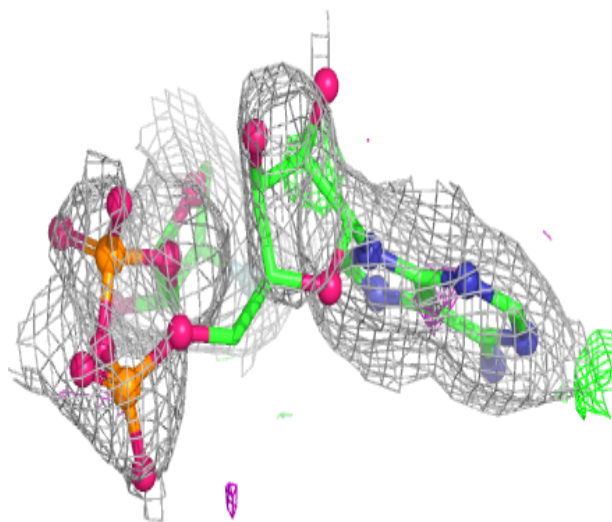
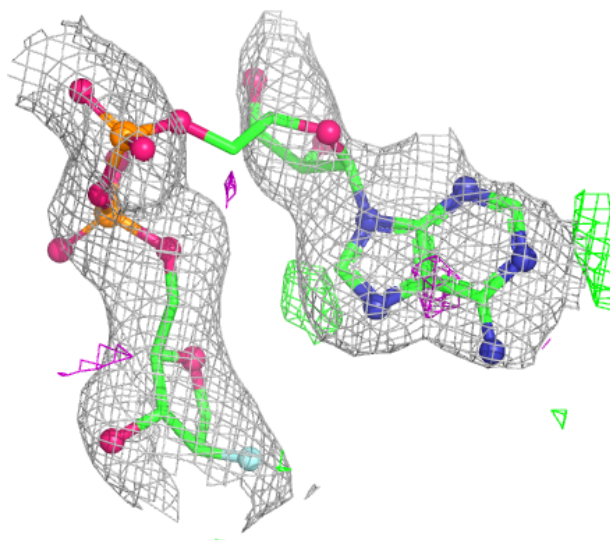
Electron density around AVU B 301:

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



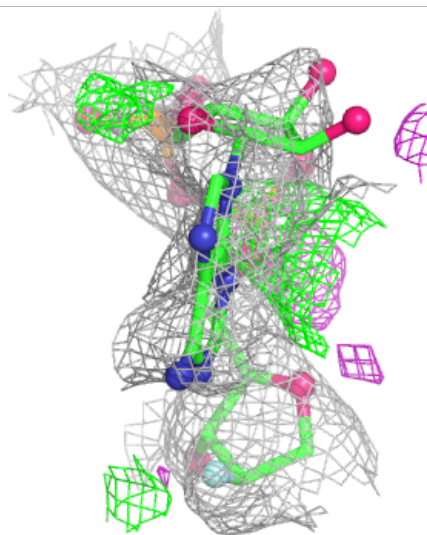
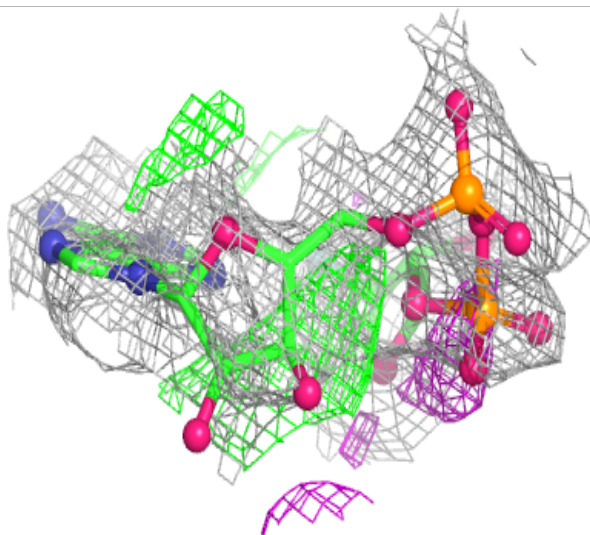
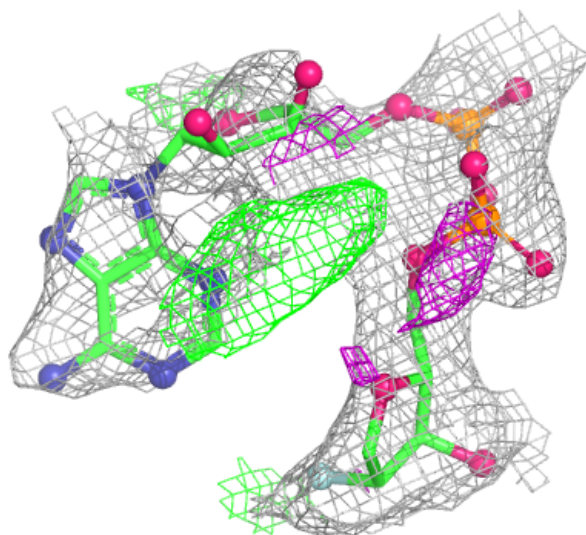
Electron density around AVU A 301:

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



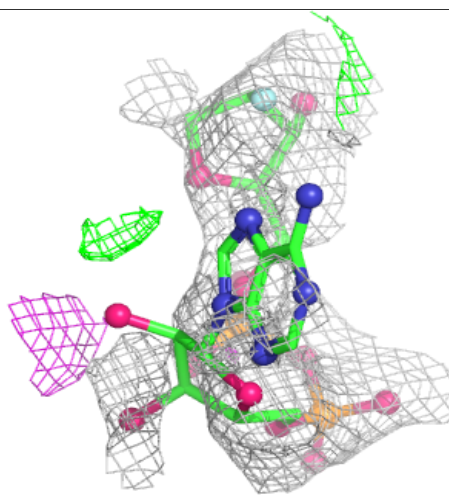
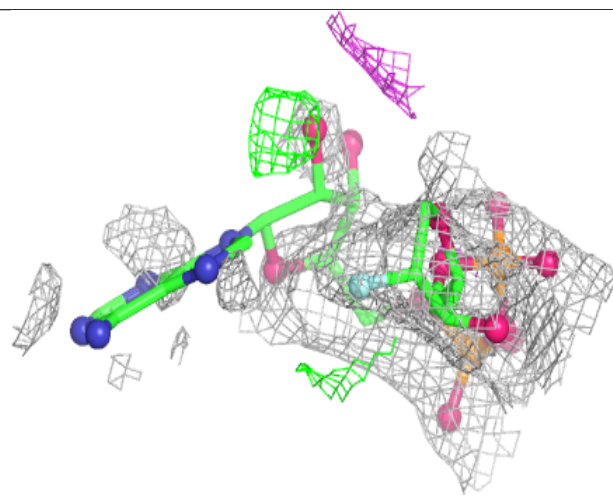
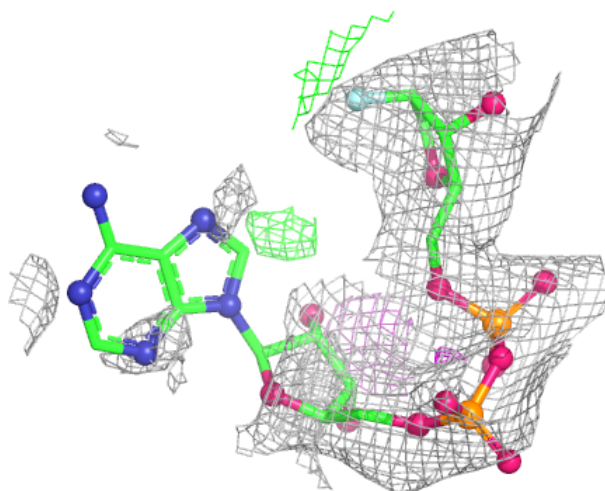
Electron density around AVU D 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



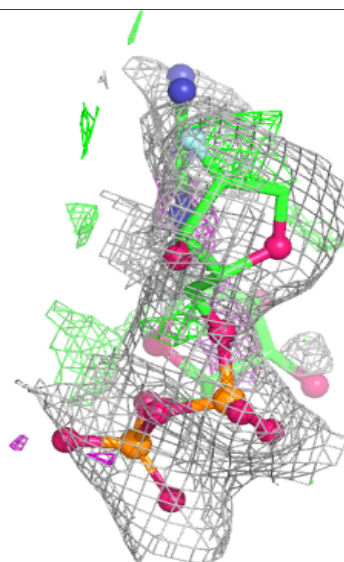
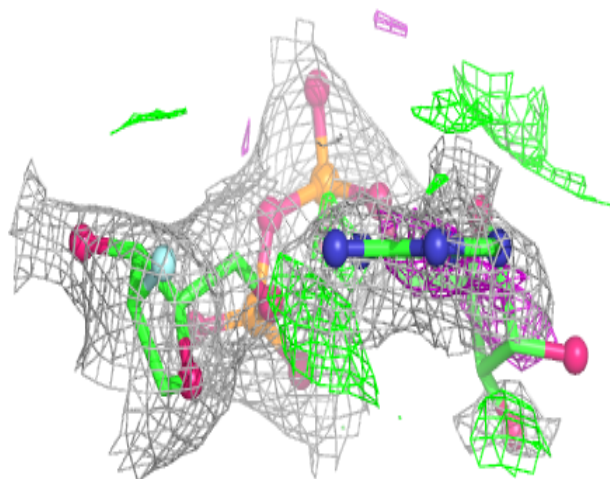
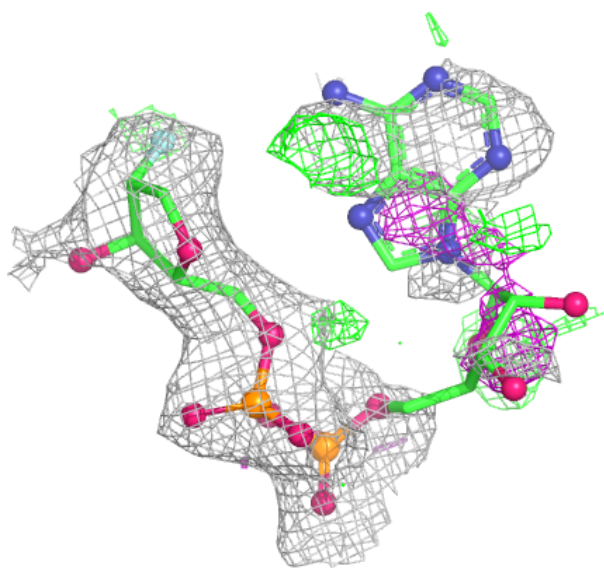
Electron density around AVU C 301:

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



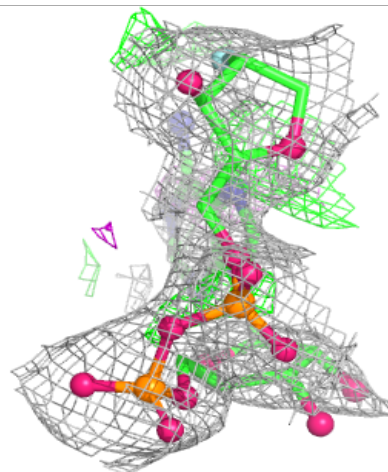
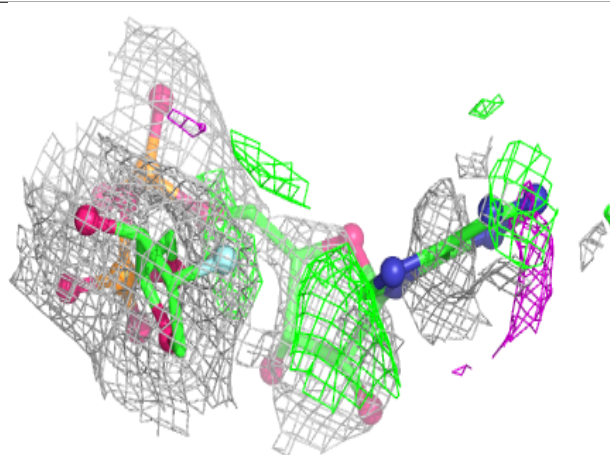
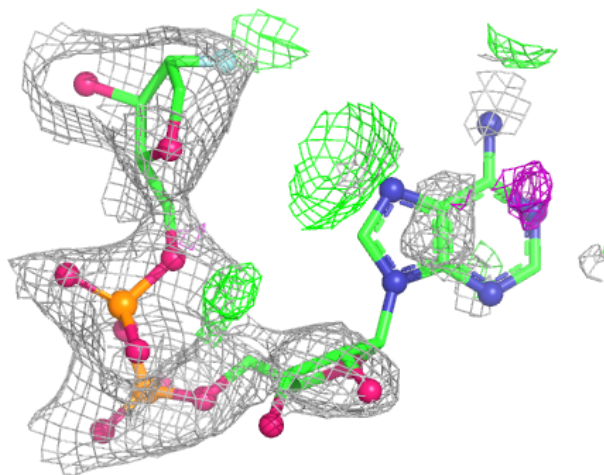
Electron density around AVU G 301:

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



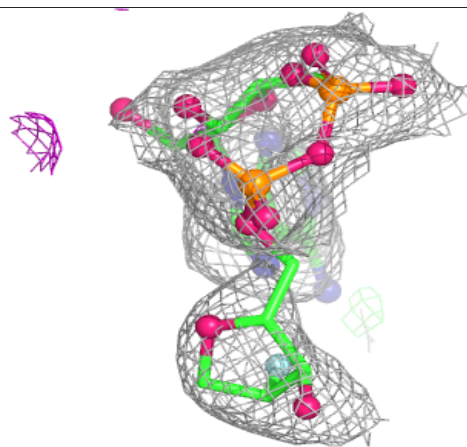
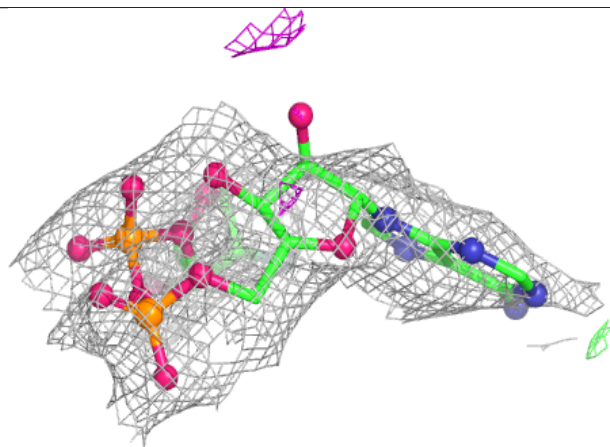
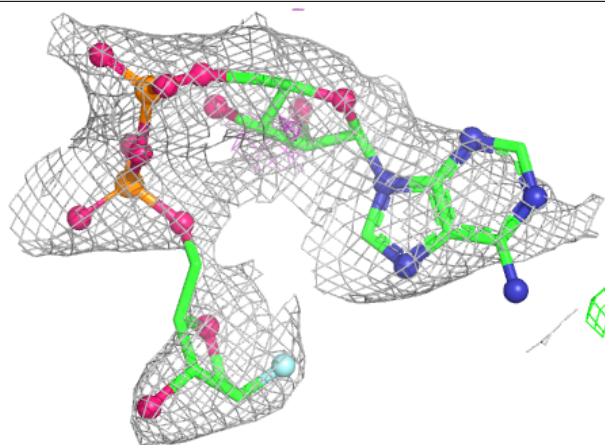
Electron density around AVU E 301:

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and green (positive)



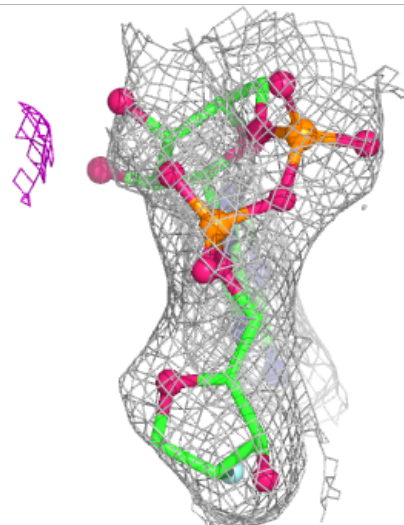
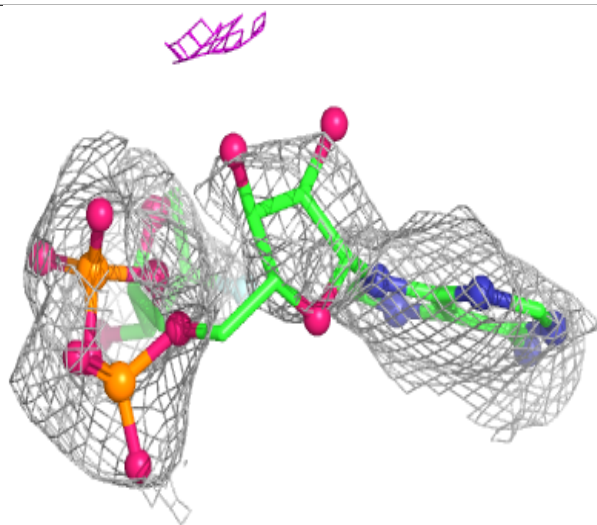
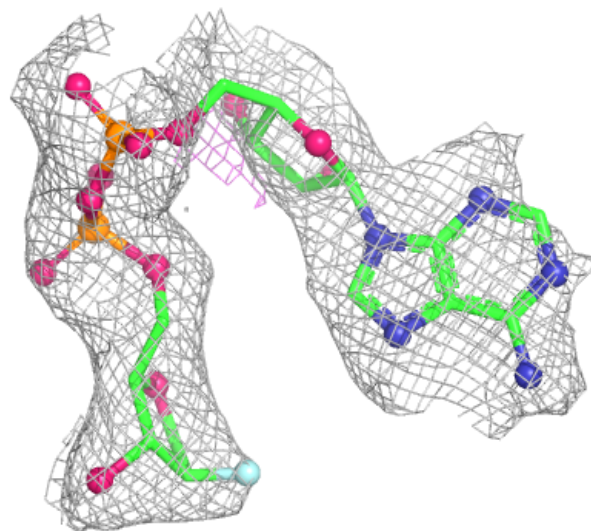
Electron density around AVU F 301:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.