



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2020 – 07:31 PM JST

PDB ID : 6LH4
Title : Crystal structural of MacroD1-ADPr complex
Authors : Yang, X.; Ma, Y.; Li, Y.
Deposited on : 2019-12-06
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

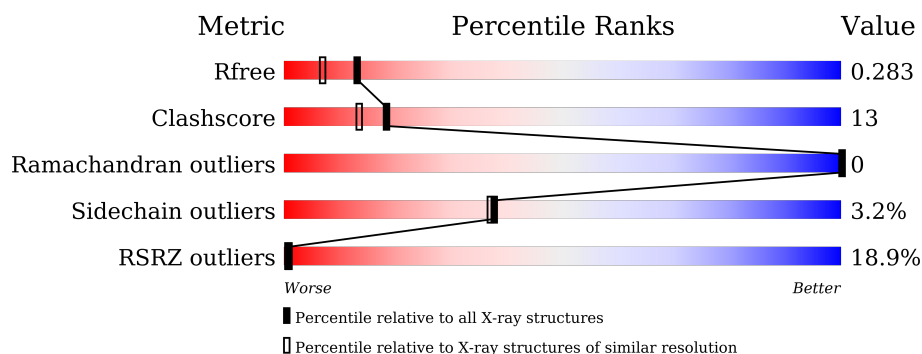
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	235	<div> <div>10%</div> <div>83%</div> <div>17%</div> </div>
1	B	235	<div> <div>8%</div> <div>86%</div> <div>14%</div> </div>
1	C	235	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
1	D	235	<div> <div>49%</div> <div>49%</div> <div>45%</div> <div>6%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AR6	D	601	-	-	X	-

2 Entry composition [i](#)

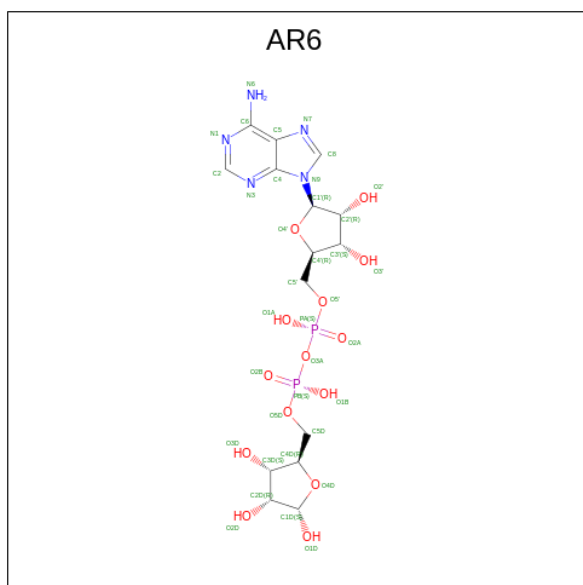
There are 3 unique types of molecules in this entry. The entry contains 7964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-ribose glycohydrolase MACROD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1851	1178	322	342	9			
1	B	235	Total	C	N	O	S	0	0	0
			1851	1178	322	342	9			
1	C	235	Total	C	N	O	S	0	0	0
			1851	1178	322	342	9			
1	D	235	Total	C	N	O	S	0	0	0
			1851	1178	322	342	9			

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	C	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		

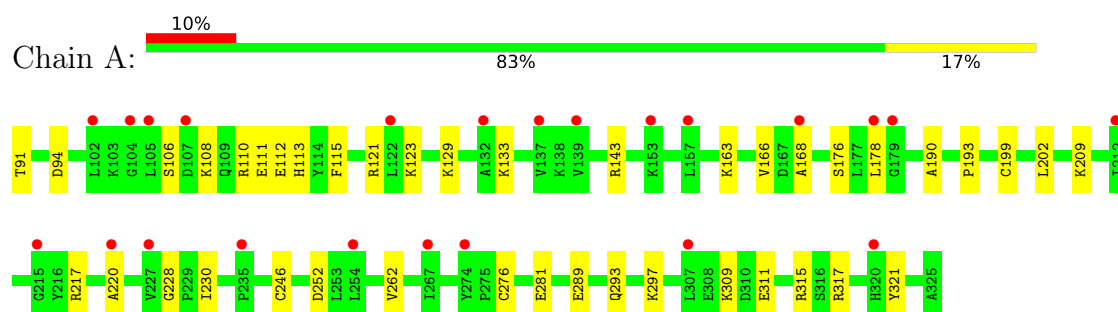
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	110	Total	O	0	0
			110	110		
3	C	101	Total	O	0	0
			101	101		
3	D	94	Total	O	0	0
			94	94		

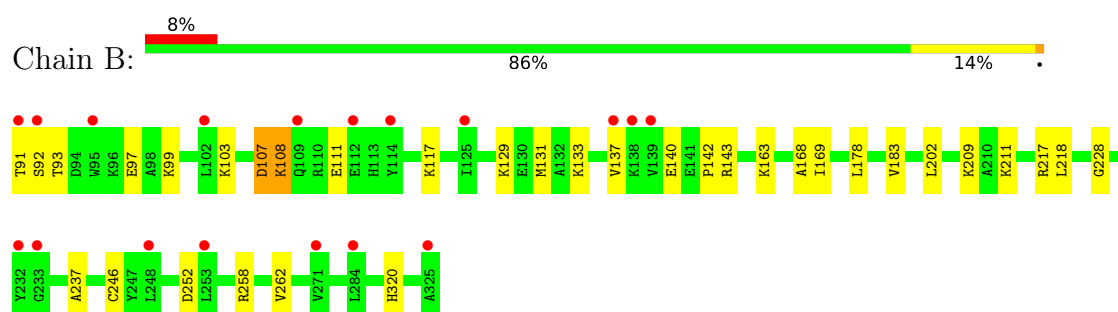
3 Residue-property plots [i](#)

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.

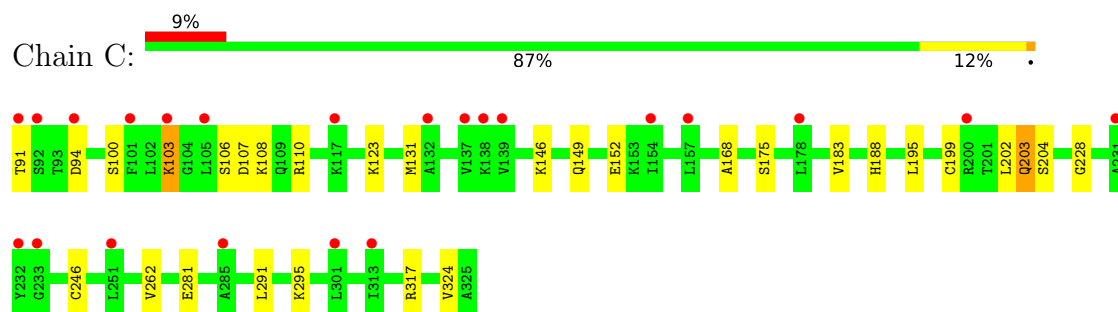
• Molecule 1: ADP-ribose glycohydrolase MACROD1



• Molecule 1: ADP-ribose glycohydrolase MACROD1

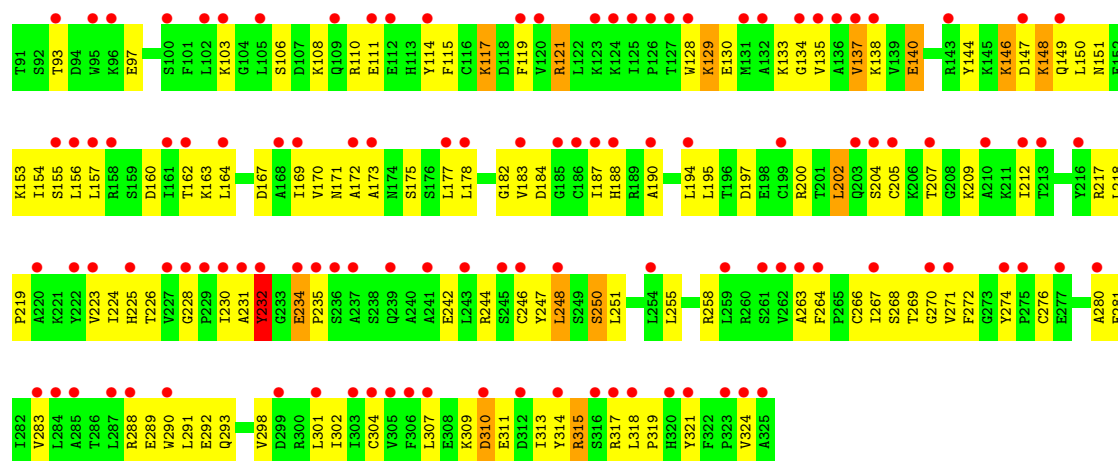


• Molecule 1: ADP-ribose glycohydrolase MACROD1



• Molecule 1: ADP-ribose glycohydrolase MACROD1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.90Å 106.20Å 79.90Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	32.90 – 2.00 32.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.90-2.00) 97.3 (32.90-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.240 , 0.285 0.241 , 0.283	Depositor DCC
R_{free} test set	3699 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.469 for -h-l,k,h 0.469 for l,k,-h-l 0.077 for h,-k,-h-l 0.074 for -h-l,-k,l 0.069 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7964	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: AR6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1888	0.62	2/2546 (0.1%)
1	B	0.45	0/1888	0.63	2/2546 (0.1%)
1	C	0.44	0/1888	0.58	0/2546
1	D	0.46	0/1888	0.75	3/2546 (0.1%)
All	All	0.45	0/7552	0.65	7/10184 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	234	GLU	CB-CA-C	5.86	122.12	110.40
1	D	232	TYR	CB-CA-C	5.80	121.99	110.40
1	D	140	GLU	CB-CA-C	5.79	121.98	110.40
1	B	107	ASP	CB-CA-C	5.69	121.78	110.40
1	B	143	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	143	ARG	NE-CZ-NH1	5.37	122.99	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1851	0	1886	26	0
1	B	1851	0	1886	24	0
1	C	1851	0	1886	24	0
1	D	1851	0	1885	126	0
2	A	36	0	20	1	0
2	B	36	0	20	3	0
2	C	36	0	20	5	0
2	D	36	0	19	10	0
3	A	111	0	0	7	1
3	B	110	0	0	8	2
3	C	101	0	0	9	1
3	D	94	0	0	15	0
All	All	7964	0	7622	201	2

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 13.

All (201) 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:D:234:GLU:CG	1:D:235:PRO:HD3	1.49	1.42
1:D:234:GLU:HG2	1:D:235:PRO:CD	1.63	1.27
1:D:163:LYS:NZ	3:D:701:HOH:O	1.69	1.23
1:D:269:THR:HG22	2:D:601:AR6:H5'	1.31	1.12
1:B:108:LYS:O	3:B:701:HOH:O	1.73	1.06
1:D:171:ASN:ND2	3:D:703:HOH:O	1.89	1.04
1:D:117:LYS:H	1:D:117:LYS:HD2	1.22	1.04
1:D:175:SER:O	1:D:204:SER:OG	1.74	1.04
1:D:293:GLN:NE2	3:D:702:HOH:O	1.85	1.03
1:A:199:CYS:O	1:A:202:LEU:O	1.77	1.01
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.25	1.00
1:D:269:THR:HG22	2:D:601:AR6:C5'	1.77	1.00
1:A:297:LYS:NZ	3:A:701:HOH:O	1.87	0.99
1:C:103:LYS:O	3:C:701:HOH:O	1.81	0.98
1:D:244:ARG:NH1	3:D:706:HOH:O	1.96	0.98
2:D:601:AR6:O4D	3:D:704:HOH:O	1.89	0.89
1:D:271:VAL:HG23	2:D:601:AR6:O1A	1.72	0.88
1:D:150:LEU:HD23	1:D:288:ARG:HD2	1.56	0.87
1:D:274:TYR:OH	3:D:705:HOH:O	1.94	0.85
1:D:234:GLU:CB	1:D:235:PRO:HD3	2.07	0.84
1:A:133:LYS:NZ	3:A:702:HOH:O	2.07	0.83
1:D:184:ASP:OD1	3:D:703:HOH:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:HD11	1:D:314:TYR:HB3	1.63	0.79
1:D:234:GLU:CB	1:D:235:PRO:CD	2.62	0.77
1:D:269:THR:CG2	2:D:601:AR6:C5'	2.42	0.77
1:D:146:LYS:HG3	1:D:146:LYS:O	1.84	0.77
1:D:150:LEU:CD2	1:D:288:ARG:HD2	2.15	0.76
1:B:131:MET:SD	3:B:790:HOH:O	2.41	0.76
1:D:121:ARG:HG2	1:D:121:ARG:NH1	1.98	0.76
1:D:175:SER:C	1:D:204:SER:HG	1.88	0.75
1:D:188:HIS:HA	1:D:195:LEU:HD23	1.69	0.73
1:D:234:GLU:CG	1:D:235:PRO:CD	2.41	0.73
1:C:131:MET:SD	3:C:778:HOH:O	2.48	0.72
1:D:129:LYS:NZ	1:D:148:LYS:HB3	2.04	0.71
1:D:154:ILE:HD13	1:D:301:LEU:HB2	1.72	0.71
1:D:258:ARG:NH1	3:D:708:HOH:O	2.05	0.70
1:B:202:LEU:HD22	1:B:211:LYS:HD3	1.74	0.70
1:D:117:LYS:CD	1:D:117:LYS:H	2.00	0.70
1:D:270:GLY:O	3:D:709:HOH:O	2.09	0.70
1:A:91:THR:O	3:A:703:HOH:O	2.09	0.69
1:D:187:ILE:O	3:D:710:HOH:O	2.11	0.69
1:C:91:THR:O	3:C:702:HOH:O	2.09	0.68
1:D:234:GLU:HG2	1:D:235:PRO:HD3	0.72	0.67
2:C:601:AR6:H1D	3:C:717:HOH:O	1.95	0.67
1:D:164:LEU:HD11	1:D:304:CYS:SG	2.36	0.66
1:A:112:GLU:N	1:A:112:GLU:OE1	2.29	0.66
2:B:601:AR6:H1D	3:B:729:HOH:O	1.95	0.66
1:D:169:ILE:HG22	1:D:263:ALA:HB3	1.78	0.66
1:D:218:LEU:HD11	3:D:710:HOH:O	1.96	0.66
1:D:129:LYS:HE3	1:D:148:LYS:HA	1.79	0.64
1:D:289:GLU:OE1	3:D:702:HOH:O	2.15	0.64
1:C:281:GLU:OE2	1:C:317:ARG:NE	2.26	0.64
1:B:252:ASP:OD1	3:B:702:HOH:O	2.14	0.64
1:B:163:LYS:NZ	3:B:704:HOH:O	2.30	0.64
1:D:175:SER:O	1:D:204:SER:CA	2.46	0.64
1:D:117:LYS:N	1:D:117:LYS:HD2	2.05	0.63
1:D:150:LEU:CD2	1:D:288:ARG:CD	2.77	0.63
1:D:138:LYS:HE2	1:D:140:GLU:HB3	1.81	0.63
1:A:176:SER:OG	1:A:178:LEU:HG	2.00	0.62
1:D:150:LEU:CD2	1:D:288:ARG:NE	2.63	0.62
1:C:103:LYS:NZ	3:C:706:HOH:O	2.31	0.62
1:D:150:LEU:HD23	1:D:288:ARG:CD	2.30	0.62
1:D:115:PHE:HZ	1:D:162:THR:HB	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:SER:O	1:D:204:SER:HA	2.01	0.60
1:D:175:SER:O	1:D:205:CYS:N	2.34	0.60
1:D:175:SER:O	1:D:204:SER:CB	2.49	0.60
1:D:232:TYR:HD1	1:D:232:TYR:N	2.00	0.60
1:D:232:TYR:H	1:D:232:TYR:HD1	1.48	0.59
1:D:114:TYR:CE1	1:D:219:PRO:HA	2.38	0.59
1:D:182:GLY:HA3	2:D:601:AR6:PA	2.43	0.58
1:D:271:VAL:HG21	2:D:601:AR6:O4D	2.03	0.58
1:D:135:VAL:HG11	1:D:315:ARG:NH2	2.18	0.58
1:C:175:SER:O	1:C:204:SER:HB2	2.04	0.58
1:D:194:LEU:HB2	3:D:719:HOH:O	2.02	0.58
1:D:232:TYR:CD1	1:D:232:TYR:N	2.72	0.58
1:B:91:THR:HG22	1:B:92:SER:H	1.69	0.57
1:D:128:TRP:CE3	1:D:318:LEU:HD13	2.40	0.57
1:D:271:VAL:HB	2:D:601:AR6:O5D	2.05	0.56
1:B:91:THR:O	3:B:703:HOH:O	2.17	0.56
1:C:123:LYS:HG2	3:C:757:HOH:O	2.04	0.56
1:D:121:ARG:NH1	1:D:121:ARG:H	2.04	0.56
1:D:310:ASP:HA	1:D:313:ILE:HG12	1.88	0.56
1:B:133:LYS:O	1:C:103:LYS:HE3	2.06	0.56
1:D:175:SER:HA	1:D:205:CYS:O	2.05	0.55
1:D:280:ALA:HB2	1:D:313:ILE:HD12	1.89	0.55
1:A:94:ASP:HB2	3:A:703:HOH:O	2.06	0.54
1:C:149:GLN:OE1	1:C:295:LYS:NZ	2.38	0.54
1:D:133:LYS:HD2	1:D:134:GLY:H	1.73	0.54
1:D:147:ASP:OD2	1:D:149:GLN:HB2	2.08	0.54
1:D:172:ALA:H	1:D:183:VAL:CG1	2.21	0.54
1:D:129:LYS:HZ1	1:D:148:LYS:HB3	1.71	0.53
1:B:129:LYS:NZ	3:B:707:HOH:O	2.41	0.53
1:D:156:LEU:HD11	1:D:314:TYR:CB	2.38	0.53
1:D:172:ALA:H	1:D:183:VAL:HG11	1.73	0.53
1:D:263:ALA:HA	1:D:302:ILE:HB	1.91	0.53
1:A:252:ASP:OD2	3:A:704:HOH:O	2.19	0.53
1:A:193:PRO:HB2	1:B:237:ALA:HB1	1.92	0.52
1:A:108:LYS:HA	1:A:111:GLU:HG3	1.91	0.52
1:D:170:VAL:HG21	1:D:264:PHE:CE1	2.44	0.52
1:D:288:ARG:O	1:D:292:GLU:HG2	2.10	0.52
1:C:199:CYS:O	1:C:202:LEU:O	2.27	0.52
1:D:195:LEU:HD11	1:D:225:HIS:HE1	1.75	0.52
1:B:183:VAL:HG22	2:B:601:AR6:N9	2.25	0.52
1:A:113:HIS:O	1:A:217:ARG:NE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD13	1:D:290:TRP:CD2	2.44	0.51
1:D:111:GLU:HG2	1:D:119:PHE:CZ	2.45	0.51
1:C:94:ASP:HB2	3:C:702:HOH:O	2.10	0.51
1:C:228:GLY:HA2	1:C:246:CYS:SG	2.51	0.51
1:C:183:VAL:HG22	2:C:601:AR6:N9	2.27	0.51
1:B:183:VAL:HG22	2:B:601:AR6:C4	2.41	0.50
1:A:289:GLU:OE1	1:A:293:GLN:NE2	2.41	0.50
1:D:231:ALA:N	1:D:272:PHE:O	2.44	0.50
1:B:140:GLU:HG3	1:B:320:HIS:NE2	2.26	0.50
1:D:106:SER:HB3	1:D:108:LYS:NZ	2.26	0.50
1:D:268:SER:HA	1:D:272:PHE:HB2	1.94	0.48
1:D:178:LEU:HD21	1:D:200:ARG:HH21	1.77	0.48
1:B:169:ILE:HD11	1:B:218:LEU:HD13	1.95	0.48
1:B:107:ASP:O	1:B:111:GLU:HG3	2.13	0.48
1:D:110:ARG:NH2	1:D:219:PRO:O	2.40	0.48
1:D:276:CYS:SG	1:D:313:ILE:HG21	2.54	0.48
1:D:317:ARG:HH11	1:D:321:TYR:HE1	1.61	0.48
1:C:168:ALA:O	1:C:262:VAL:HA	2.15	0.47
1:D:156:LEU:CD1	1:D:314:TYR:HB3	2.39	0.47
1:D:234:GLU:HB3	1:D:235:PRO:CD	2.43	0.47
1:D:129:LYS:NZ	1:D:148:LYS:CB	2.77	0.47
1:D:183:VAL:HG23	2:D:601:AR6:C4	2.45	0.47
1:D:224:ILE:HG21	1:D:250:SER:HB3	1.97	0.46
1:D:266:CYS:O	1:D:269:THR:HB	2.16	0.46
1:D:202:LEU:CD1	1:D:202:LEU:N	2.77	0.46
1:D:212:ILE:HG13	1:D:223:VAL:O	2.15	0.46
1:D:255:LEU:HD11	1:D:290:TRP:HZ2	1.79	0.46
1:D:307:LEU:HB2	1:D:310:ASP:OD1	2.16	0.46
1:A:281:GLU:OE1	1:A:321:TYR:OH	2.24	0.46
1:D:129:LYS:HZ2	1:D:148:LYS:HB3	1.80	0.46
1:C:183:VAL:HG22	2:C:601:AR6:C4	2.46	0.46
1:A:163:LYS:NZ	3:A:705:HOH:O	2.28	0.46
1:D:144:TYR:CE2	1:D:288:ARG:HG2	2.51	0.46
1:A:115:PHE:CE1	1:A:190:ALA:HB1	2.51	0.46
1:D:171:ASN:HD21	1:D:184:ASP:CG	2.19	0.45
1:B:93:THR:O	1:B:97:GLU:HG3	2.16	0.45
2:A:601:AR6:H1D	3:A:722:HOH:O	2.16	0.45
1:D:311:GLU:O	1:D:315:ARG:HB2	2.17	0.45
1:D:269:THR:CG2	2:D:601:AR6:H5'	2.18	0.45
1:D:266:CYS:HB2	1:D:269:THR:HB	1.98	0.45
1:B:228:GLY:HA2	1:B:246:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:OE2	1:A:317:ARG:NE	2.33	0.44
1:D:184:ASP:OD2	3:D:712:HOH:O	2.21	0.44
1:D:226:THR:HG21	1:D:246:CYS:HB3	2.00	0.44
1:A:168:ALA:O	1:A:262:VAL:HA	2.17	0.44
1:D:108:LYS:HB2	1:D:108:LYS:HE2	1.77	0.44
1:D:171:ASN:ND2	1:D:173:ALA:HB2	2.33	0.44
1:A:106:SER:O	1:A:110:ARG:HG3	2.16	0.44
1:C:203:GLN:CD	1:C:203:GLN:H	2.19	0.43
1:B:209:LYS:HD3	1:B:209:LYS:HA	1.82	0.43
1:B:258:ARG:NH1	3:B:705:HOH:O	2.37	0.43
1:C:291:LEU:O	1:C:295:LYS:HB3	2.18	0.43
1:A:111:GLU:OE2	1:A:121:ARG:NH1	2.49	0.43
1:D:247:TYR:CZ	1:D:283:VAL:HG22	2.53	0.43
1:A:311:GLU:HG2	1:A:315:ARG:HE	1.84	0.43
1:D:128:TRP:HD1	1:D:151:ASN:HB3	1.84	0.43
1:D:153:LYS:HE3	1:D:298:VAL:O	2.18	0.43
1:D:114:TYR:HA	1:D:217:ARG:O	2.19	0.43
1:D:154:ILE:HD11	1:D:291:LEU:HD11	2.00	0.43
1:B:168:ALA:O	1:B:262:VAL:HA	2.19	0.43
1:D:171:ASN:ND2	1:D:184:ASP:OD1	2.49	0.43
1:D:228:GLY:HA2	1:D:246:CYS:SG	2.58	0.43
1:D:266:CYS:O	1:D:269:THR:HG22	2.19	0.43
1:A:276:CYS:SG	1:A:309:LYS:HE3	2.59	0.42
1:D:121:ARG:CG	1:D:121:ARG:HH11	2.09	0.42
1:D:93:THR:O	1:D:97:GLU:HG3	2.18	0.42
1:A:209:LYS:HA	1:A:209:LYS:HD3	1.89	0.42
1:D:177:LEU:HD22	3:D:716:HOH:O	2.18	0.42
1:D:309:LYS:HB2	1:D:309:LYS:HE3	1.76	0.42
1:A:230:ILE:HD13	1:B:142:PRO:HD2	2.02	0.42
1:C:183:VAL:HG22	2:C:601:AR6:C8	2.49	0.42
1:B:99:LYS:O	1:B:103:LYS:HG2	2.20	0.42
1:C:100:SER:O	1:C:103:LYS:HB2	2.20	0.42
1:D:115:PHE:CE1	1:D:190:ALA:HB1	2.54	0.42
1:A:228:GLY:HA2	1:A:246:CYS:SG	2.60	0.42
1:B:117:LYS:HA	1:B:117:LYS:HD3	1.80	0.42
1:C:106:SER:O	1:C:110:ARG:HG3	2.20	0.42
1:D:226:THR:CG2	1:D:267:ILE:HD13	2.50	0.42
1:D:150:LEU:HD22	1:D:288:ARG:NE	2.35	0.42
1:D:248:LEU:HA	1:D:248:LEU:HD12	1.80	0.41
1:C:183:VAL:HG23	2:C:601:AR6:O2A	2.21	0.41
1:D:160:ASP:O	1:D:163:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:HIS:HA	1:C:195:LEU:HD23	2.03	0.41
1:D:207:THR:OG1	1:D:242:GLU:HG2	2.20	0.41
1:D:155:SER:HB2	1:D:302:ILE:HD13	2.03	0.41
1:C:152:GLU:OE1	3:C:703:HOH:O	2.21	0.41
1:C:146:LYS:HE3	1:C:324:VAL:O	2.21	0.41
1:D:197:ASP:O	1:D:200:ARG:HB3	2.21	0.41
1:A:129:LYS:HD3	1:A:129:LYS:HA	1.72	0.41
1:A:166:VAL:O	1:A:220:ALA:HA	2.20	0.41
1:D:128:TRP:CD1	1:D:151:ASN:HB3	2.55	0.40
1:D:187:ILE:HG22	1:D:195:LEU:HD22	2.03	0.40
1:D:137:VAL:HG23	1:D:319:PRO:HG2	2.04	0.40
1:D:157:LEU:HA	1:D:157:LEU:HD23	1.79	0.40
1:B:137:VAL:HG12	3:C:730:HOH:O	2.22	0.40
1:D:114:TYR:HD2	1:D:119:PHE:CD2	2.39	0.40
1:D:281:GLU:OE2	1:D:317:ARG:NH1	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:727:HOH:O	3:B:736:HOH:O[2_645]	1.81	0.39
3:B:773:HOH:O	3:C:782:HOH:O[2_656]	2.12	0.08

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	233/235 (99%)	228 (98%)	5 (2%)	0	100	100
1	B	233/235 (99%)	230 (99%)	3 (1%)	0	100	100
1	C	233/235 (99%)	225 (97%)	8 (3%)	0	100	100
1	D	233/235 (99%)	223 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	932/940 (99%)	906 (97%)	26 (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	A	200/200 (100%)	199 (100%)	1 (0%)	88	92
1	B	200/200 (100%)	197 (98%)	3 (2%)	65	69
1	C	200/200 (100%)	196 (98%)	4 (2%)	55	58
1	D	200/200 (100%)	182 (91%)	18 (9%)	9	6
All	All	800/800 (100%)	774 (97%)	26 (3%)	38	37

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	B	108	LYS
1	B	178	LEU
1	B	217	ARG
1	C	103	LYS
1	C	107	ASP
1	C	108	LYS
1	C	203	GLN
1	D	103	LYS
1	D	117	LYS
1	D	121	ARG
1	D	129	LYS
1	D	130	GLU
1	D	137	VAL
1	D	146	LYS
1	D	148	LYS
1	D	167	ASP

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Mol	Chain	Res	Type
1	D	202	LEU
1	D	209	LYS
1	D	230	ILE
1	D	232	TYR
1	D	248	LEU
1	D	250	SER
1	D	310	ASP
1	D	315	ARG
1	D	324	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	601	-	34,39,39	1.39	4 (11%)	40,60,60	1.14	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AR6	C	601	-	34,39,39	1.36	4 (11%)	40,60,60	1.10	3 (7%)
2	AR6	B	601	-	34,39,39	1.32	2 (5%)	40,60,60	1.14	3 (7%)
2	AR6	D	601	1	34,39,39	0.85	0	40,60,60	1.30	7 (17%)

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	A	601	-	-	1/18/54/54	0/4/4/4
2	AR6	C	601	-	-	2/18/54/54	0/4/4/4
2	AR6	B	601	-	-	1/18/54/54	0/4/4/4
2	AR6	D	601	1	-	4/18/54/54	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	AR6	O4D-C1D	-5.63	1.36	1.43
2	C	601	AR6	O4D-C1D	-5.49	1.36	1.43
2	B	601	AR6	O4D-C1D	-5.35	1.36	1.43
2	A	601	AR6	C8-N7	-2.17	1.30	1.34
2	C	601	AR6	C8-N7	-2.14	1.30	1.34
2	C	601	AR6	PB-O1B	-2.11	1.45	1.55
2	A	601	AR6	PA-O1A	-2.10	1.45	1.55
2	C	601	AR6	PA-O1A	-2.05	1.45	1.55
2	B	601	AR6	C8-N7	-2.04	1.31	1.34
2	A	601	AR6	PB-O1B	-2.01	1.45	1.55

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	AR6	O2'-C2'-C1'	3.34	123.18	110.85
2	D	601	AR6	O2'-C2'-C3'	3.24	122.31	111.82
2	A	601	AR6	O4'-C1'-C2'	-3.07	102.44	106.93
2	B	601	AR6	O4'-C1'-C2'	-2.80	102.83	106.93
2	D	601	AR6	C3'-C2'-C1'	2.72	105.08	100.98
2	C	601	AR6	O4'-C1'-C2'	-2.68	103.01	106.93
2	B	601	AR6	C5-C6-N6	2.46	124.10	120.35
2	A	601	AR6	C5-C6-N6	2.32	123.87	120.35
2	D	601	AR6	C1D-C2D-C3D	2.28	105.15	102.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AR6	O1D-C1D-O4D	2.25	114.02	111.13
2	A	601	AR6	O2D-C2D-C1D	2.17	117.81	111.82
2	D	601	AR6	O3'-C3'-C2'	2.11	118.65	111.82
2	C	601	AR6	O2D-C2D-C1D	2.11	117.64	111.82
2	C	601	AR6	C5-C6-N6	2.11	123.55	120.35
2	D	601	AR6	C5-C6-N6	2.09	123.53	120.35
2	D	601	AR6	O4'-C1'-C2'	-2.04	103.94	106.93
2	B	601	AR6	O1A-PA-O2A	2.03	122.28	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	AR6	C5'-O5'-PA-O2A
2	D	601	AR6	C5'-O5'-PA-O3A
2	C	601	AR6	O4'-C4'-C5'-O5'
2	C	601	AR6	C3'-C4'-C5'-O5'
2	B	601	AR6	O4'-C4'-C5'-O5'
2	D	601	AR6	C3'-C4'-C5'-O5'
2	A	601	AR6	O4'-C4'-C5'-O5'
2	D	601	AR6	C5'-O5'-PA-O1A

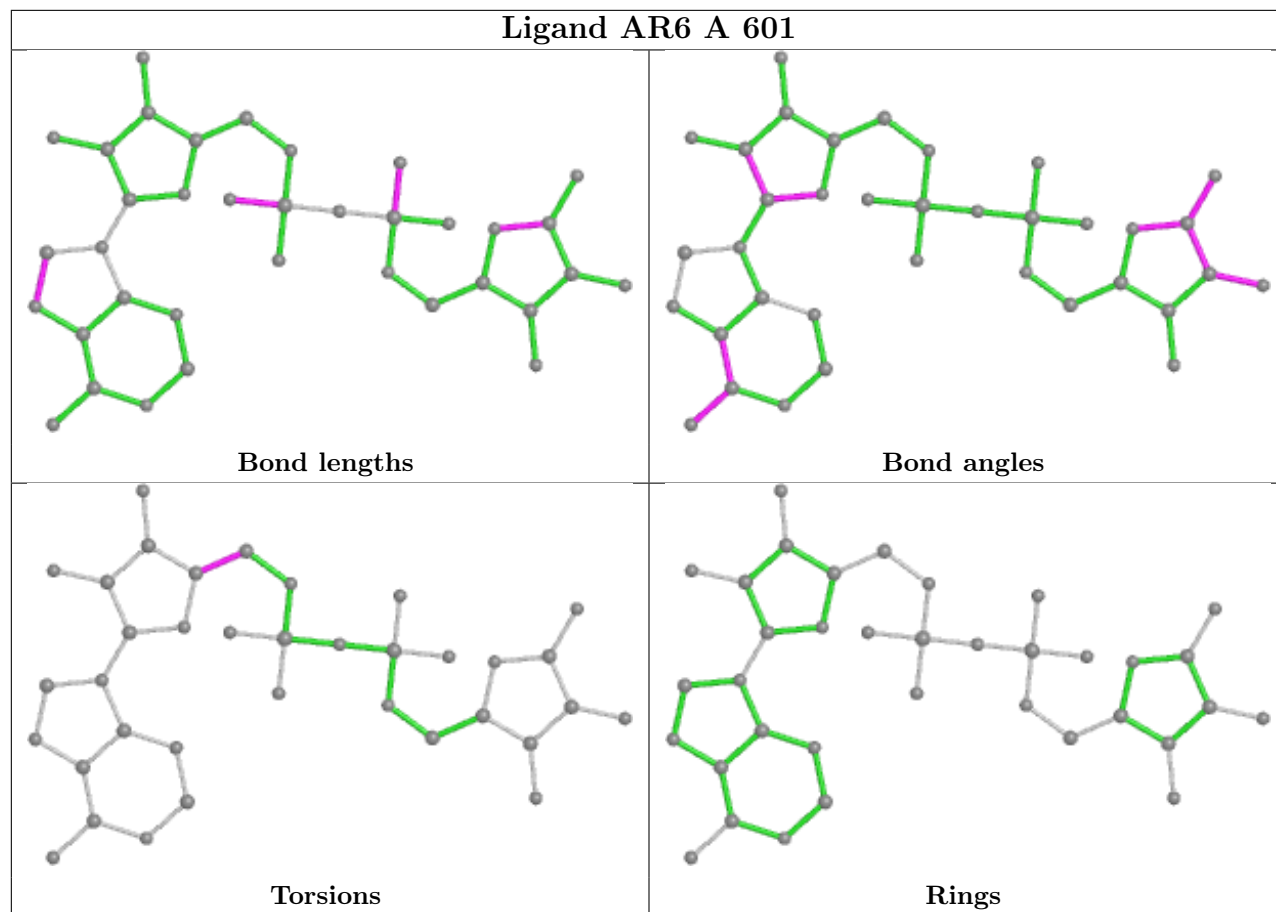
There are no ring outliers.

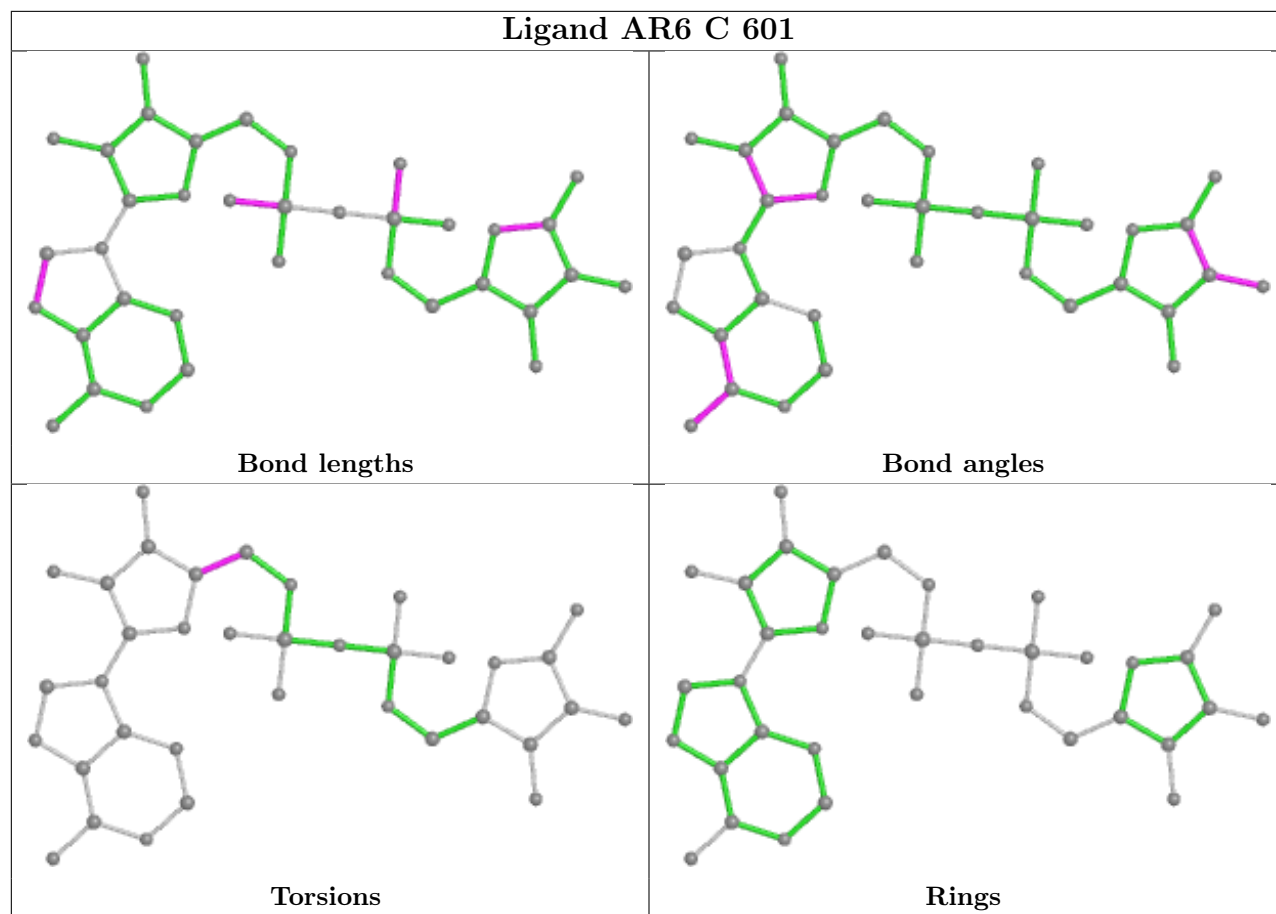
4 monomers are involved in 19 short contacts:

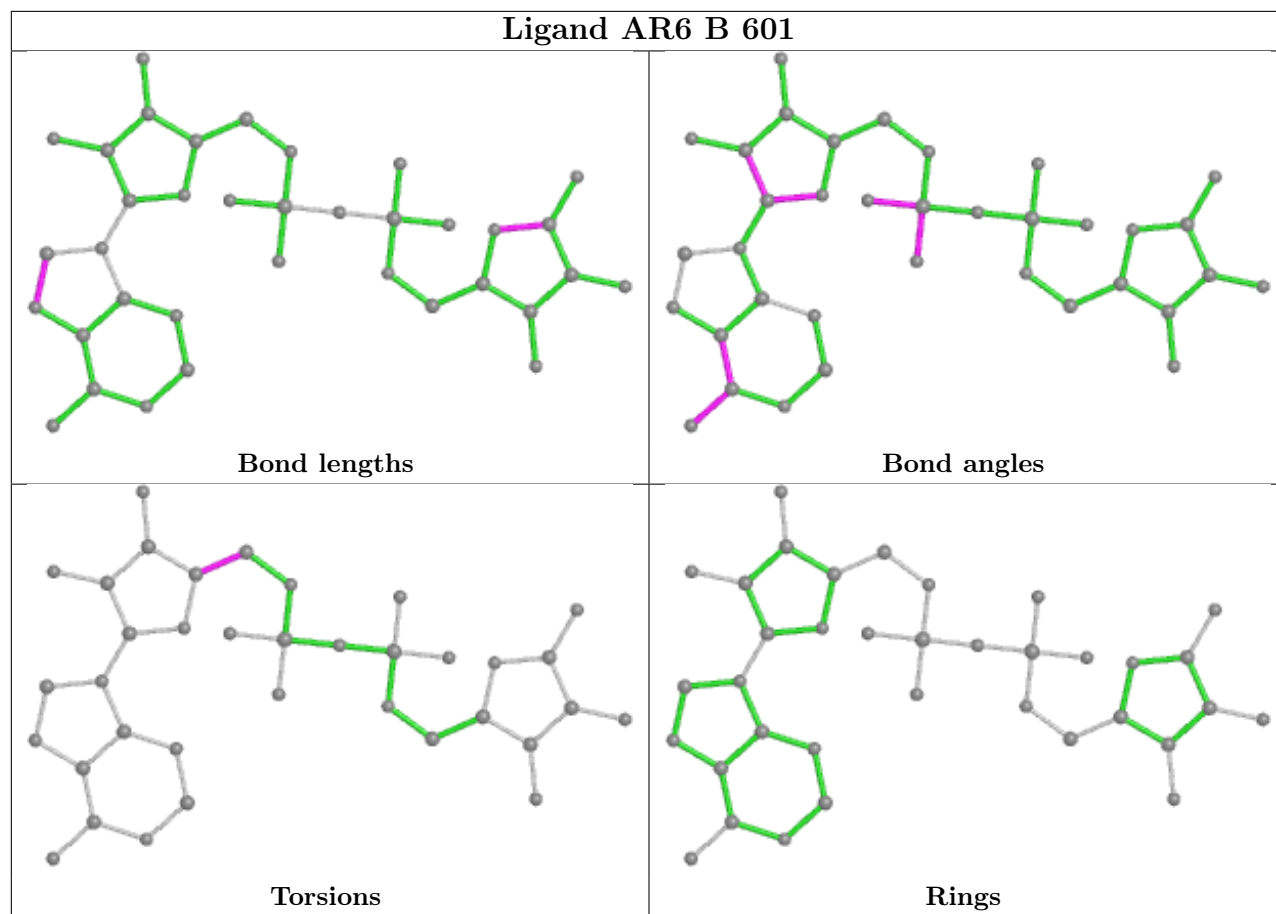
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AR6	1	0
2	C	601	AR6	5	0
2	B	601	AR6	3	0
2	D	601	AR6	10	0

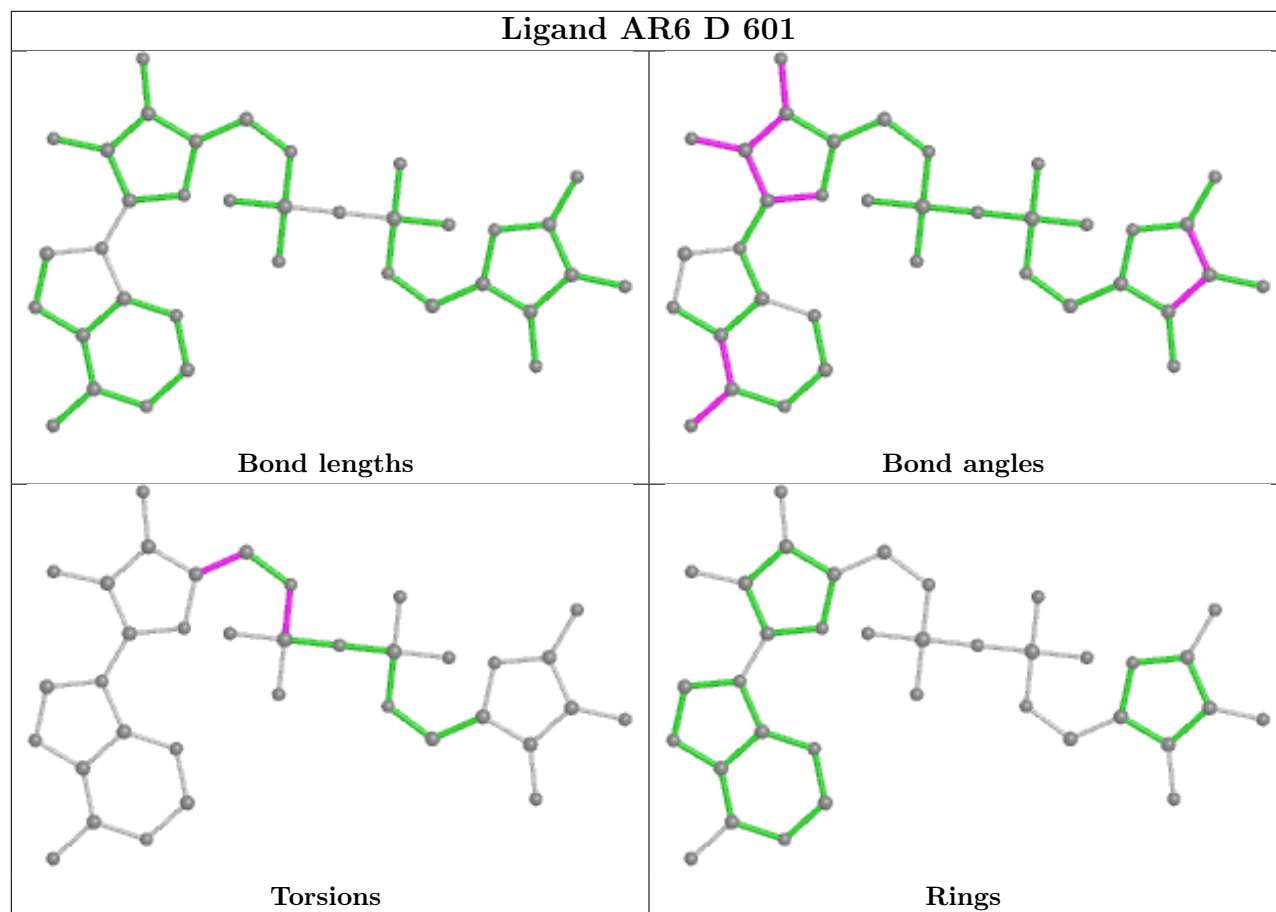
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	235/235 (100%)	0.86	23 (9%) 7 7	23, 33, 55, 65	0
1	B	235/235 (100%)	0.78	18 (7%) 13 12	24, 33, 57, 69	0
1	C	235/235 (100%)	0.85	22 (9%) 8 8	23, 33, 55, 68	0
1	D	235/235 (100%)	2.34	115 (48%) 0 0	30, 81, 104, 136	0
All	All	940/940 (100%)	1.21	178 (18%) 1 1	23, 37, 91, 136	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	VAL	15.0
1	D	134	GLY	10.0
1	D	263	ALA	9.5
1	D	137	VAL	9.2
1	D	262	VAL	8.9
1	C	139	VAL	8.1
1	D	164	LEU	7.4
1	D	248	LEU	7.2
1	D	172	ALA	6.9
1	D	230	ILE	6.5
1	D	194	LEU	6.1
1	D	235	PRO	6.1
1	D	213	THR	6.0
1	D	132	ALA	6.0
1	C	92	SER	5.8
1	D	227	VAL	5.8
1	D	271	VAL	5.4
1	D	305	VAL	5.0
1	D	162	THR	4.9
1	D	199	CYS	4.9
1	A	220	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	138	LYS	4.7
1	D	136	ALA	4.7
1	D	225	HIS	4.7
1	D	149	GLN	4.7
1	C	233	GLY	4.6
1	D	155	SER	4.5
1	D	120	VAL	4.5
1	D	131	MET	4.5
1	D	283	VAL	4.3
1	D	274	TYR	4.3
1	D	306	PHE	4.2
1	B	92	SER	4.2
1	C	103	LYS	4.2
1	C	91	THR	4.1
1	D	303	ILE	4.1
1	A	105	LEU	4.1
1	D	314	TYR	4.1
1	D	236	SER	4.1
1	A	139	VAL	4.1
1	D	102	LEU	4.0
1	D	119	PHE	4.0
1	D	123	LYS	3.9
1	B	125	ILE	3.9
1	D	204	SER	3.9
1	C	232	TYR	3.9
1	B	271	VAL	3.8
1	A	179	GLY	3.8
1	C	154	ILE	3.8
1	D	318	LEU	3.8
1	D	237	ALA	3.7
1	C	132	ALA	3.6
1	B	232	TYR	3.6
1	D	307	LEU	3.6
1	D	183	VAL	3.6
1	D	239	GLN	3.6
1	D	324	VAL	3.6
1	D	138	LYS	3.6
1	D	125	ILE	3.5
1	D	325	ALA	3.5
1	D	222	TYR	3.5
1	B	109	GLN	3.5
1	D	156	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	234	GLU	3.5
1	D	232	TYR	3.4
1	D	323	PRO	3.4
1	A	102	LEU	3.4
1	D	241	ALA	3.4
1	D	207	THR	3.4
1	D	128	TRP	3.3
1	B	139	VAL	3.3
1	D	216	TYR	3.3
1	D	321	TYR	3.2
1	D	157	LEU	3.2
1	D	264	PHE	3.1
1	C	105	LEU	3.1
1	D	161	ILE	3.0
1	C	231	ALA	3.0
1	D	190	ALA	3.0
1	D	245	SER	3.0
1	D	111	GLU	3.0
1	D	178	LEU	3.0
1	D	277	GLU	3.0
1	D	270	GLY	2.9
1	C	200	ARG	2.9
1	D	124	LYS	2.9
1	D	299	ASP	2.9
1	D	186	CYS	2.9
1	A	153	LYS	2.9
1	D	228	GLY	2.8
1	D	246	CYS	2.8
1	D	223	VAL	2.8
1	C	313	ILE	2.8
1	D	114	TYR	2.8
1	D	169	ILE	2.8
1	C	251	LEU	2.7
1	A	320	HIS	2.7
1	D	100	SER	2.7
1	D	212	ILE	2.7
1	B	233	GLY	2.7
1	A	235	PRO	2.7
1	D	203	GLN	2.7
1	D	229	PRO	2.7
1	B	95	TRP	2.7
1	D	320	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	126	PRO	2.7
1	D	317	ARG	2.7
1	B	248	LEU	2.6
1	D	259	LEU	2.6
1	D	185	GLY	2.6
1	A	122	LEU	2.6
1	C	138	LYS	2.6
1	C	137	VAL	2.6
1	D	96	LYS	2.6
1	D	93	THR	2.6
1	D	127	THR	2.6
1	D	112	GLU	2.5
1	C	101	PHE	2.5
1	D	301	LEU	2.5
1	A	178	LEU	2.5
1	A	274	TYR	2.5
1	D	173	ALA	2.5
1	A	157	LEU	2.5
1	C	117	LYS	2.4
1	A	254	LEU	2.4
1	A	215	GLY	2.4
1	D	210	ALA	2.4
1	D	220	ALA	2.4
1	B	91	THR	2.4
1	D	143	ARG	2.4
1	D	158	ARG	2.4
1	C	94	ASP	2.4
1	B	102	LEU	2.4
1	C	157	LEU	2.4
1	D	285	ALA	2.4
1	D	275	PRO	2.4
1	D	254	LEU	2.4
1	A	212	ILE	2.4
1	D	103	LYS	2.3
1	D	310	ASP	2.3
1	D	177	LEU	2.3
1	B	253	LEU	2.3
1	D	188	HIS	2.3
1	D	187	ILE	2.3
1	D	280	ALA	2.3
1	C	301	LEU	2.3
1	D	243	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	2.3
1	D	261	SER	2.3
1	B	114	TYR	2.3
1	D	288	ARG	2.3
1	A	137	VAL	2.3
1	D	316	SER	2.3
1	D	231	ALA	2.2
1	D	147	ASP	2.2
1	D	95	TRP	2.2
1	D	105	LEU	2.2
1	A	132	ALA	2.2
1	D	109	GLN	2.2
1	B	137	VAL	2.2
1	D	290	TRP	2.2
1	C	285	ALA	2.2
1	D	287	LEU	2.2
1	B	325	ALA	2.2
1	D	168	ALA	2.2
1	B	284	LEU	2.1
1	A	168	ALA	2.1
1	A	227	VAL	2.1
1	D	304	CYS	2.1
1	D	205	CYS	2.1
1	A	267	ILE	2.1
1	B	112	GLU	2.1
1	D	267	ILE	2.1
1	A	307	LEU	2.1
1	A	104	GLY	2.0
1	C	178	LEU	2.0
1	A	107	ASP	2.0
1	D	312	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

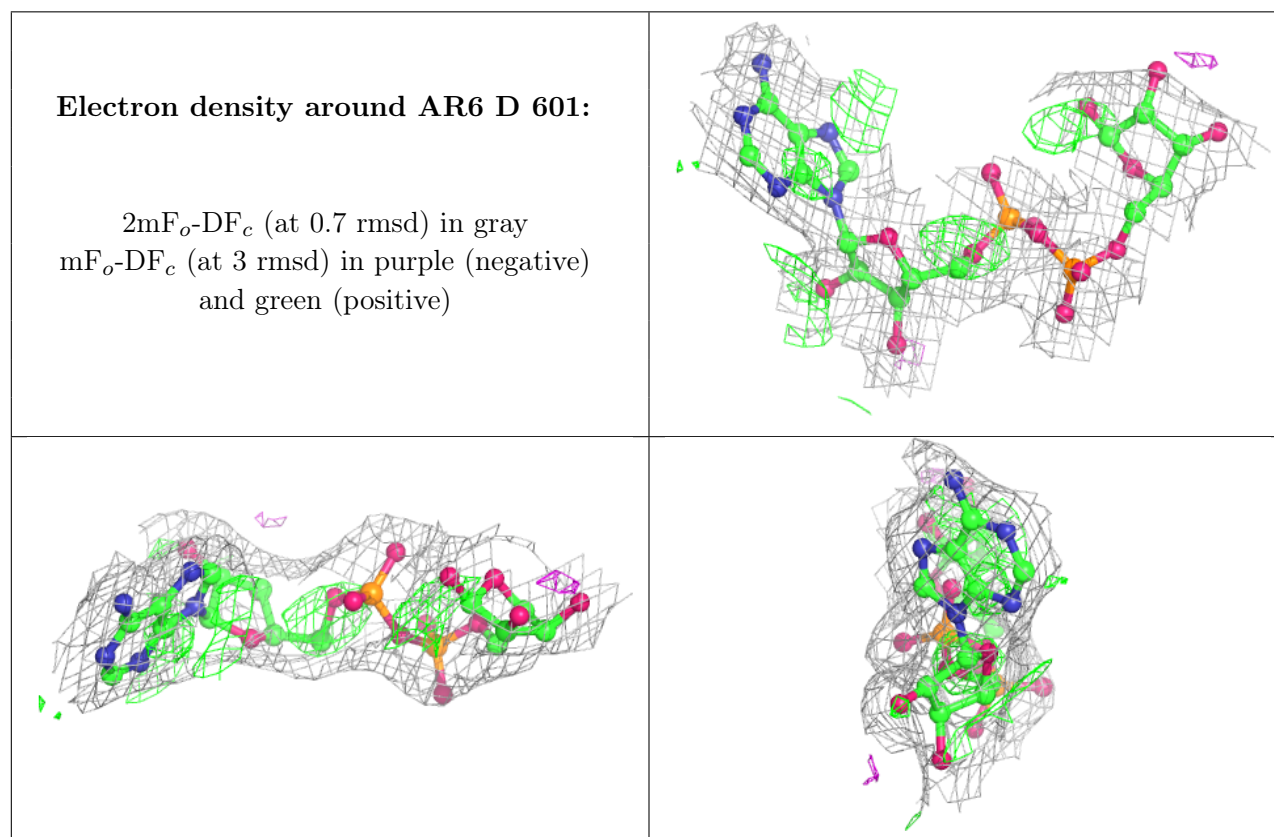
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

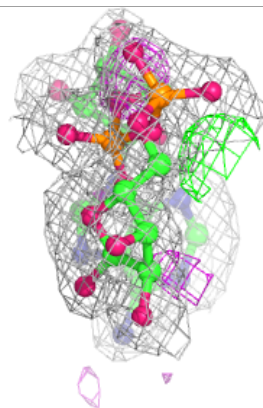
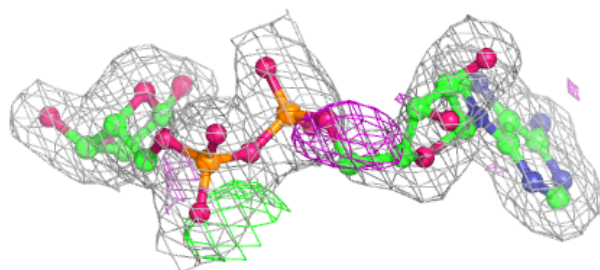
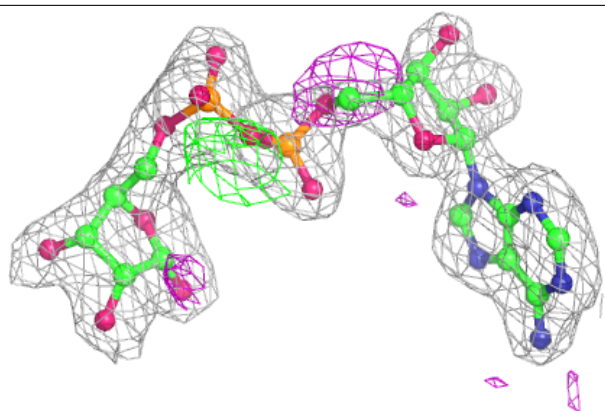
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AR6	D	601	36/36	0.88	0.19	77,83,89,90	0
2	AR6	C	601	36/36	0.94	0.15	26,30,34,43	0
2	AR6	B	601	36/36	0.94	0.15	26,30,33,42	0
2	AR6	A	601	36/36	0.94	0.16	24,29,33,41	0

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.

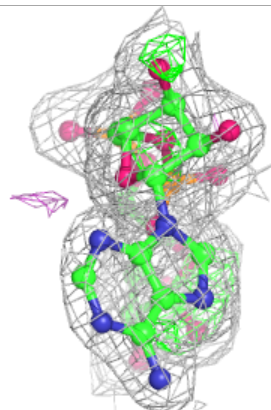
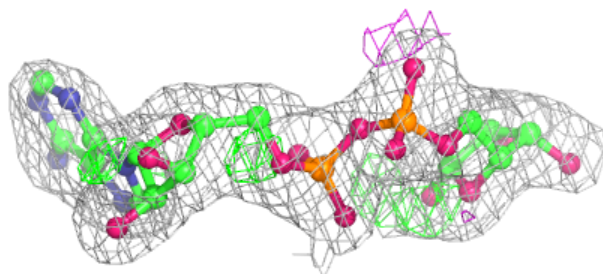
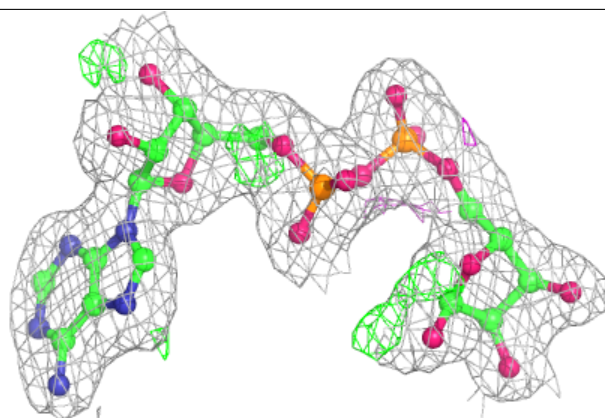


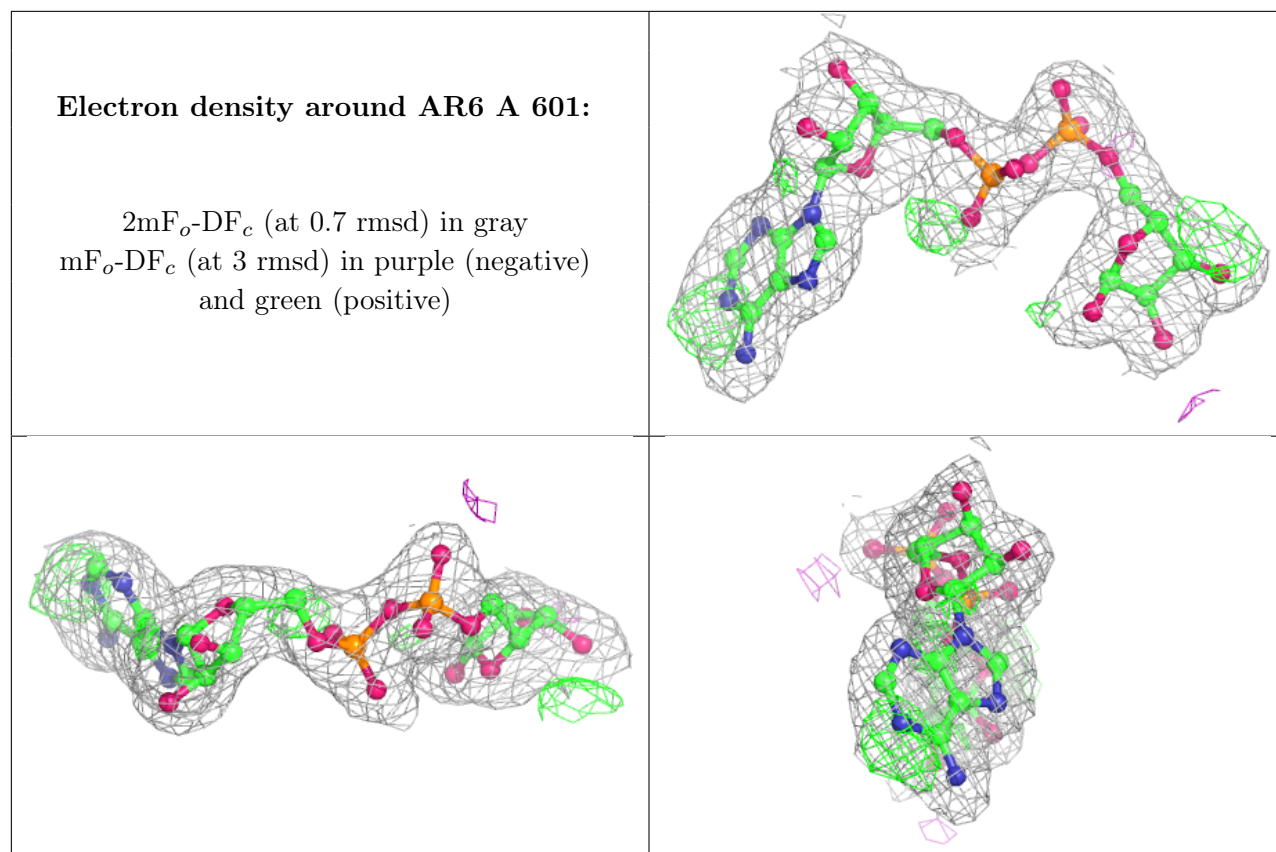
Electron density around AR6 C 601:

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

**Electron density around AR6 B 601:**

$2mF_o-DF_c$ (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.