



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:31 AM EDT

PDB ID : 5ZDC / pdb_00005zdc
Title : Crystal structure of poly(ADP-ribose) glycohydrolase (PARG) from *Deinococcus radiodurans* in complex with ADP-ribose (P32)
Authors : Cho, C.C.; Hsu, C.H.
Deposited on : 2018-02-23
Resolution : 1.98 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

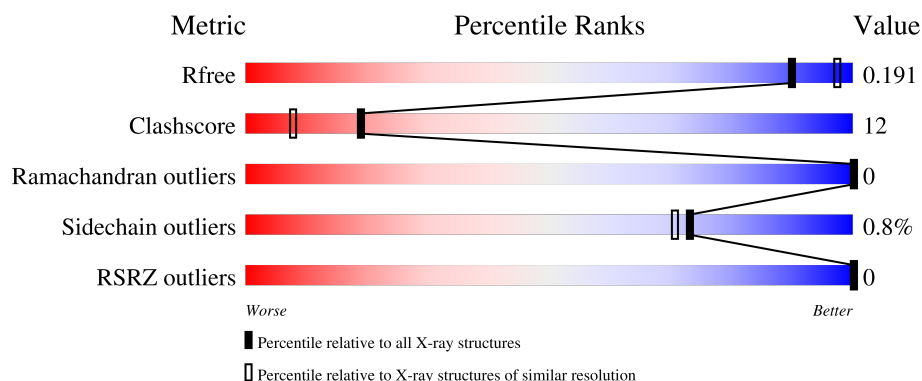
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	C	253	85% 15%
1	D	253	78% 20% .
1	F	253	80% 19%
1	H	253	79% 19% ..
1	J	253	75% 22% ..

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Mol	Chain	Length	Quality of chain
1	L	253	 80%17%..

2 Entry composition [i](#)

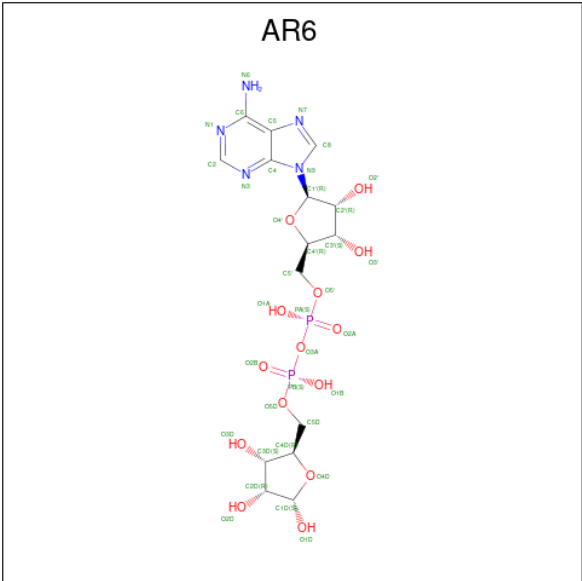
There are 4 unique types of molecules in this entry. The entry contains 12800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 poly ADP-ribose glycohydrolase.

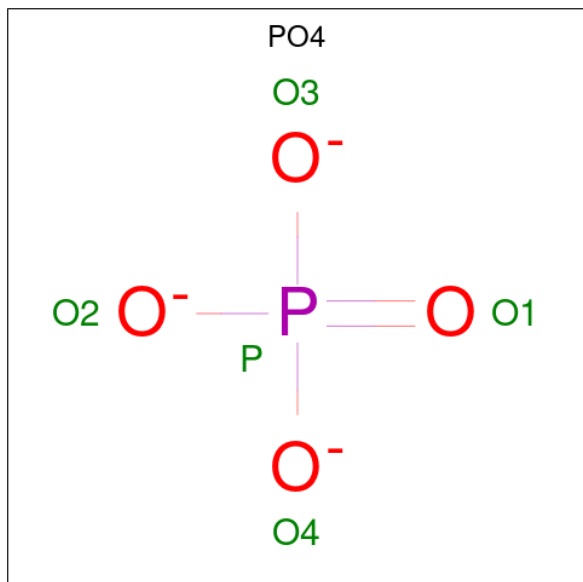
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	253	Total	C	N	O	S	0	0	0
			1944	1218	363	357	6			
1	F	252	Total	C	N	O	S	0	0	0
			1937	1213	362	356	6			
1	H	250	Total	C	N	O	S	0	0	0
			1928	1208	360	354	6			
1	J	250	Total	C	N	O	S	0	0	0
			1928	1208	360	354	6			
1	L	248	Total	C	N	O	S	0	0	0
			1916	1200	358	352	6			
1	D	249	Total	C	N	O	S	0	0	0
			1923	1205	359	353	6			

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLA N-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-Y L]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	F	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	H	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	J	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	L	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	161	Total	O	0	0
			161	161		

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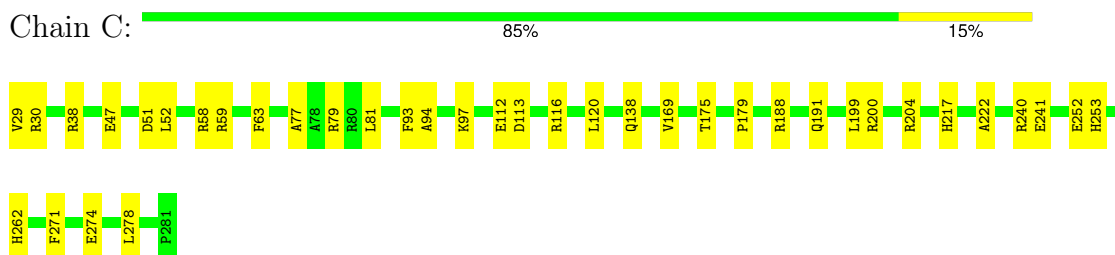
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	184	Total 184	O 184	0	0
4	H	142	Total 142	O 142	0	0
4	J	167	Total 167	O 167	0	0
4	L	197	Total 197	O 197	0	0
4	D	142	Total 142	O 142	0	0

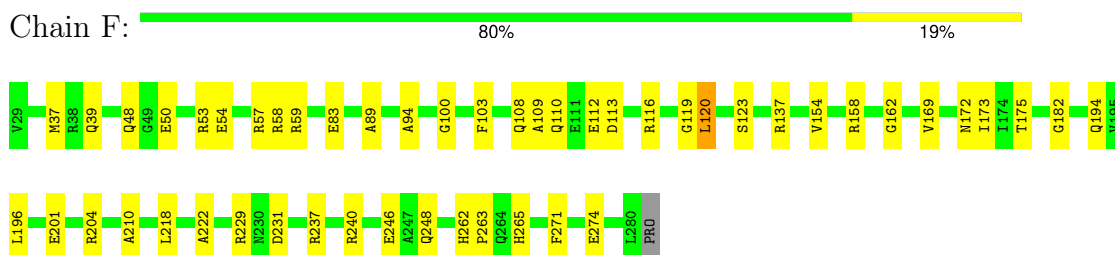
3 Residue-property plots

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.

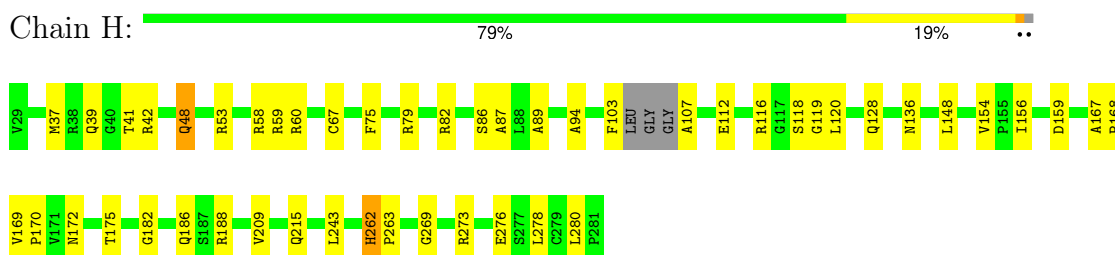
- Molecule 1: poly ADP-ribose glycohydrolase



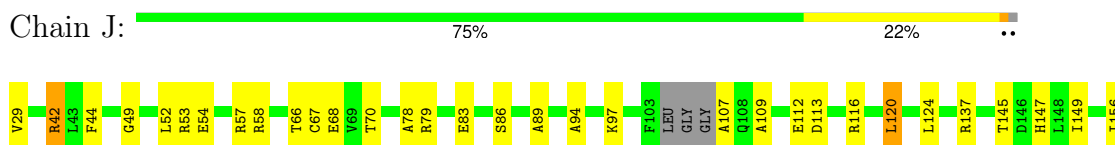
- Molecule 1: poly ADP-ribose glycohydrolase



- Molecule 1: poly ADP-ribose glycohydrolase



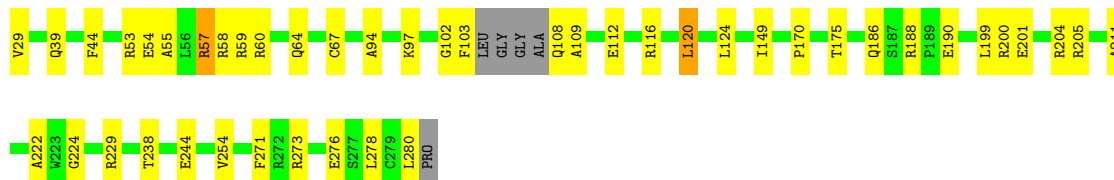
- Molecule 1: poly ADP-ribose glycohydrolase





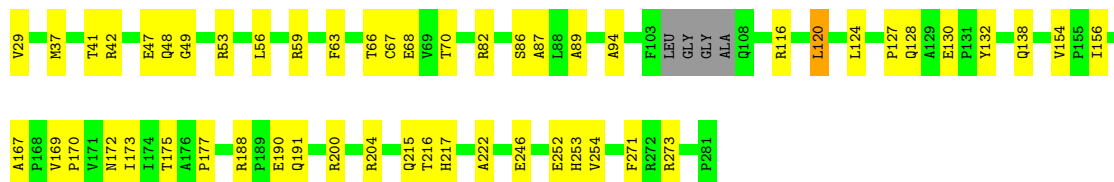
- Molecule 1: poly ADP-ribose glycohydrolase

Chain L: 80% 17% ..



- Molecule 1: poly ADP-ribose glycohydrolase

Chain D: 78% 20% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	108.50Å 108.50Å 130.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.03 – 1.98 28.03 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.4 (28.03-1.98) 1.4 (28.03-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.144 , 0.191 0.146 , 0.191	Depositor DCC
R_{free} test set	2030 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.7	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12800	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: AR6, PO4

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	C	0.34	0/1989	0.56	0/2705
1	D	0.34	0/1967	0.57	0/2674
1	F	0.38	0/1981	0.56	0/2693
1	H	0.36	0/1972	0.57	0/2681
1	J	0.35	0/1972	0.57	0/2681
1	L	0.46	2/1959 (0.1%)	0.59	0/2662
All	All	0.37	2/11840 (0.0%)	0.57	0/16096

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	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	57	ARG	CZ-NH1	9.55	1.46	1.32
1	L	57	ARG	NE-CZ	5.27	1.38	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	262	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1944	0	1917	33	0
1	D	1923	0	1894	47	0
1	F	1937	0	1910	51	0
1	H	1928	0	1899	41	0
1	J	1928	0	1899	58	0
1	L	1916	0	1887	48	0
2	C	36	0	19	1	0
2	D	36	0	19	1	0
2	F	36	0	19	3	0
2	H	36	0	19	1	0
2	J	36	0	19	4	0
2	L	36	0	19	2	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	C	161	0	0	12	0
4	D	142	0	0	12	0
4	F	184	0	0	20	0
4	H	142	0	0	10	0
4	J	167	0	0	18	0
4	L	197	0	0	22	0
All	All	12800	0	11520	276	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (276) 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)
2:D:301:AR6:O4'	2:D:301:AR6:C1'	1.64	1.29
1:H:59:ARG:NH1	1:D:86:SER:OG	1.75	1.19
2:L:301:AR6:O4'	2:L:301:AR6:C1'	1.64	1.18
2:J:301:AR6:O4'	2:J:301:AR6:C1'	1.65	1.18
2:H:301:AR6:O4'	2:H:301:AR6:C1'	1.65	1.17
2:F:301:AR6:O4'	2:F:301:AR6:C1'	1.65	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:GLU:HA	4:L:406:HOH:O	1.48	1.12
2:C:301:AR6:O4'	2:C:301:AR6:C1'	1.64	1.12
1:F:37:MET:SD	4:F:418:HOH:O	2.07	1.10
1:L:58:ARG:NH1	4:L:401:HOH:O	1.88	1.05
1:F:113:ASP:OD2	1:F:116:ARG:NH1	1.96	0.97
1:J:53:ARG:HH22	1:J:208:GLY:HA3	1.30	0.96
1:D:132:TYR:OH	1:D:177:PRO:HD3	1.66	0.96
1:F:53:ARG:HH11	1:F:57:ARG:HH22	0.99	0.94
1:C:30:ARG:NH2	4:C:402:HOH:O	1.99	0.92
1:J:182:GLY:O	4:J:501:HOH:O	1.86	0.91
1:H:136:ASN:ND2	4:H:401:HOH:O	2.02	0.91
1:F:58:ARG:NH1	4:F:404:HOH:O	2.05	0.90
1:L:200:ARG:NH1	4:L:404:HOH:O	2.06	0.89
1:L:276:GLU:HG3	1:L:280:LEU:HD23	1.52	0.89
1:L:108:GLN:N	4:L:405:HOH:O	2.07	0.86
1:J:201:GLU:OE2	1:J:204:ARG:NH2	2.09	0.86
1:H:39:GLN:OE1	1:D:48:GLN:NE2	2.09	0.85
1:F:39:GLN:OE1	4:F:401:HOH:O	1.95	0.85
1:D:82:ARG:NH2	1:D:86:SER:O	2.09	0.85
1:D:273:ARG:NH2	4:D:404:HOH:O	2.11	0.82
1:F:246:GLU:OE2	4:F:403:HOH:O	1.97	0.81
1:C:59:ARG:NH2	1:J:86:SER:OG	2.13	0.81
1:D:200:ARG:NH1	4:D:403:HOH:O	2.11	0.81
1:C:113:ASP:OD2	1:C:116:ARG:NH1	2.14	0.80
1:F:53:ARG:HH11	1:F:57:ARG:NH2	1.80	0.79
1:H:86:SER:OG	1:D:59:ARG:NH2	2.13	0.79
1:D:167:ALA:O	4:D:401:HOH:O	2.00	0.78
1:F:194:GLN:NE2	4:F:407:HOH:O	2.12	0.77
1:F:53:ARG:NH1	1:F:57:ARG:HH22	1.79	0.77
1:L:109:ALA:N	4:L:408:HOH:O	2.19	0.76
1:C:191:GLN:OE1	4:C:403:HOH:O	2.03	0.76
1:J:79:ARG:NH1	4:J:505:HOH:O	2.14	0.76
1:L:57:ARG:HD2	4:L:406:HOH:O	1.86	0.75
1:H:79:ARG:O	4:H:402:HOH:O	2.05	0.75
1:D:246:GLU:O	4:D:402:HOH:O	2.05	0.74
1:L:103:PHE:HD1	1:L:112:GLU:HG3	1.53	0.74
1:J:83:GLU:OE2	4:J:502:HOH:O	2.04	0.73
1:J:116:ARG:NH1	4:J:508:HOH:O	2.17	0.73
1:L:108:GLN:NE2	4:L:410:HOH:O	2.21	0.72
1:F:240:ARG:NH2	1:F:274:GLU:OE2	2.23	0.72
1:C:51:ASP:OD1	4:C:406:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:ARG:HG3	1:L:211:ALA:HB1	1.73	0.71
1:F:229:ARG:NH2	4:F:413:HOH:O	2.23	0.70
1:L:54:GLU:OE1	4:L:406:HOH:O	2.08	0.70
1:F:100:GLY:O	4:F:405:HOH:O	2.10	0.70
1:L:29:VAL:N	4:L:411:HOH:O	2.25	0.69
1:H:82:ARG:NH2	1:H:86:SER:O	2.24	0.69
1:J:53:ARG:NH2	1:J:208:GLY:HA3	2.07	0.69
1:L:199:LEU:HD23	1:L:238:THR:HG21	1.74	0.69
1:F:54:GLU:OE1	4:F:406:HOH:O	2.10	0.69
1:C:52:LEU:HB2	1:C:204:ARG:HH22	1.58	0.69
1:C:240:ARG:NH2	1:C:274:GLU:OE2	2.24	0.69
1:L:188:ARG:HA	1:L:188:ARG:HE	1.58	0.69
1:C:179:PRO:HD2	1:C:199:LEU:HD12	1.75	0.68
1:J:145:THR:OG1	4:J:503:HOH:O	2.11	0.68
4:F:401:HOH:O	1:L:44:PHE:HA	1.93	0.68
1:H:188:ARG:NH1	4:H:406:HOH:O	2.27	0.68
1:C:262:HIS:ND1	4:C:410:HOH:O	2.27	0.67
1:L:244:GLU:OE2	4:L:407:HOH:O	2.13	0.67
1:J:158:ARG:O	4:J:504:HOH:O	2.13	0.67
1:J:159:ASP:OD2	1:J:163:GLN:HB2	1.95	0.67
1:D:246:GLU:OE2	1:D:246:GLU:N	2.19	0.66
1:D:246:GLU:H	1:D:246:GLU:CD	2.01	0.65
1:D:191:GLN:OE1	4:D:406:HOH:O	2.14	0.65
1:F:237:ARG:NH1	4:F:411:HOH:O	2.21	0.65
1:L:186:GLN:NE2	1:L:229:ARG:NH1	2.47	0.63
1:D:200:ARG:NH1	4:D:410:HOH:O	2.31	0.63
1:F:48:GLN:NE2	1:L:39:GLN:OE1	2.31	0.63
1:F:39:GLN:NE2	4:F:414:HOH:O	2.26	0.62
1:J:29:VAL:O	4:J:507:HOH:O	2.16	0.61
1:L:103:PHE:N	4:L:414:HOH:O	2.34	0.61
1:D:29:VAL:N	4:D:412:HOH:O	2.33	0.61
1:C:188:ARG:NH1	4:C:401:HOH:O	1.84	0.61
1:D:49:GLY:O	1:D:53:ARG:HG2	1.99	0.61
1:D:204:ARG:NH2	4:D:413:HOH:O	2.33	0.61
1:J:185:ALA:HB3	4:J:501:HOH:O	2.01	0.60
1:D:63:PHE:CD2	1:D:252:GLU:HG2	2.37	0.60
1:H:67:CYS:HB3	1:H:278:LEU:HG	1.84	0.60
1:F:37:MET:HE1	1:F:119:GLY:O	2.02	0.59
1:H:167:ALA:O	4:H:405:HOH:O	2.16	0.58
1:D:47:GLU:OE1	4:D:407:HOH:O	2.17	0.58
1:J:188:ARG:NE	4:J:513:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:ARG:HD3	4:J:543:HOH:O	2.03	0.58
1:L:103:PHE:CD1	1:L:112:GLU:HG3	2.38	0.58
1:H:276:GLU:O	1:H:280:LEU:HG	2.04	0.58
1:F:204:ARG:HD2	1:F:246:GLU:OE2	2.04	0.58
1:J:53:ARG:NH2	1:J:205:ARG:HA	2.18	0.57
1:L:116:ARG:NH1	4:L:419:HOH:O	2.37	0.57
1:F:158:ARG:NH2	1:F:162:GLY:O	2.37	0.57
1:L:53:ARG:HG2	1:L:204:ARG:NH1	2.20	0.57
1:D:216:THR:HB	1:D:252:GLU:HG3	1.86	0.56
1:H:82:ARG:NH1	1:H:170:PRO:O	2.35	0.56
1:C:58:ARG:NH1	4:C:404:HOH:O	2.05	0.56
1:H:58:ARG:HD3	4:D:438:HOH:O	2.05	0.55
1:J:42:ARG:NE	4:J:517:HOH:O	2.39	0.55
1:H:182:GLY:O	1:H:186:GLN:HG3	2.06	0.55
1:L:170:PRO:HB3	4:L:562:HOH:O	2.06	0.55
1:H:58:ARG:NH2	4:H:414:HOH:O	2.40	0.55
1:C:97:LYS:NZ	4:C:405:HOH:O	2.07	0.55
1:H:60:ARG:NH2	4:H:403:HOH:O	2.39	0.55
1:F:120:LEU:HG	1:F:173:ILE:HD12	1.88	0.54
1:H:156:ILE:HB	1:H:169:VAL:HG22	1.90	0.54
1:J:53:ARG:HH21	1:J:205:ARG:HA	1.71	0.54
1:C:63:PHE:CD1	1:C:252:GLU:HG3	2.43	0.54
1:F:53:ARG:NH1	1:F:57:ARG:HH12	2.05	0.54
1:D:132:TYR:CZ	1:D:177:PRO:HD3	2.41	0.54
1:H:59:ARG:HH11	1:D:86:SER:HG	1.52	0.53
1:J:149:ILE:HB	1:J:175:THR:HB	1.89	0.53
1:J:53:ARG:HH22	1:J:208:GLY:CA	2.13	0.53
1:J:156:ILE:HD12	1:J:169:VAL:HG22	1.90	0.53
2:F:301:AR6:O2'	4:F:408:HOH:O	2.18	0.53
1:J:54:GLU:HG3	1:J:58:ARG:HH11	1.74	0.53
1:F:182:GLY:HA3	1:F:229:ARG:HD2	1.91	0.53
1:C:38:ARG:HD3	4:C:534:HOH:O	2.09	0.53
1:F:201:GLU:OE2	1:F:204:ARG:NH2	2.39	0.53
1:C:58:ARG:HD3	4:C:404:HOH:O	2.09	0.53
1:L:64:GLN:OE1	4:L:409:HOH:O	2.19	0.52
1:J:57:ARG:HD2	4:J:539:HOH:O	2.09	0.52
1:H:37:MET:HE1	1:H:119:GLY:O	2.09	0.52
1:F:94:ALA:HB2	1:F:175:THR:HG23	1.91	0.52
1:D:94:ALA:HB2	1:D:175:THR:HG23	1.92	0.51
1:L:55:ALA:O	1:L:59:ARG:HG2	2.10	0.51
1:F:113:ASP:OD1	4:F:409:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:TYR:OH	1:D:177:PRO:CD	2.51	0.51
1:F:53:ARG:HG3	4:F:403:HOH:O	2.10	0.51
1:J:66:THR:O	1:J:253:HIS:HA	2.10	0.51
1:C:59:ARG:NH2	1:J:86:SER:HG	2.05	0.51
1:J:42:ARG:HD3	1:J:42:ARG:C	2.36	0.51
1:C:58:ARG:NH2	4:C:411:HOH:O	2.33	0.51
1:H:53:ARG:HG3	4:H:474:HOH:O	2.11	0.51
1:C:63:PHE:CE1	1:C:252:GLU:HG3	2.46	0.51
1:F:37:MET:HE1	1:F:119:GLY:C	2.36	0.50
1:F:240:ARG:NE	1:F:274:GLU:OE2	2.43	0.50
1:D:138:GLN:O	1:D:138:GLN:HG2	2.11	0.50
1:J:42:ARG:HD2	1:J:44:PHE:CE2	2.46	0.50
1:J:89:ALA:HA	1:J:172:ASN:O	2.12	0.50
1:F:231:ASP:OD1	4:F:410:HOH:O	2.20	0.50
1:J:268:LEU:HD21	1:J:272:ARG:NH1	2.26	0.50
1:D:53:ARG:NH2	1:D:204:ARG:O	2.45	0.50
1:C:200:ARG:NH1	1:C:241:GLU:OE2	2.40	0.50
1:F:37:MET:SD	1:F:123:SER:HB2	2.52	0.50
1:F:37:MET:HE2	1:F:154:VAL:HG13	1.93	0.50
1:F:240:ARG:CZ	1:F:274:GLU:OE2	2.59	0.50
1:F:50:GLU:CD	1:F:50:GLU:H	2.20	0.50
1:C:217:HIS:CD2	1:C:253:HIS:HB3	2.47	0.49
1:H:262:HIS:HB3	1:H:263:PRO:HD2	1.93	0.49
1:L:200:ARG:HD2	1:L:200:ARG:O	2.12	0.49
1:C:79:ARG:HG2	1:C:169:VAL:HG21	1.94	0.49
1:F:108:GLN:N	4:F:402:HOH:O	2.46	0.49
1:C:138:GLN:OE1	4:C:407:HOH:O	2.20	0.49
1:J:109:ALA:HB1	2:J:301:AR6:H1D	1.94	0.49
1:D:156:ILE:HB	1:D:169:VAL:HG22	1.94	0.49
1:D:222:ALA:HA	1:D:271:PHE:CZ	2.47	0.49
1:D:252:GLU:OE1	4:D:408:HOH:O	2.20	0.49
1:F:196:LEU:HD11	4:F:507:HOH:O	2.11	0.49
1:H:75:PHE:CE2	1:H:118:SER:HB3	2.48	0.49
1:J:97:LYS:HG2	1:J:137:ARG:HG3	1.95	0.49
1:D:67:CYS:HB2	1:D:254:VAL:HB	1.95	0.49
1:D:217:HIS:CD2	1:D:253:HIS:HB3	2.48	0.49
1:L:186:GLN:NE2	1:L:229:ARG:HH12	2.11	0.49
1:J:67:CYS:SG	1:J:278:LEU:HB3	2.53	0.48
1:L:60:ARG:NH2	4:L:427:HOH:O	2.45	0.48
1:J:54:GLU:HG3	1:J:58:ARG:NH1	2.27	0.48
1:J:268:LEU:O	1:J:272:ARG:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:HH21	1:D:48:GLN:NE2	2.12	0.48
1:J:52:LEU:HB3	1:J:53:ARG:NH2	2.28	0.48
1:D:154:VAL:HG21	1:D:173:ILE:HD12	1.96	0.48
1:F:109:ALA:N	4:F:402:HOH:O	1.96	0.48
1:F:50:GLU:CD	1:F:50:GLU:N	2.72	0.48
1:L:103:PHE:C	4:L:414:HOH:O	2.57	0.48
1:L:120:LEU:HD22	1:L:124:LEU:HG	1.95	0.48
1:F:89:ALA:HA	1:F:172:ASN:O	2.13	0.47
1:H:42:ARG:HH21	1:H:48:GLN:NE2	2.12	0.47
1:L:199:LEU:CD2	1:L:238:THR:HG21	2.44	0.47
1:L:273:ARG:NH2	4:L:428:HOH:O	2.46	0.47
1:C:112:GLU:O	1:C:116:ARG:HG3	2.13	0.47
1:J:42:ARG:NH1	4:J:512:HOH:O	2.31	0.47
1:D:41:THR:O	1:D:128:GLN:HG3	2.13	0.47
1:C:240:ARG:HG2	1:C:278:LEU:HD12	1.96	0.47
1:J:67:CYS:HA	1:J:254:VAL:O	2.14	0.47
1:D:188:ARG:HG3	1:D:190:GLU:OE2	2.14	0.47
1:H:86:SER:CB	1:D:59:ARG:HH21	2.24	0.47
1:J:186:GLN:HG3	4:J:501:HOH:O	2.14	0.47
1:F:109:ALA:HB1	2:F:301:AR6:H1D	1.96	0.47
1:F:262:HIS:O	1:F:265:HIS:ND1	2.48	0.47
1:J:210:ALA:HB1	1:J:218:LEU:HD21	1.97	0.47
1:D:87:ALA:HB1	1:D:215:GLN:HA	1.97	0.47
1:H:269:GLY:O	1:H:273:ARG:HB2	2.15	0.46
1:L:188:ARG:HD3	1:L:190:GLU:OE2	2.15	0.46
1:C:47:GLU:CD	1:C:47:GLU:H	2.24	0.46
1:C:94:ALA:HB2	1:C:175:THR:HG23	1.98	0.46
1:L:222:ALA:HA	1:L:271:PHE:CZ	2.51	0.46
1:J:94:ALA:HB2	1:J:175:THR:HG23	1.98	0.46
1:J:186:GLN:N	4:J:501:HOH:O	2.49	0.46
1:J:187:SER:O	1:J:188:ARG:HD3	2.15	0.46
1:H:156:ILE:O	1:H:168:PRO:HA	2.15	0.45
1:J:78:ALA:HB1	1:J:171:VAL:HG11	1.98	0.45
1:L:149:ILE:HB	1:L:175:THR:HB	1.97	0.45
1:J:49:GLY:O	1:J:53:ARG:HG2	2.16	0.45
1:H:103:PHE:HD1	1:H:112:GLU:HG3	1.82	0.45
1:H:87:ALA:HB1	1:H:215:GLN:HA	1.99	0.45
1:H:107:ALA:N	4:H:419:HOH:O	2.50	0.45
1:L:97:LYS:HB2	1:L:97:LYS:HE3	1.55	0.45
1:H:89:ALA:HA	1:H:172:ASN:O	2.16	0.45
1:H:112:GLU:O	1:H:116:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:ARG:HD3	4:F:440:HOH:O	2.16	0.45
1:J:147:HIS:HB2	4:J:503:HOH:O	2.17	0.45
1:F:103:PHE:HD1	1:F:112:GLU:HG3	1.81	0.45
1:F:222:ALA:HA	1:F:271:PHE:CZ	2.52	0.45
1:J:42:ARG:HG2	4:J:512:HOH:O	2.17	0.45
1:H:94:ALA:HB2	1:H:175:THR:HG23	1.99	0.44
1:H:154:VAL:O	1:H:170:PRO:HA	2.17	0.44
1:F:274:GLU:OE2	1:F:274:GLU:O	2.35	0.44
1:J:120:LEU:HD22	1:J:124:LEU:HG	2.00	0.44
1:C:188:ARG:HA	1:C:188:ARG:NE	2.33	0.44
1:H:148:LEU:HD22	1:H:209:VAL:HG21	2.00	0.44
1:L:201:GLU:OE2	1:L:205:ARG:NE	2.48	0.44
1:D:89:ALA:HA	1:D:172:ASN:O	2.17	0.44
1:J:268:LEU:HD21	1:J:272:ARG:HH12	1.83	0.44
1:D:63:PHE:CE2	1:D:252:GLU:HG2	2.52	0.44
1:D:66:THR:O	1:D:253:HIS:HA	2.18	0.44
1:L:67:CYS:SG	1:L:278:LEU:HB3	2.58	0.44
1:L:200:ARG:NE	4:L:426:HOH:O	2.45	0.43
1:J:107:ALA:HA	1:J:112:GLU:OE1	2.18	0.43
1:J:226:GLY:HA3	2:J:301:AR6:O1A	2.18	0.43
1:H:53:ARG:HD2	1:H:53:ARG:HA	1.70	0.43
1:C:77:ALA:O	1:C:81:LEU:HG	2.19	0.43
1:L:94:ALA:HB2	1:L:175:THR:HG23	2.00	0.43
1:L:200:ARG:HH11	1:L:200:ARG:HG3	1.84	0.43
1:C:94:ALA:CB	1:C:175:THR:HG23	2.49	0.42
1:C:29:VAL:N	4:C:426:HOH:O	2.52	0.42
1:H:87:ALA:CB	1:H:215:GLN:HA	2.48	0.42
1:L:102:GLY:C	4:L:414:HOH:O	2.60	0.42
1:C:116:ARG:HD2	4:H:434:HOH:O	2.19	0.42
1:J:244:GLU:HB2	4:J:526:HOH:O	2.20	0.42
1:J:53:ARG:HA	1:J:53:ARG:NH1	2.34	0.42
1:J:244:GLU:HG3	1:J:278:LEU:HD11	2.02	0.42
1:J:94:ALA:CB	1:J:175:THR:HG23	2.50	0.42
1:F:248:GLN:HA	4:F:447:HOH:O	2.19	0.42
1:L:67:CYS:HA	1:L:254:VAL:O	2.20	0.42
1:D:37:MET:HE2	1:D:37:MET:HB3	1.98	0.42
1:C:222:ALA:HA	1:C:271:PHE:CZ	2.55	0.41
1:L:57:ARG:HG3	4:L:474:HOH:O	2.19	0.41
1:D:120:LEU:HD22	1:D:124:LEU:HG	2.02	0.41
1:H:58:ARG:CZ	1:D:170:PRO:HG2	2.50	0.41
1:L:53:ARG:NH2	4:L:404:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:ARG:HD3	4:L:452:HOH:O	2.19	0.41
1:J:68:GLU:HG3	1:J:70:THR:HG23	2.02	0.41
1:L:224:GLY:HA2	2:L:301:AR6:O2B	2.19	0.41
1:D:116:ARG:NH2	4:D:433:HOH:O	2.50	0.41
1:D:68:GLU:HG3	1:D:70:THR:HG23	2.03	0.41
1:F:103:PHE:CD1	1:F:112:GLU:HG3	2.55	0.41
1:H:243:LEU:HD23	1:H:243:LEU:HA	1.85	0.41
1:J:226:GLY:N	2:J:301:AR6:H5'	2.35	0.41
1:D:94:ALA:CB	1:D:175:THR:HG23	2.50	0.41
1:C:93:PHE:N	1:C:93:PHE:CD2	2.88	0.41
1:L:94:ALA:CB	1:L:175:THR:HG23	2.50	0.41
1:F:110:GLN:O	1:F:113:ASP:HB2	2.20	0.41
1:H:41:THR:O	1:H:128:GLN:HG3	2.21	0.41
1:D:127:PRO:HA	1:D:130:GLU:HG3	2.02	0.41
1:F:262:HIS:HA	1:F:263:PRO:HD3	1.89	0.41
1:F:137:ARG:HH11	1:F:137:ARG:HD2	1.77	0.40
1:H:159:ASP:OD2	1:H:159:ASP:C	2.64	0.40
1:H:167:ALA:N	4:H:405:HOH:O	2.44	0.40
1:H:94:ALA:CB	1:H:175:THR:HG23	2.52	0.40
1:F:83:GLU:H	1:F:83:GLU:HG3	1.41	0.40
1:J:217:HIS:CD2	1:J:253:HIS:HB3	2.57	0.40
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.92	0.40
1:F:210:ALA:HB1	1:F:218:LEU:HD21	2.04	0.40
1:J:113:ASP:HA	1:J:116:ARG:NH1	2.37	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	C	251/253 (99%)	244 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	245/253 (97%)	238 (97%)	7 (3%)	0	100	100
1	F	250/253 (99%)	242 (97%)	8 (3%)	0	100	100
1	H	246/253 (97%)	237 (96%)	9 (4%)	0	100	100
1	J	246/253 (97%)	237 (96%)	9 (4%)	0	100	100
1	L	244/253 (96%)	238 (98%)	6 (2%)	0	100	100
All	All	1482/1518 (98%)	1436 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	198/198 (100%)	197 (100%)	1 (0%)	81	79
1	D	197/198 (100%)	196 (100%)	1 (0%)	81	79
1	F	197/198 (100%)	195 (99%)	2 (1%)	68	65
1	H	197/198 (100%)	195 (99%)	2 (1%)	68	65
1	J	197/198 (100%)	194 (98%)	3 (2%)	57	52
1	L	196/198 (99%)	195 (100%)	1 (0%)	81	79
All	All	1182/1188 (100%)	1172 (99%)	10 (1%)	73	71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	120	LEU
1	F	120	LEU
1	F	169	VAL
1	H	48	GLN
1	H	120	LEU
1	J	42	ARG
1	J	120	LEU
1	J	169	VAL

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Mol	Chain	Res	Type
1	L	120	LEU
1	D	120	LEU

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

Mol	Chain	Res	Type
1	C	138	GLN
1	C	186	GLN
1	F	153	GLN
1	H	153	GLN
1	H	191	GLN
1	H	230	ASN
1	J	153	GLN
1	J	163	GLN
1	J	191	GLN
1	J	248	GLN
1	L	186	GLN
1	D	153	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	AR6	H	301	-	39,39,39	3.80	16 (41%)	56,60,60	1.91	14 (25%)
2	AR6	D	301	-	39,39,39	3.89	16 (41%)	56,60,60	1.89	12 (21%)
2	AR6	L	301	-	39,39,39	3.76	16 (41%)	56,60,60	2.00	12 (21%)
3	PO4	C	302	-	4,4,4	1.06	0	6,6,6	0.62	0
2	AR6	C	301	-	39,39,39	3.75	15 (38%)	56,60,60	2.04	15 (26%)
2	AR6	F	301	-	39,39,39	3.84	17 (43%)	56,60,60	1.87	13 (23%)
3	PO4	F	302	-	4,4,4	1.07	0	6,6,6	0.64	0
2	AR6	J	301	-	39,39,39	3.85	17 (43%)	56,60,60	1.98	14 (25%)
3	PO4	D	302	-	4,4,4	1.11	0	6,6,6	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AR6	H	301	-	-	4/22/54/54	0/4/4/4
2	AR6	D	301	-	-	9/22/54/54	0/4/4/4
2	AR6	L	301	-	-	4/22/54/54	0/4/4/4
2	AR6	C	301	-	-	4/22/54/54	0/4/4/4
2	AR6	F	301	-	-	5/22/54/54	0/4/4/4
2	AR6	J	301	-	-	3/22/54/54	0/4/4/4

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	AR6	O4D-C1D	12.71	1.58	1.43
2	J	301	AR6	O4D-C1D	12.56	1.58	1.43
2	D	301	AR6	O4D-C1D	12.00	1.57	1.43
2	H	301	AR6	O4D-C1D	11.68	1.57	1.43
2	C	301	AR6	O4D-C1D	11.42	1.57	1.43
2	L	301	AR6	O4D-C1D	11.29	1.56	1.43
2	J	301	AR6	O4'-C1'	10.02	1.65	1.42
2	H	301	AR6	O4'-C1'	9.95	1.65	1.42
2	F	301	AR6	O4'-C1'	9.95	1.65	1.42
2	C	301	AR6	O4'-C1'	9.84	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	AR6	O4'-C1'	9.81	1.64	1.42
2	L	301	AR6	O4'-C1'	9.57	1.64	1.42
2	D	301	AR6	C3D-C2D	-7.47	1.33	1.53
2	L	301	AR6	C3D-C2D	-7.30	1.33	1.53
2	F	301	AR6	C3D-C2D	-7.18	1.33	1.53
2	C	301	AR6	C3D-C2D	-7.03	1.34	1.53
2	H	301	AR6	C3D-C2D	-7.02	1.34	1.53
2	J	301	AR6	C3D-C2D	-6.77	1.35	1.53
2	H	301	AR6	O4D-C4D	-6.72	1.30	1.45
2	D	301	AR6	O4D-C4D	-6.60	1.30	1.45
2	J	301	AR6	O4D-C4D	-6.53	1.30	1.45
2	F	301	AR6	O4D-C4D	-6.39	1.30	1.45
2	C	301	AR6	O4'-C4'	-6.34	1.30	1.45
2	C	301	AR6	O4D-C4D	-6.30	1.31	1.45
2	F	301	AR6	O4'-C4'	-6.17	1.31	1.45
2	L	301	AR6	O4D-C4D	-6.14	1.31	1.45
2	J	301	AR6	O4'-C4'	-6.13	1.31	1.45
2	D	301	AR6	O4'-C4'	-6.11	1.31	1.45
2	D	301	AR6	C2'-C1'	-6.07	1.34	1.53
2	L	301	AR6	PB-O3A	6.04	1.66	1.59
2	L	301	AR6	O4'-C4'	-6.00	1.31	1.45
2	H	301	AR6	O4'-C4'	-5.85	1.32	1.45
2	C	301	AR6	C2'-C1'	-5.83	1.35	1.53
2	F	301	AR6	C2'-C1'	-5.80	1.35	1.53
2	J	301	AR6	C2'-C1'	-5.79	1.35	1.53
2	H	301	AR6	C2'-C1'	-5.73	1.35	1.53
2	L	301	AR6	C2'-C1'	-5.59	1.35	1.53
2	D	301	AR6	PA-O3A	5.49	1.65	1.59
2	L	301	AR6	PA-O3A	5.39	1.65	1.59
2	D	301	AR6	C6-N6	5.23	1.47	1.34
2	D	301	AR6	PB-O3A	5.01	1.64	1.59
2	H	301	AR6	PA-O3A	4.95	1.64	1.59
2	C	301	AR6	PA-O3A	4.89	1.64	1.59
2	C	301	AR6	C6-N6	4.86	1.46	1.34
2	H	301	AR6	C6-N6	4.80	1.46	1.34
2	F	301	AR6	C6-N6	4.57	1.45	1.34
2	L	301	AR6	C6-N6	4.57	1.45	1.34
2	J	301	AR6	PA-O3A	4.54	1.64	1.59
2	H	301	AR6	PB-O3A	4.52	1.64	1.59
2	J	301	AR6	C6-N6	4.33	1.45	1.34
2	H	301	AR6	O1D-C1D	-4.17	1.26	1.39
2	C	301	AR6	PB-O3A	4.17	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	AR6	PA-O3A	4.11	1.63	1.59
2	L	301	AR6	C3D-C4D	3.98	1.63	1.53
2	F	301	AR6	C3D-C4D	3.98	1.63	1.53
2	C	301	AR6	O1D-C1D	-3.96	1.27	1.39
2	L	301	AR6	O1D-C1D	-3.95	1.27	1.39
2	J	301	AR6	C5-N7	-3.88	1.32	1.39
2	D	301	AR6	O3'-C3'	-3.88	1.33	1.43
2	D	301	AR6	O1D-C1D	-3.86	1.27	1.39
2	C	301	AR6	O3'-C3'	-3.85	1.33	1.43
2	J	301	AR6	O1D-C1D	-3.76	1.27	1.39
2	J	301	AR6	O3'-C3'	-3.75	1.33	1.43
2	F	301	AR6	O1D-C1D	-3.73	1.27	1.39
2	D	301	AR6	C3D-C4D	3.73	1.62	1.53
2	J	301	AR6	C3D-C4D	3.65	1.62	1.53
2	L	301	AR6	O3'-C3'	-3.59	1.34	1.43
2	H	301	AR6	C3D-C4D	3.58	1.62	1.53
2	C	301	AR6	C3D-C4D	3.51	1.61	1.53
2	F	301	AR6	O3'-C3'	-3.49	1.34	1.43
2	J	301	AR6	PB-O3A	3.49	1.63	1.59
2	H	301	AR6	O3'-C3'	-3.47	1.34	1.43
2	J	301	AR6	C5-C4	-3.44	1.32	1.39
2	F	301	AR6	PB-O3A	3.42	1.63	1.59
2	F	301	AR6	C5-N7	-3.24	1.33	1.39
2	H	301	AR6	C5-N7	-3.24	1.33	1.39
2	H	301	AR6	C5-C4	-2.83	1.34	1.39
2	C	301	AR6	C5-C4	-2.79	1.34	1.39
2	D	301	AR6	C3'-C4'	2.64	1.59	1.53
2	D	301	AR6	C5-N7	-2.62	1.34	1.39
2	D	301	AR6	C5-C4	-2.58	1.34	1.39
2	L	301	AR6	C5-N7	-2.55	1.34	1.39
2	F	301	AR6	C3'-C4'	2.53	1.59	1.53
2	C	301	AR6	C5-N7	-2.51	1.34	1.39
2	F	301	AR6	C5-C4	-2.47	1.34	1.39
2	J	301	AR6	C3'-C4'	2.40	1.59	1.53
2	J	301	AR6	O2'-C2'	2.37	1.48	1.43
2	F	301	AR6	O2'-C2'	2.37	1.48	1.43
2	C	301	AR6	C3'-C4'	2.35	1.58	1.53
2	H	301	AR6	C3'-C4'	2.24	1.58	1.53
2	L	301	AR6	C5-C4	-2.23	1.35	1.39
2	J	301	AR6	C8-N9	-2.22	1.33	1.37
2	D	301	AR6	C4-N9	-2.17	1.33	1.37
2	F	301	AR6	O2D-C2D	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	AR6	O2'-C2'	2.09	1.48	1.43
2	H	301	AR6	O2D-C2D	2.09	1.48	1.43
2	L	301	AR6	C3'-C4'	2.02	1.58	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	AR6	N6-C6-N1	-6.74	103.38	118.38
2	C	301	AR6	N6-C6-N1	-6.29	104.38	118.38
2	H	301	AR6	N3-C2-N1	-6.05	119.43	128.58
2	J	301	AR6	N3-C2-N1	-5.97	119.55	128.58
2	D	301	AR6	N3-C2-N1	-5.76	119.86	128.58
2	L	301	AR6	C5-C6-N6	5.75	137.52	123.29
2	L	301	AR6	N3-C2-N1	-5.61	120.09	128.58
2	C	301	AR6	N3-C2-N1	-5.54	120.19	128.58
2	F	301	AR6	N3-C2-N1	-5.54	120.20	128.58
2	J	301	AR6	C5-C4-N3	-5.38	119.31	126.72
2	J	301	AR6	N6-C6-N1	-5.21	106.77	118.38
2	H	301	AR6	N6-C6-N1	-5.20	106.80	118.38
2	C	301	AR6	C5-C6-N6	5.17	136.09	123.29
2	F	301	AR6	N6-C6-N1	-5.16	106.88	118.38
2	F	301	AR6	C5-C4-N3	-4.75	120.18	126.72
2	H	301	AR6	C5-C4-N3	-4.73	120.21	126.72
2	D	301	AR6	N6-C6-N1	-4.62	108.10	118.38
2	D	301	AR6	C5-C6-N6	4.40	134.17	123.29
2	F	301	AR6	C5-C6-N6	4.32	133.99	123.29
2	L	301	AR6	C5-C4-N3	-4.28	120.82	126.72
2	H	301	AR6	C5-C6-N6	4.25	133.80	123.29
2	C	301	AR6	C5-C4-N3	-4.24	120.88	126.72
2	J	301	AR6	C5-C6-N6	4.13	133.51	123.29
2	C	301	AR6	N9-C8-N7	-3.61	108.82	113.94
2	D	301	AR6	O1D-C1D-O4D	-3.56	106.58	111.12
2	J	301	AR6	C2-N3-C4	3.53	120.46	111.83
2	D	301	AR6	O4'-C1'-N9	3.51	114.82	108.09
2	D	301	AR6	N9-C8-N7	-3.43	109.07	113.94
2	F	301	AR6	N9-C8-N7	-3.41	109.10	113.94
2	D	301	AR6	C5-C4-N3	-3.37	122.08	126.72
2	J	301	AR6	N9-C8-N7	-3.37	109.16	113.94
2	H	301	AR6	C2-N3-C4	3.35	120.00	111.83
2	C	301	AR6	C1D-C2D-C3D	3.32	106.37	102.29
2	J	301	AR6	N3-C4-N9	3.17	132.55	127.17
2	L	301	AR6	C2-N3-C4	3.13	119.48	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	AR6	C5-C4-N9	3.08	109.17	105.81
2	L	301	AR6	O1D-C1D-O4D	-2.98	107.32	111.12
2	C	301	AR6	C2-N3-C4	2.98	119.10	111.83
2	F	301	AR6	C2-N3-C4	2.94	119.01	111.83
2	C	301	AR6	O3A-PB-O2B	-2.94	101.87	110.70
2	F	301	AR6	N3-C4-N9	2.88	132.07	127.17
2	H	301	AR6	O1D-C1D-O4D	-2.76	107.60	111.12
2	H	301	AR6	O1B-PB-O3A	2.73	114.66	107.27
2	J	301	AR6	C6-C5-C4	2.65	120.79	117.18
2	F	301	AR6	O1A-PA-O3A	2.65	114.42	107.27
2	C	301	AR6	O4'-C1'-N9	2.62	113.12	108.09
2	F	301	AR6	O1B-PB-O3A	2.60	114.31	107.27
2	H	301	AR6	N9-C8-N7	-2.59	110.27	113.94
2	L	301	AR6	O3A-PB-O2B	-2.53	103.10	110.70
2	H	301	AR6	O4'-C1'-N9	2.50	112.90	108.09
2	D	301	AR6	C2-N3-C4	2.49	117.92	111.83
2	F	301	AR6	C6-C5-C4	2.49	120.58	117.18
2	J	301	AR6	C5-N7-C8	2.48	107.35	103.45
2	H	301	AR6	C5-C4-N9	2.48	108.52	105.81
2	C	301	AR6	C5-N7-C8	2.48	107.35	103.45
2	C	301	AR6	C5-C4-N9	2.46	108.49	105.81
2	D	301	AR6	C2-N1-C6	2.42	122.71	118.73
2	H	301	AR6	N3-C4-N9	2.41	131.27	127.17
2	C	301	AR6	O1D-C1D-O4D	-2.40	108.06	111.12
2	J	301	AR6	O1B-PB-O3A	2.40	113.76	107.27
2	F	301	AR6	O3A-PB-O2B	-2.37	103.57	110.70
2	L	301	AR6	N9-C8-N7	-2.37	110.57	113.94
2	F	301	AR6	C5-N7-C8	2.37	107.17	103.45
2	J	301	AR6	O5D-C5D-C4D	-2.35	100.99	108.99
2	H	301	AR6	C1D-C2D-C3D	2.34	105.17	102.29
2	H	301	AR6	C6-C5-C4	2.18	120.15	117.18
2	C	301	AR6	C4-C5-N7	-2.17	108.10	110.58
2	H	301	AR6	C3'-C2'-C1'	2.15	105.52	101.46
2	L	301	AR6	C3'-C2'-C1'	2.14	105.52	101.46
2	J	301	AR6	C5-C4-N9	2.14	108.14	105.81
2	J	301	AR6	O2'-C2'-C3'	-2.12	105.03	111.82
2	L	301	AR6	O1B-PB-O3A	2.10	112.95	107.27
2	D	301	AR6	C3'-C2'-C1'	2.09	105.41	101.46
2	D	301	AR6	O1B-PB-O3A	2.09	112.91	107.27
2	F	301	AR6	C3'-C2'-C1'	2.09	105.41	101.46
2	J	301	AR6	O1A-PA-O3A	2.08	112.90	107.27
2	D	301	AR6	C5D-C4D-C3D	-2.06	107.81	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	AR6	C1D-C2D-C3D	2.05	104.81	102.29
2	C	301	AR6	N3-C4-N9	2.03	130.62	127.17
2	C	301	AR6	O1B-PB-O3A	2.01	112.71	107.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

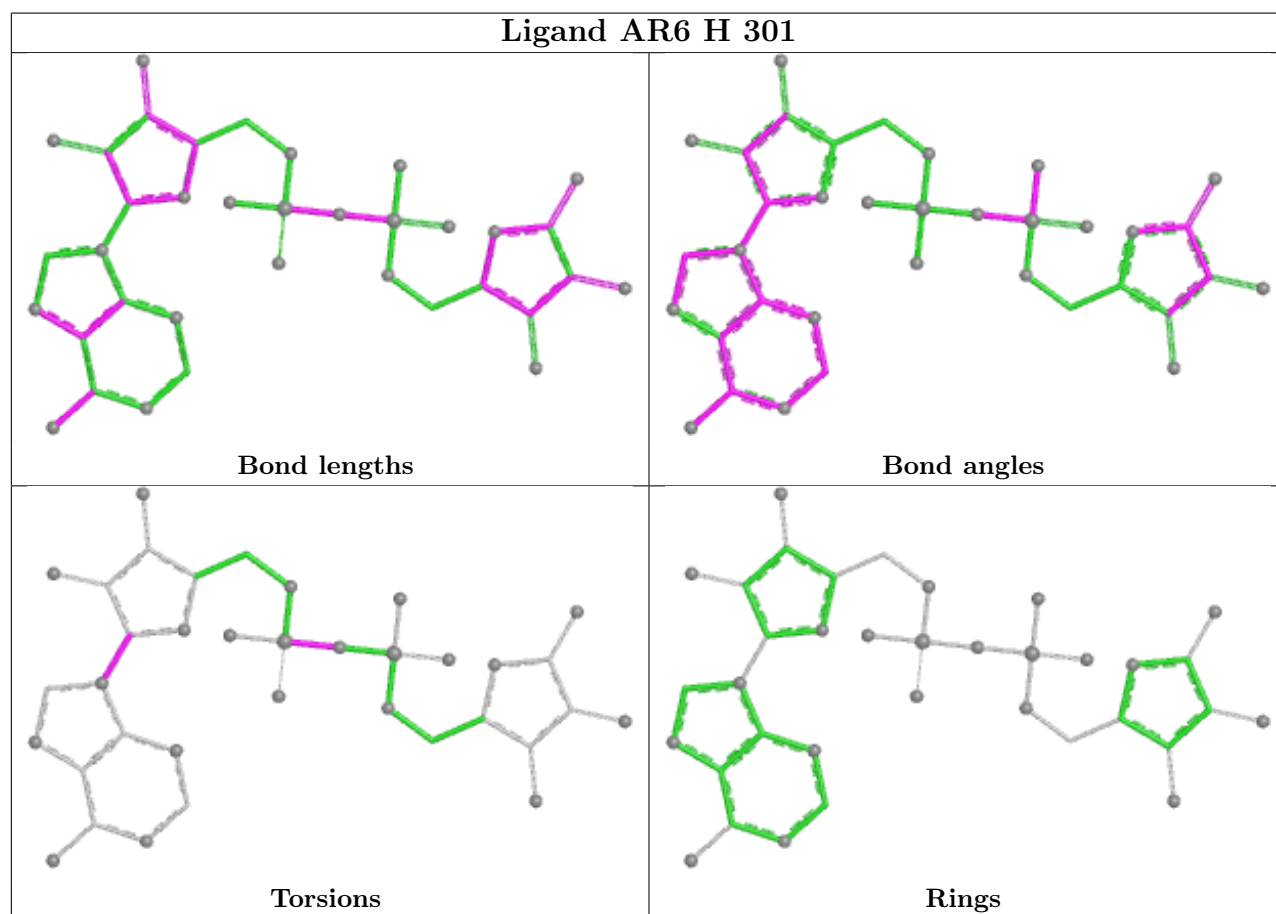
Mol	Chain	Res	Type	Atoms
2	C	301	AR6	PA-O3A-PB-O5D
2	D	301	AR6	C5D-O5D-PB-O2B
2	D	301	AR6	PA-O3A-PB-O5D
2	C	301	AR6	C2'-C1'-N9-C8
2	F	301	AR6	C2'-C1'-N9-C8
2	H	301	AR6	C2'-C1'-N9-C8
2	J	301	AR6	C2'-C1'-N9-C8
2	L	301	AR6	C2'-C1'-N9-C8
2	D	301	AR6	C2'-C1'-N9-C8
2	F	301	AR6	PB-O3A-PA-O1A
2	H	301	AR6	PB-O3A-PA-O1A
2	D	301	AR6	C5D-O5D-PB-O1B
2	D	301	AR6	C5D-O5D-PB-O3A
2	J	301	AR6	PB-O3A-PA-O1A
2	L	301	AR6	PB-O3A-PA-O1A
2	D	301	AR6	C3D-C4D-C5D-O5D
2	J	301	AR6	O4'-C1'-N9-C8
2	F	301	AR6	O4'-C1'-N9-C8
2	H	301	AR6	O4'-C1'-N9-C8
2	D	301	AR6	O4'-C1'-N9-C8
2	F	301	AR6	PB-O3A-PA-O2A
2	H	301	AR6	PB-O3A-PA-O2A
2	D	301	AR6	PB-O3A-PA-O1A
2	C	301	AR6	O4'-C1'-N9-C8
2	L	301	AR6	O4'-C1'-N9-C8
2	C	301	AR6	C2'-C1'-N9-C4
2	F	301	AR6	C2'-C1'-N9-C4
2	D	301	AR6	C2'-C1'-N9-C4
2	L	301	AR6	PB-O3A-PA-O2A

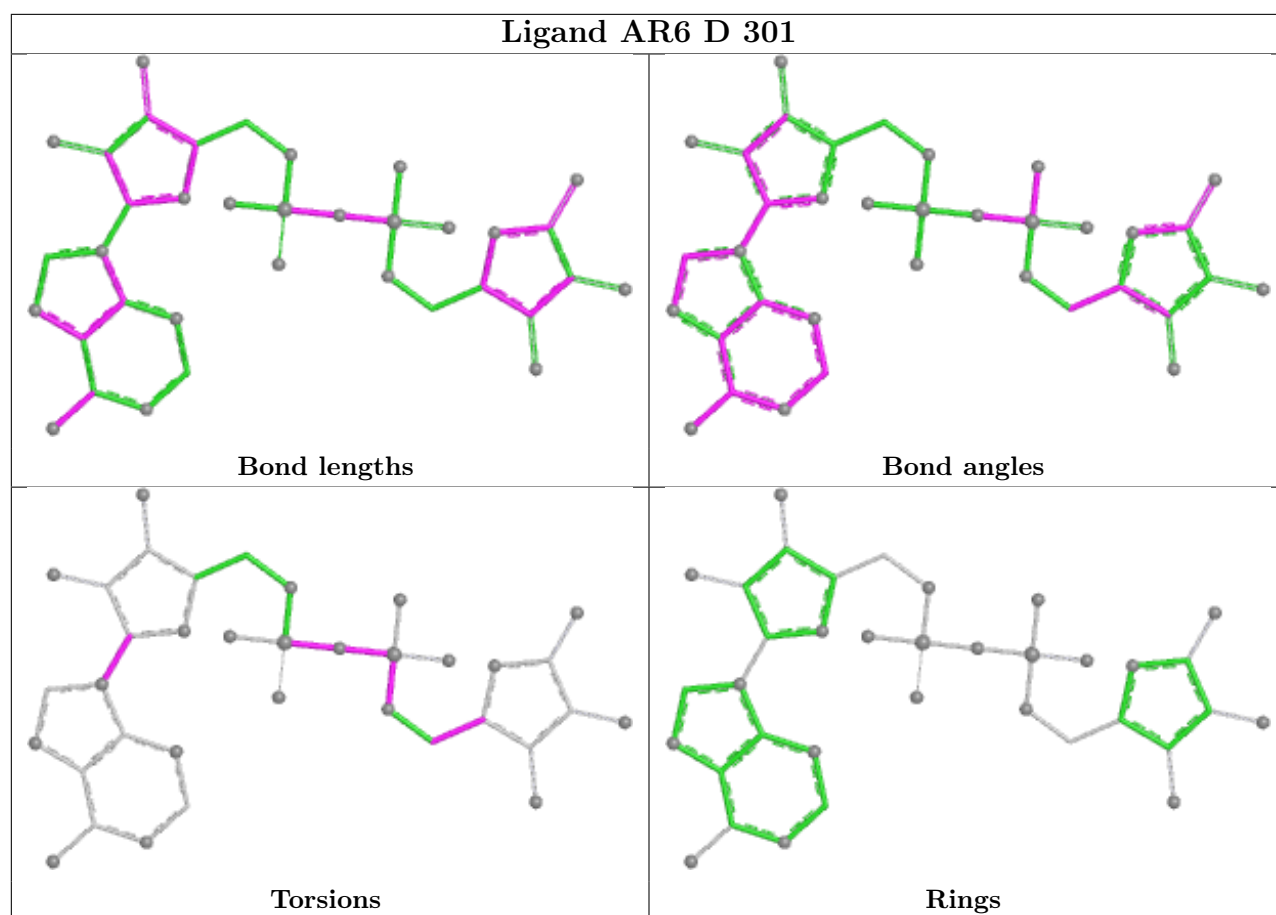
There are no ring outliers.

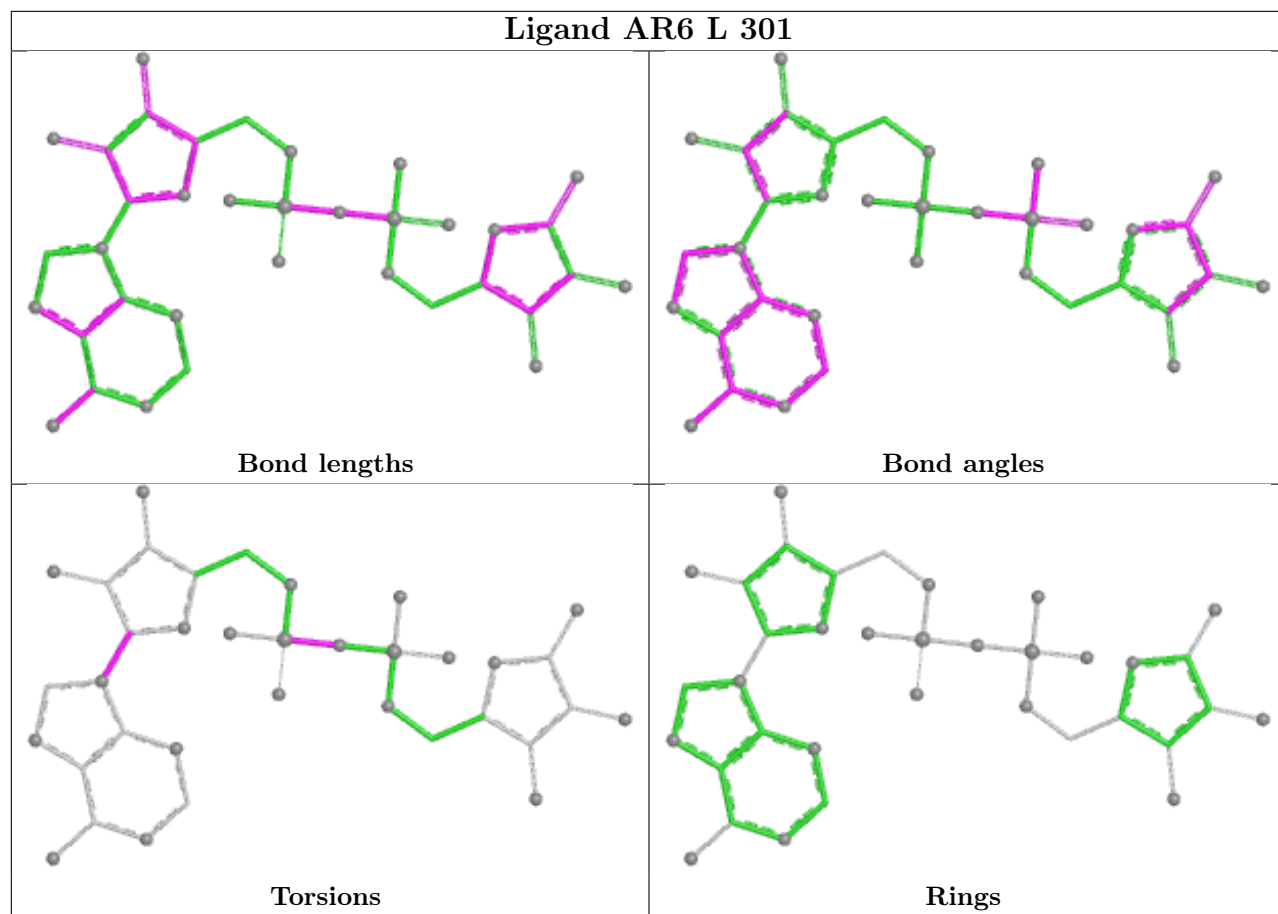
6 monomers are involved in 12 short contacts:

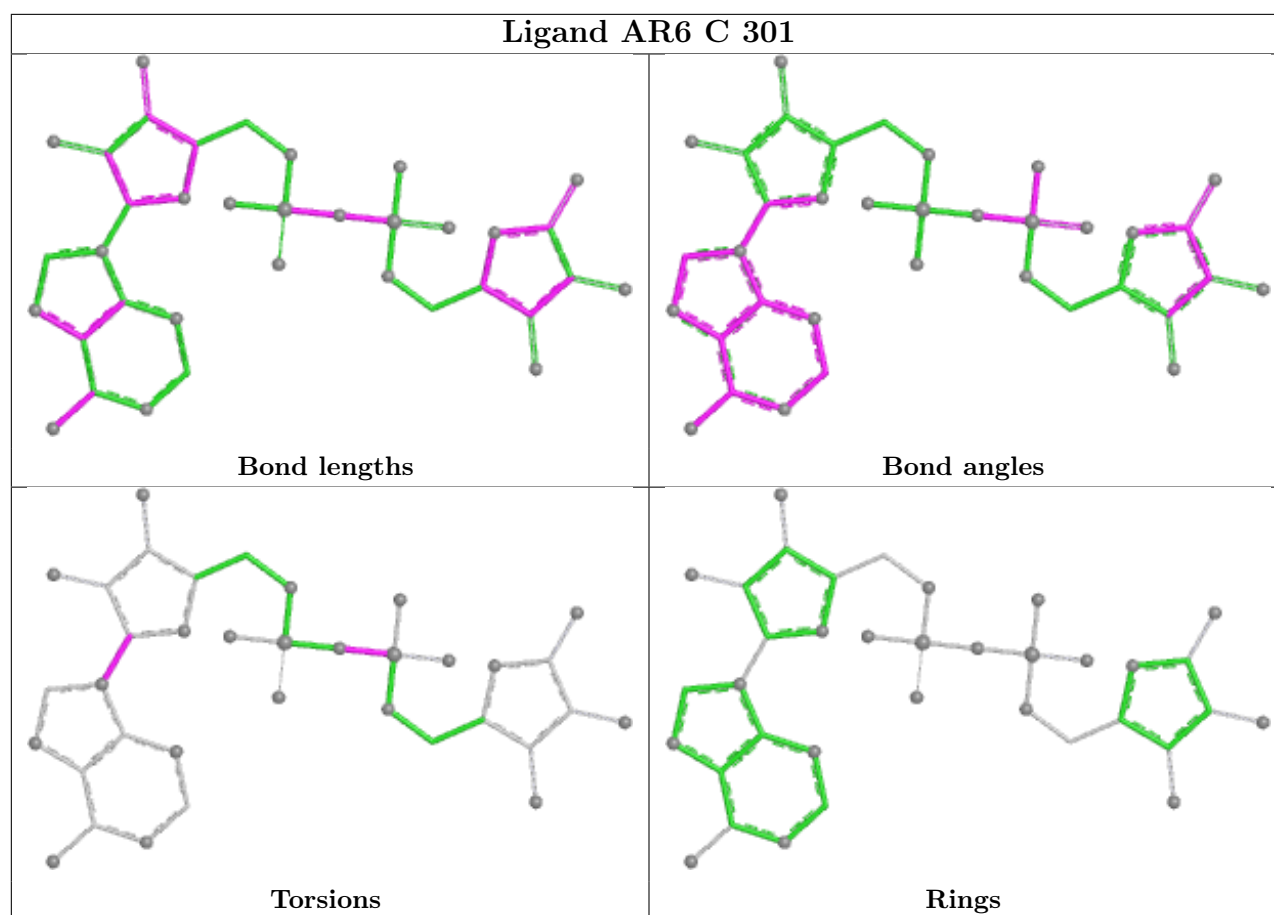
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	AR6	1	0
2	D	301	AR6	1	0
2	L	301	AR6	2	0
2	C	301	AR6	1	0
2	F	301	AR6	3	0
2	J	301	AR6	4	0

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.

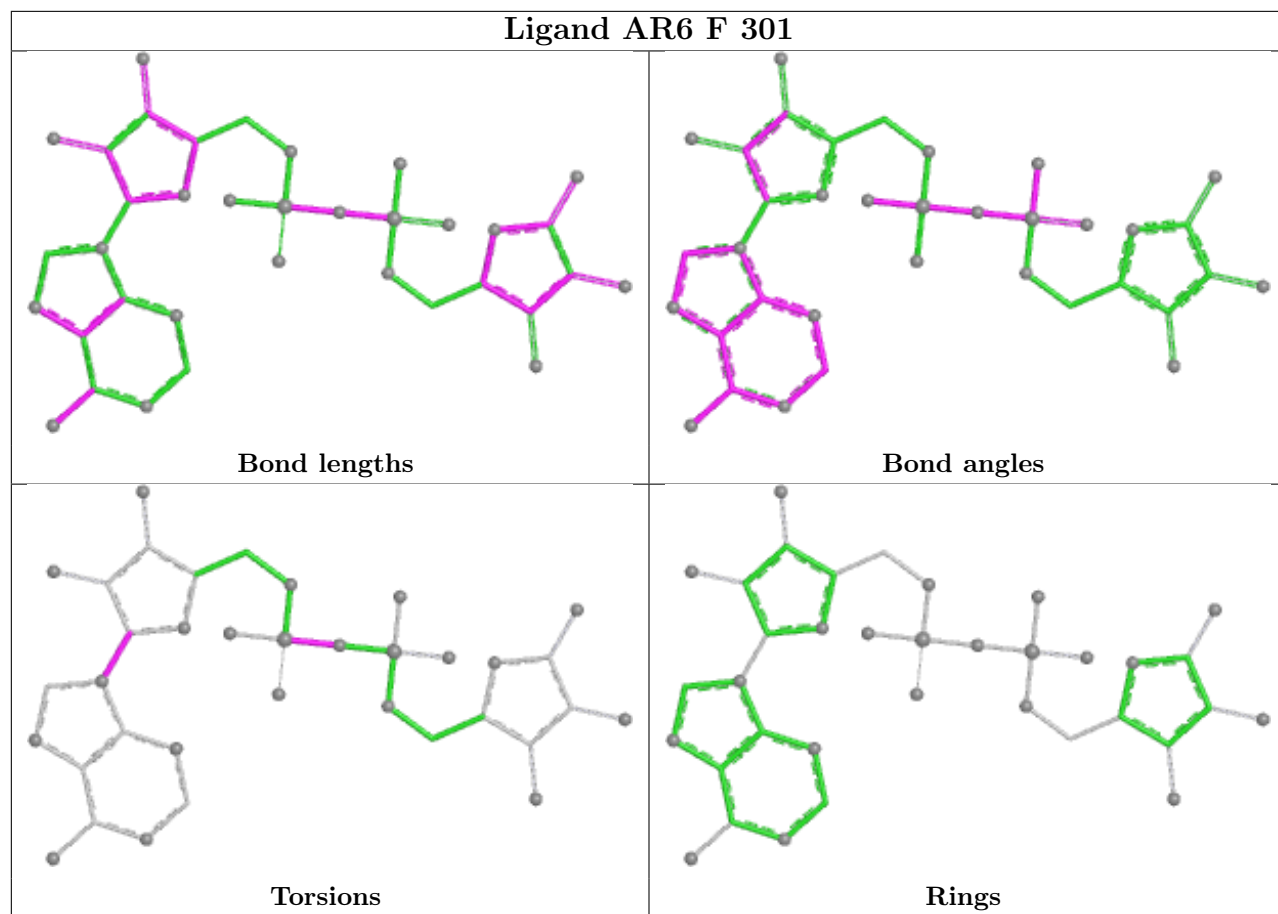


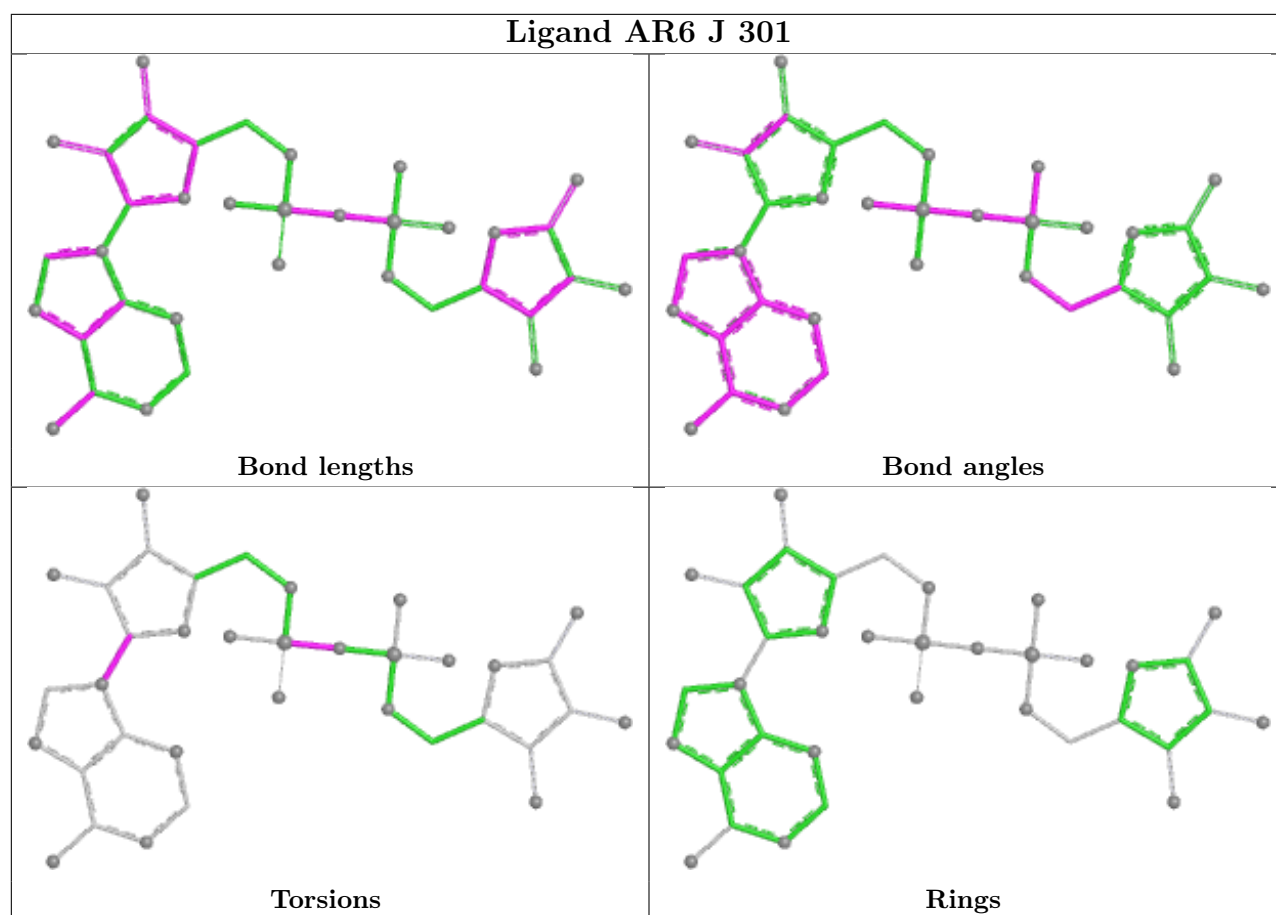






Ligand AR6 F 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	253/253 (100%)	-1.94	0 100 100	15, 27, 52, 85	0
1	D	249/253 (98%)	-1.91	0 100 100	19, 28, 49, 70	0
1	F	252/253 (99%)	-1.91	0 100 100	15, 27, 48, 69	0
1	H	250/253 (98%)	-1.93	0 100 100	18, 31, 56, 98	0
1	J	250/253 (98%)	-1.93	0 100 100	14, 30, 55, 82	0
1	L	248/253 (98%)	-1.90	0 100 100	14, 25, 46, 63	0
All	All	1502/1518 (98%)	-1.92	0 100 100	14, 28, 52, 98	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	AR6	F	301	36/36	0.99	0.01	17,26,33,36	0

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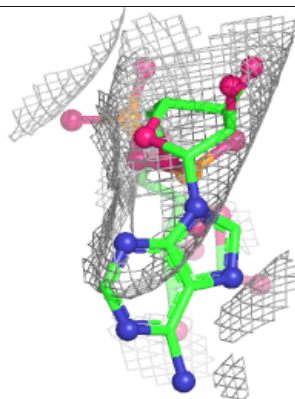
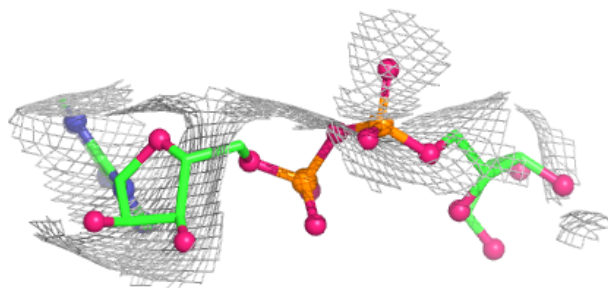
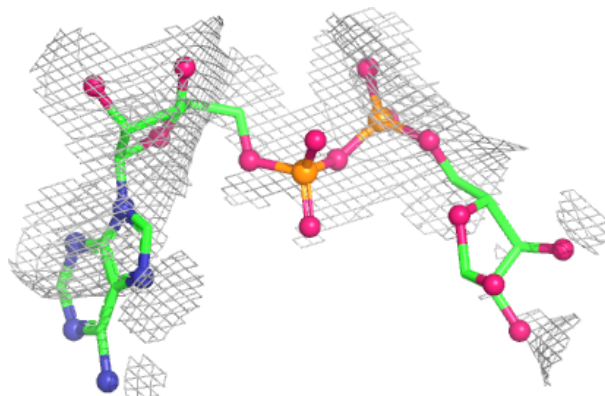
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AR6	J	301	36/36	0.99	0.01	17,25,30,32	0
2	AR6	H	301	36/36	1.00	0.01	16,23,29,33	0
2	AR6	C	301	36/36	1.00	0.01	13,22,32,38	0
2	AR6	L	301	36/36	1.00	0.01	17,23,27,32	0
2	AR6	D	301	36/36	1.00	0.01	13,25,32,34	0
3	PO4	C	302	5/5	1.00	0.01	68,70,74,75	0
3	PO4	F	302	5/5	1.00	0.01	65,65,69,70	0
3	PO4	D	302	5/5	1.00	0.00	48,54,58,59	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.

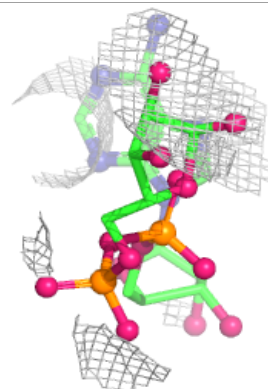
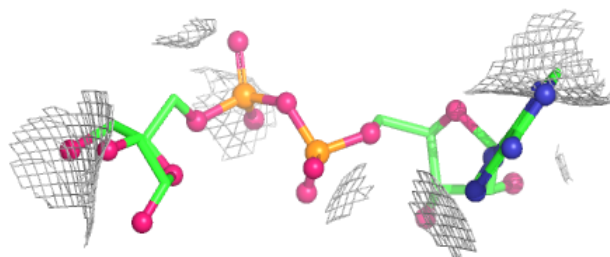
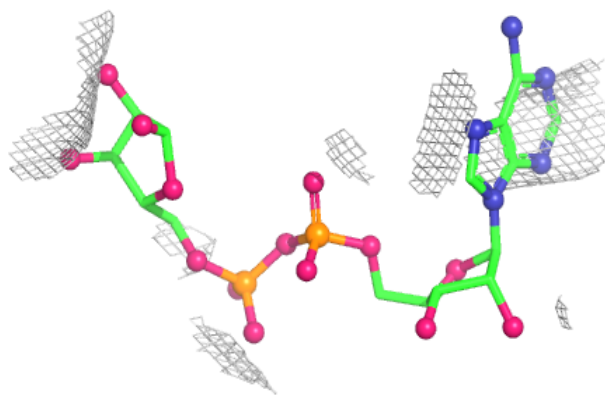
Electron density around AR6 F 301:

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



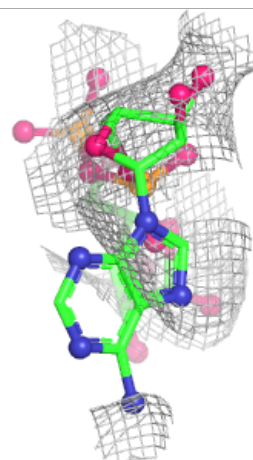
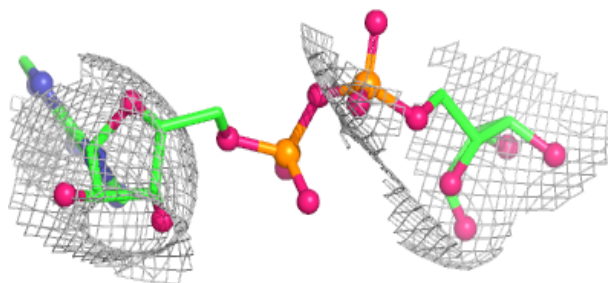
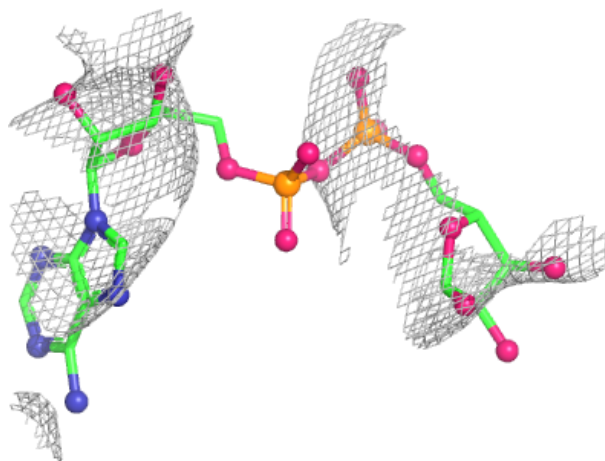
Electron density around AR6 J 301:

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



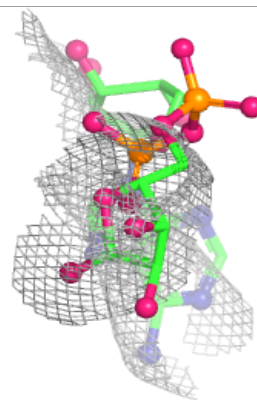
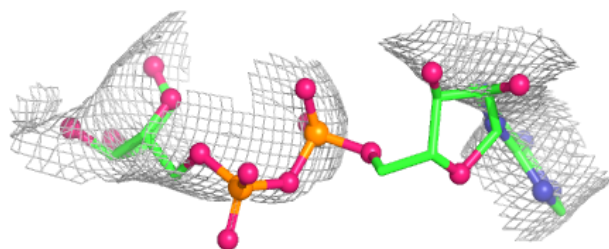
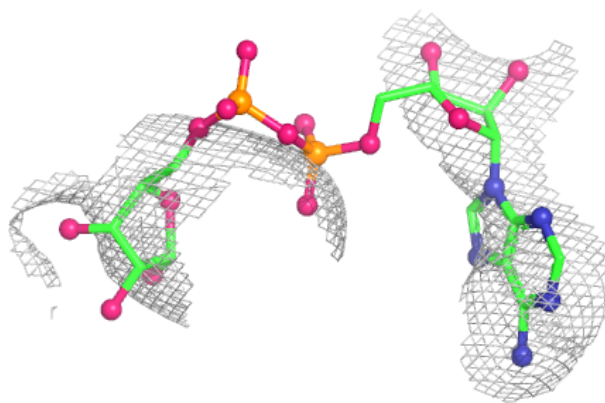
Electron density around AR6 H 301:

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

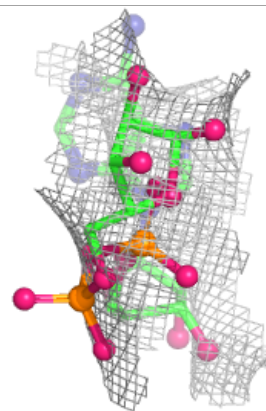
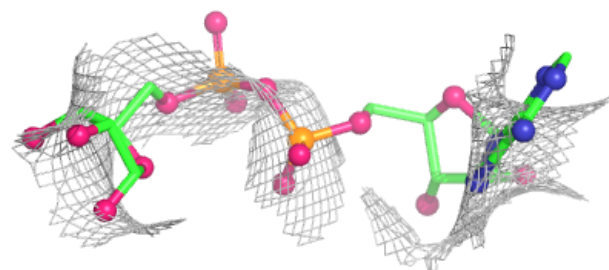
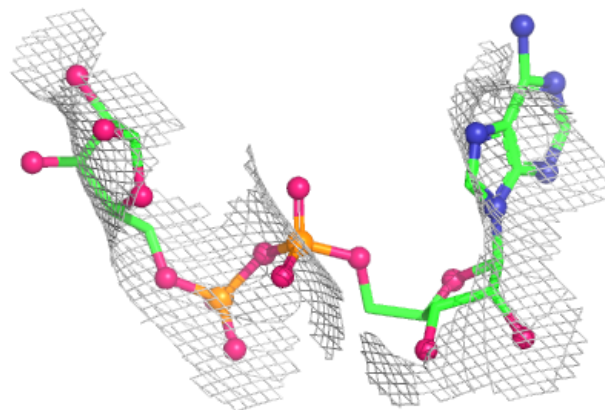


Electron density around AR6 C 301:

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

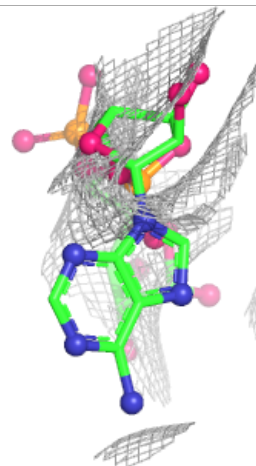
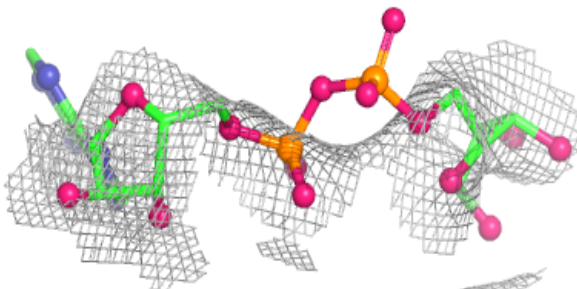
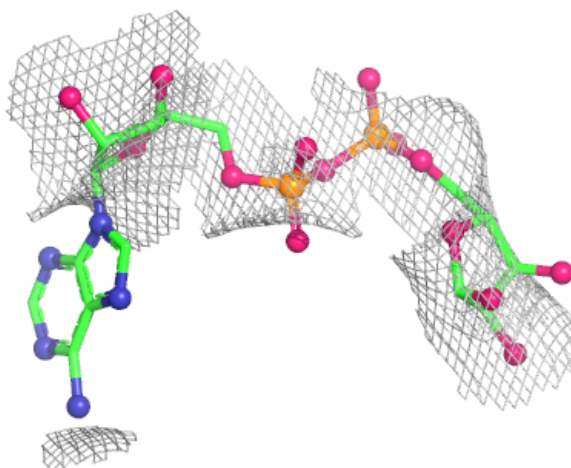
**Electron density around AR6 L 301:**

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



Electron density around AR6 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 [i](#)

There are no such residues in this entry.