



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 8DMU / pdb_00008dmu
Title : Crystal structure of macrodomain CG3568 from *Drosophila melanogaster* in complex with ADP-ribose
Authors : Zhang, Z.; Das, C.
Deposited on : 2022-07-08
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 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

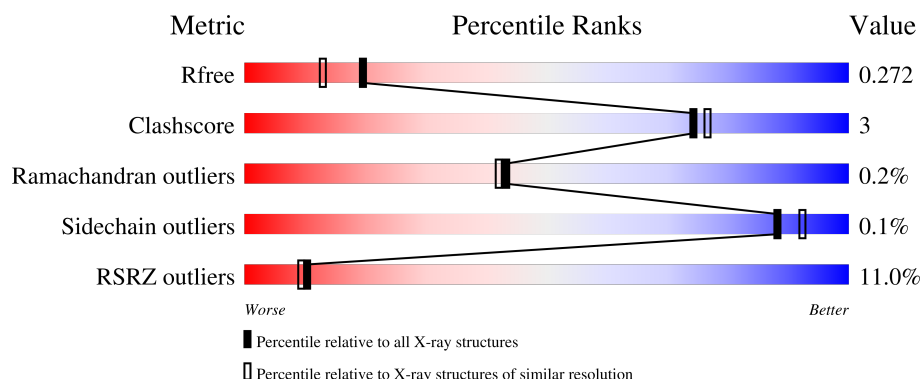
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	489	4% 91% 7%
1	B	489	7% 92% 6%
1	C	489	17% 87% 10%
1	D	489	15% 90% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	608	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16466 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.

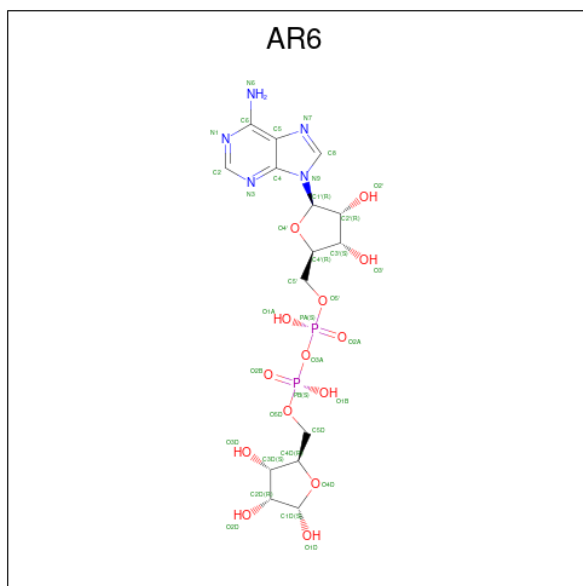
- Molecule 1 is a protein called CG3568.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3715	2355	655	689	16			
1	B	476	Total	C	N	O	S	0	0	0
			3720	2361	654	689	16			
1	C	474	Total	C	N	O	S	0	1	0
			3702	2340	654	692	16			
1	D	475	Total	C	N	O	S	0	0	0
			3717	2352	658	691	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q9W4J9
A	21	PRO	-	expression tag	UNP Q9W4J9
A	22	LEU	-	expression tag	UNP Q9W4J9
A	23	GLY	-	expression tag	UNP Q9W4J9
A	24	SER	-	expression tag	UNP Q9W4J9
B	20	GLY	-	expression tag	UNP Q9W4J9
B	21	PRO	-	expression tag	UNP Q9W4J9
B	22	LEU	-	expression tag	UNP Q9W4J9
B	23	GLY	-	expression tag	UNP Q9W4J9
B	24	SER	-	expression tag	UNP Q9W4J9
C	20	GLY	-	expression tag	UNP Q9W4J9
C	21	PRO	-	expression tag	UNP Q9W4J9
C	22	LEU	-	expression tag	UNP Q9W4J9
C	23	GLY	-	expression tag	UNP Q9W4J9
C	24	SER	-	expression tag	UNP Q9W4J9
D	20	GLY	-	expression tag	UNP Q9W4J9
D	21	PRO	-	expression tag	UNP Q9W4J9
D	22	LEU	-	expression tag	UNP Q9W4J9
D	23	GLY	-	expression tag	UNP Q9W4J9
D	24	SER	-	expression tag	UNP Q9W4J9

- 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 (CCD ID: AR6) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
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 NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

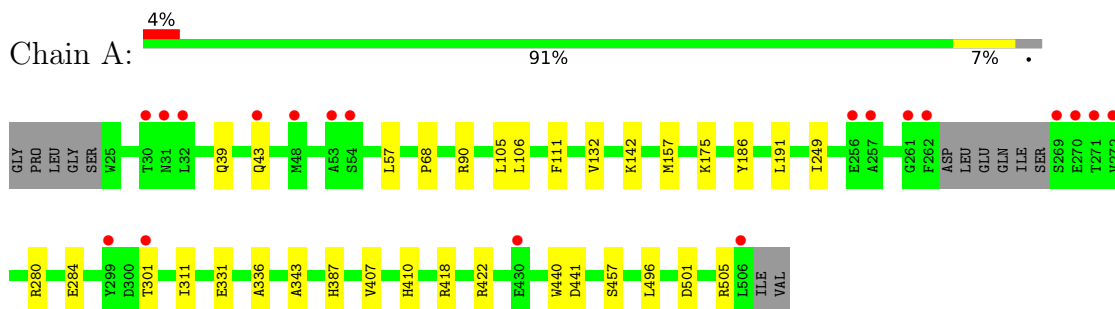
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	377	Total	O	0	0
			377	377		
6	C	312	Total	O	0	0
			312	312		
6	D	342	Total	O	0	0
			342	342		

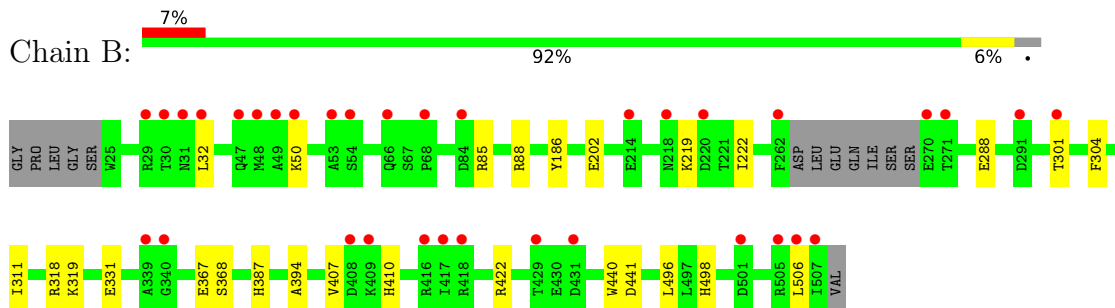
3 Residue-property plots

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.

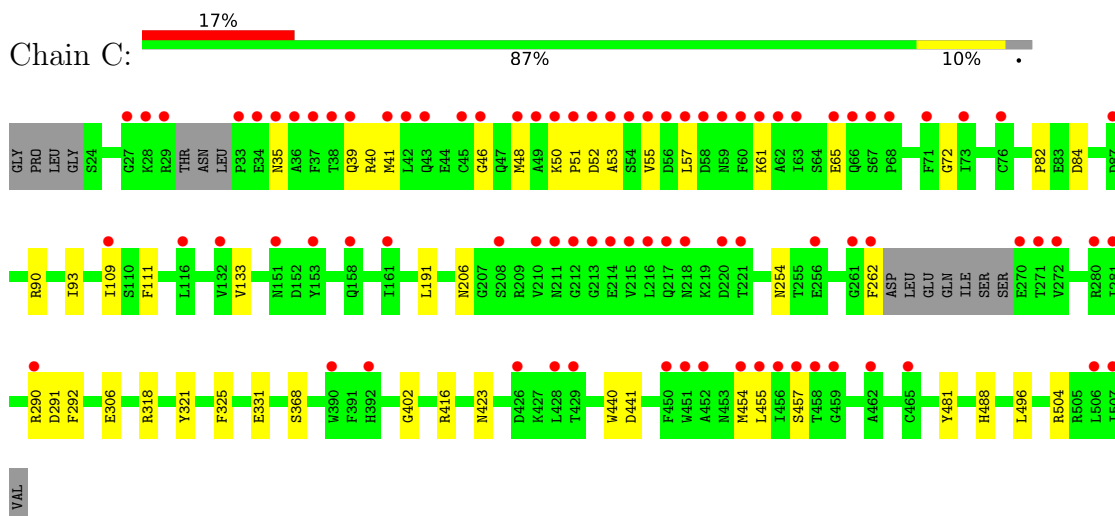
• Molecule 1: CG3568



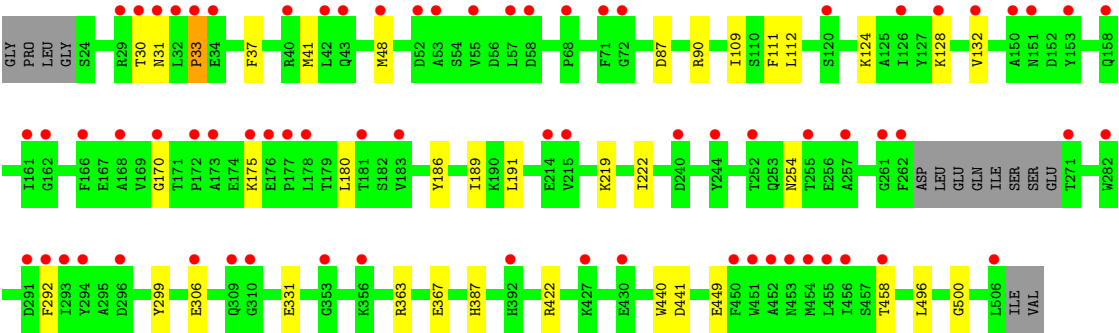
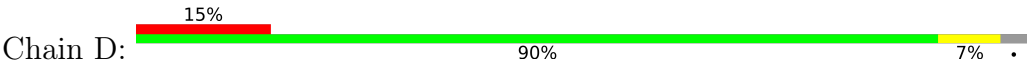
• Molecule 1: CG3568



• Molecule 1: CG3568



● Molecule 1: CG3568



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.05Å 129.81Å 199.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.25 – 2.00 92.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (92.25-2.00) 99.9 (92.25-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.232 , 0.273 0.234 , 0.272	Depositor DCC
R_{free} test set	9004 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16466	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6160e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NI, AR6, CL

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	0.38	0/3801	0.55	0/5159
1	B	0.40	0/3806	0.57	0/5164
1	C	0.35	0/3785	0.56	0/5134
1	D	0.39	0/3802	0.58	0/5157
All	All	0.38	0/15194	0.57	0/20614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3564	20	0
1	B	3720	0	3584	16	0
1	C	3702	0	3543	30	0
1	D	3717	0	3577	27	0
2	A	36	0	21	0	0
2	B	36	0	21	0	0
2	C	36	0	21	0	0
2	D	36	0	21	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	3	0
5	D	1	0	0	0	0
6	A	379	0	0	3	0
6	B	377	0	0	6	0
6	C	312	0	0	2	0
6	D	342	0	0	1	0
All	All	16466	0	14352	92	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 3.

All (92) 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)
5:B:608:CL:CL	6:B:961:HOH:O	2.23	0.92
1:C:50:LYS:HG3	1:C:51:PRO:HD2	1.60	0.83
1:C:50:LYS:HE2	1:C:488:HIS:CE1	2.21	0.76
5:B:608:CL:CL	6:B:1071:HOH:O	2.41	0.74
1:B:331:GLU:HA	1:B:496:LEU:HD13	1.76	0.67
1:C:46:GLY:O	1:C:504:ARG:NH1	2.29	0.65
1:A:407:VAL:HB	1:A:410:HIS:HB2	1.83	0.61
1:A:331:GLU:HA	1:A:496:LEU:HD13	1.83	0.61
1:C:50:LYS:HE2	1:C:488:HIS:HE1	1.62	0.60
1:A:142:LYS:NZ	6:A:706:HOH:O	2.34	0.59
1:A:175:LYS:HB3	6:A:743:HOH:O	2.03	0.58
1:D:331:GLU:HA	1:D:496:LEU:HD13	1.87	0.57
1:D:41:MET:HE1	1:D:112:LEU:HD12	1.87	0.57
1:D:387:HIS:CE1	1:D:422:ARG:HD2	2.39	0.57
1:D:219:LYS:HD3	1:D:222:ILE:HD11	1.87	0.56
1:B:85:ARG:NH2	1:B:202:GLU:OE1	2.39	0.56
1:C:40:ARG:NH2	6:C:708:HOH:O	2.38	0.56
1:D:37:PHE:CE1	1:D:41:MET:HE2	2.40	0.56
1:B:387:HIS:CE1	1:B:422:ARG:HD2	2.41	0.56
1:D:41:MET:HE3	1:D:109:ILE:HG12	1.88	0.56
1:B:219:LYS:HD3	1:B:222:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:O	1:A:284:GLU:HG3	2.06	0.55
1:A:311:ILE:HD11	1:D:299:TYR:CE2	2.41	0.55
1:C:50:LYS:CG	1:C:51:PRO:HD2	2.35	0.55
1:D:37:PHE:HE1	1:D:41:MET:HE2	1.73	0.53
1:C:65:GLU:HG3	6:C:713:HOH:O	2.07	0.53
1:B:50:LYS:HE2	1:B:498:HIS:HB2	1.88	0.53
1:C:440:TRP:CG	1:C:441:ASP:H	2.26	0.53
1:C:331:GLU:HA	1:C:496:LEU:HD13	1.90	0.53
1:D:31:ASN:C	1:D:33:PRO:HD3	2.34	0.53
1:D:170:GLY:HA2	1:D:180:LEU:HD22	1.90	0.53
1:D:124:LYS:O	1:D:128:LYS:HG2	2.09	0.52
1:A:418:ARG:NE	6:A:705:HOH:O	2.34	0.52
1:A:501:ASP:O	1:A:505:ARG:HG3	2.10	0.52
1:D:41:MET:HE3	1:D:109:ILE:HG23	1.91	0.52
1:B:318:ARG:HG3	1:B:368:SER:HB2	1.91	0.52
1:A:440:TRP:CG	1:A:441:ASP:H	2.27	0.52
1:C:402:GLY:O	1:C:416:ARG:NH1	2.43	0.51
1:A:387:HIS:CE1	1:A:422:ARG:HD2	2.46	0.50
1:B:440:TRP:CG	1:B:441:ASP:H	2.28	0.50
1:D:87:ASP:OD1	1:D:90:ARG:NH2	2.45	0.50
1:B:32:LEU:HD21	1:B:506:LEU:HD13	1.95	0.49
5:B:608:CL:CL	6:B:1017:HOH:O	2.57	0.49
1:B:407:VAL:HB	1:B:410:HIS:HB2	1.93	0.49
1:C:48:MET:SD	1:C:133:VAL:HG21	2.53	0.49
1:D:363:ARG:O	1:D:367:GLU:HG3	2.12	0.49
1:C:41:MET:HG3	1:C:109:ILE:HG23	1.95	0.49
1:D:440:TRP:CG	1:D:441:ASP:H	2.31	0.48
1:C:318:ARG:HG3	1:C:368:SER:HB2	1.95	0.48
1:C:52:ASP:O	1:C:481:TYR:CE1	2.67	0.48
1:A:249:ILE:HB	1:A:311:ILE:HB	1.96	0.47
1:D:124:LYS:HB3	1:D:128:LYS:HE2	1.95	0.47
1:B:288:GLU:OE1	1:B:319:LYS:NZ	2.43	0.47
1:A:336:ALA:HB2	1:A:343:ALA:HB2	1.97	0.47
1:D:48:MET:HB2	1:D:500:GLY:CA	2.45	0.47
1:C:52:ASP:O	1:C:481:TYR:OH	2.33	0.47
1:C:72:GLY:HA3	1:C:455:LEU:HD21	1.97	0.47
1:D:111:PHE:CG	1:D:191:LEU:HD11	2.49	0.47
1:D:186:TYR:HA	1:D:189:ILE:HD12	1.97	0.46
1:C:35:ASN:O	1:C:39:GLN:HG3	2.14	0.46
1:A:57:LEU:H	1:A:90:ARG:NH1	2.13	0.46
1:C:55:VAL:HG11	1:C:93:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:O	1:A:43:GLN:HG2	2.16	0.46
1:A:301:THR:HG23	1:D:306:GLU:OE2	2.16	0.46
1:D:449:GLU:OE1	1:D:458:THR:OG1	2.28	0.45
1:D:124:LYS:O	1:D:128:LYS:HE2	2.17	0.44
1:D:254:ASN:HB3	1:D:292:PHE:O	2.16	0.44
1:C:262:PHE:H	1:C:291:ASP:HB2	1.81	0.44
1:D:175:LYS:HE3	6:D:765:HOH:O	2.16	0.44
1:B:394:ALA:O	6:B:701:HOH:O	2.21	0.44
1:C:111:PHE:CG	1:C:191:LEU:HD11	2.53	0.43
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.77	0.43
1:D:48:MET:HB2	1:D:500:GLY:HA3	1.99	0.43
1:A:111:PHE:CG	1:A:191:LEU:HD11	2.53	0.43
1:C:57:LEU:HD13	1:C:90:ARG:HG3	2.01	0.43
1:C:206:ASN:O	1:C:423:ASN:HB3	2.18	0.43
1:C:321:TYR:HB3	1:C:325:PHE:CE2	2.53	0.43
1:C:57:LEU:HG	1:C:61:LYS:NZ	2.34	0.42
1:B:304:PHE:HB3	1:B:311:ILE:CG2	2.50	0.42
1:C:82:PRO:HB2	1:C:84:ASP:OD1	2.18	0.42
1:A:105:LEU:HD11	1:A:132:VAL:HG11	2.00	0.42
1:C:53:ALA:O	1:C:55:VAL:HG23	2.19	0.42
1:C:290:ARG:NH1	1:C:292:PHE:CE1	2.88	0.41
1:D:41:MET:SD	1:D:132:VAL:HG22	2.61	0.41
1:A:301:THR:HG23	1:D:306:GLU:CD	2.46	0.41
1:A:68:PRO:HG2	1:A:157:MET:HE1	2.02	0.41
1:B:85:ARG:HD2	1:B:85:ARG:HA	1.89	0.41
1:B:367:GLU:OE1	6:B:702:HOH:O	2.22	0.41
1:B:301:THR:HG23	1:C:306:GLU:OE1	2.21	0.40
1:B:88:ARG:NH2	6:B:714:HOH:O	2.44	0.40
1:C:254:ASN:HB3	1:C:292:PHE:O	2.22	0.40
1:C:454:MET:HE2	1:C:454:MET:HB3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	472/489 (96%)	454 (96%)	17 (4%)	1 (0%)	43	42
1	B	472/489 (96%)	456 (97%)	16 (3%)	0	100	100
1	C	469/489 (96%)	445 (95%)	23 (5%)	1 (0%)	43	42
1	D	471/489 (96%)	451 (96%)	18 (4%)	2 (0%)	30	27
All	All	1884/1956 (96%)	1806 (96%)	74 (4%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	33	PRO
1	C	457	SER
1	A	457	SER
1	D	30	THR

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	383/414 (92%)	382 (100%)	1 (0%)	86	91
1	B	385/414 (93%)	384 (100%)	1 (0%)	86	91
1	C	382/414 (92%)	382 (100%)	0	100	100
1	D	385/414 (93%)	385 (100%)	0	100	100
All	All	1535/1656 (93%)	1533 (100%)	2 (0%)	88	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	TYR
1	B	186	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	160	ASN
1	A	480	HIS
1	B	160	ASN
1	B	392	HIS
1	B	480	HIS
1	C	39	GLN
1	C	160	ASN
1	C	423	ASN
1	D	47	GLN
1	D	66	GLN
1	D	160	ASN
1	D	494	HIS

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](#)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 for Mogul analysis.

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
4	SO4	A	605	-	4,4,4	0.38	0	6,6,6	0.31	0
2	AR6	D	601	-	39,39,39	0.54	0	56,60,60	0.60	0
4	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.16	0
4	SO4	B	603	-	4,4,4	0.35	0	6,6,6	0.31	0
2	AR6	C	601	-	39,39,39	0.54	0	56,60,60	0.64	0
4	SO4	B	605	-	4,4,4	0.31	0	6,6,6	0.33	0
4	SO4	C	603	-	4,4,4	0.20	0	6,6,6	0.38	0
2	AR6	B	601	-	39,39,39	0.60	1 (2%)	56,60,60	0.63	0
4	SO4	B	604	-	4,4,4	0.27	0	6,6,6	0.06	0
4	SO4	D	603	-	4,4,4	0.29	0	6,6,6	0.39	0
4	SO4	C	602	-	4,4,4	0.26	0	6,6,6	0.38	0
4	SO4	D	602	-	4,4,4	0.30	0	6,6,6	0.26	0
2	AR6	A	601	-	39,39,39	0.57	0	56,60,60	0.65	0
4	SO4	A	603	-	4,4,4	0.29	0	6,6,6	0.12	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	C	601	-	-	3/22/54/54	0/4/4/4
2	AR6	A	601	-	-	2/22/54/54	0/4/4/4
2	AR6	D	601	-	-	4/22/54/54	0/4/4/4
2	AR6	B	601	-	-	2/22/54/54	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	AR6	PA-O3A	2.04	1.61	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	AR6	C2'-C1'-N9-C4
2	A	601	AR6	C2'-C1'-N9-C8
2	B	601	AR6	C2'-C1'-N9-C4
2	B	601	AR6	C2'-C1'-N9-C8

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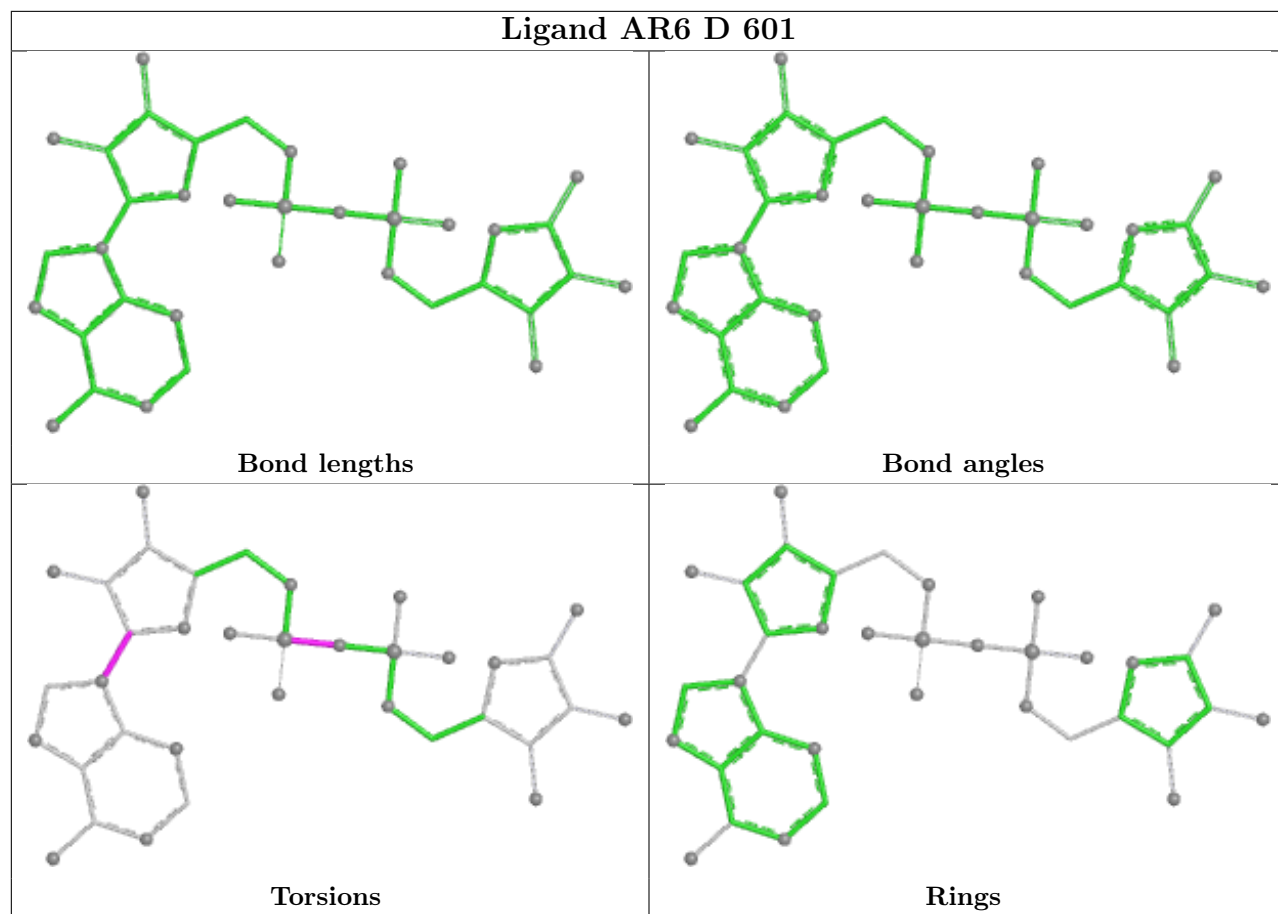
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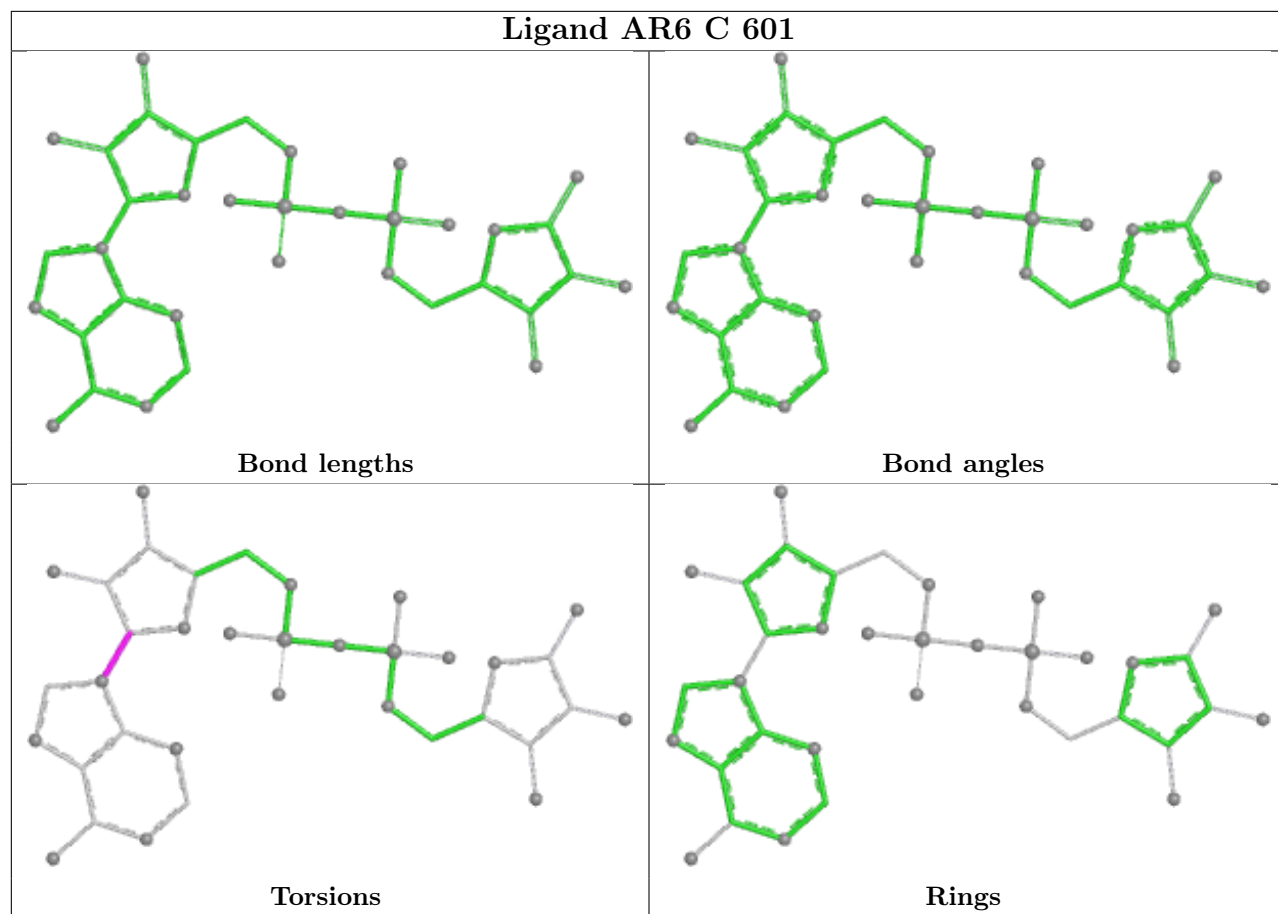
Mol	Chain	Res	Type	Atoms
2	C	601	AR6	C2'-C1'-N9-C8
2	D	601	AR6	C2'-C1'-N9-C8
2	C	601	AR6	C2'-C1'-N9-C4
2	D	601	AR6	C2'-C1'-N9-C4
2	D	601	AR6	PB-O3A-PA-O2A
2	D	601	AR6	PB-O3A-PA-O1A
2	C	601	AR6	O4'-C1'-N9-C8

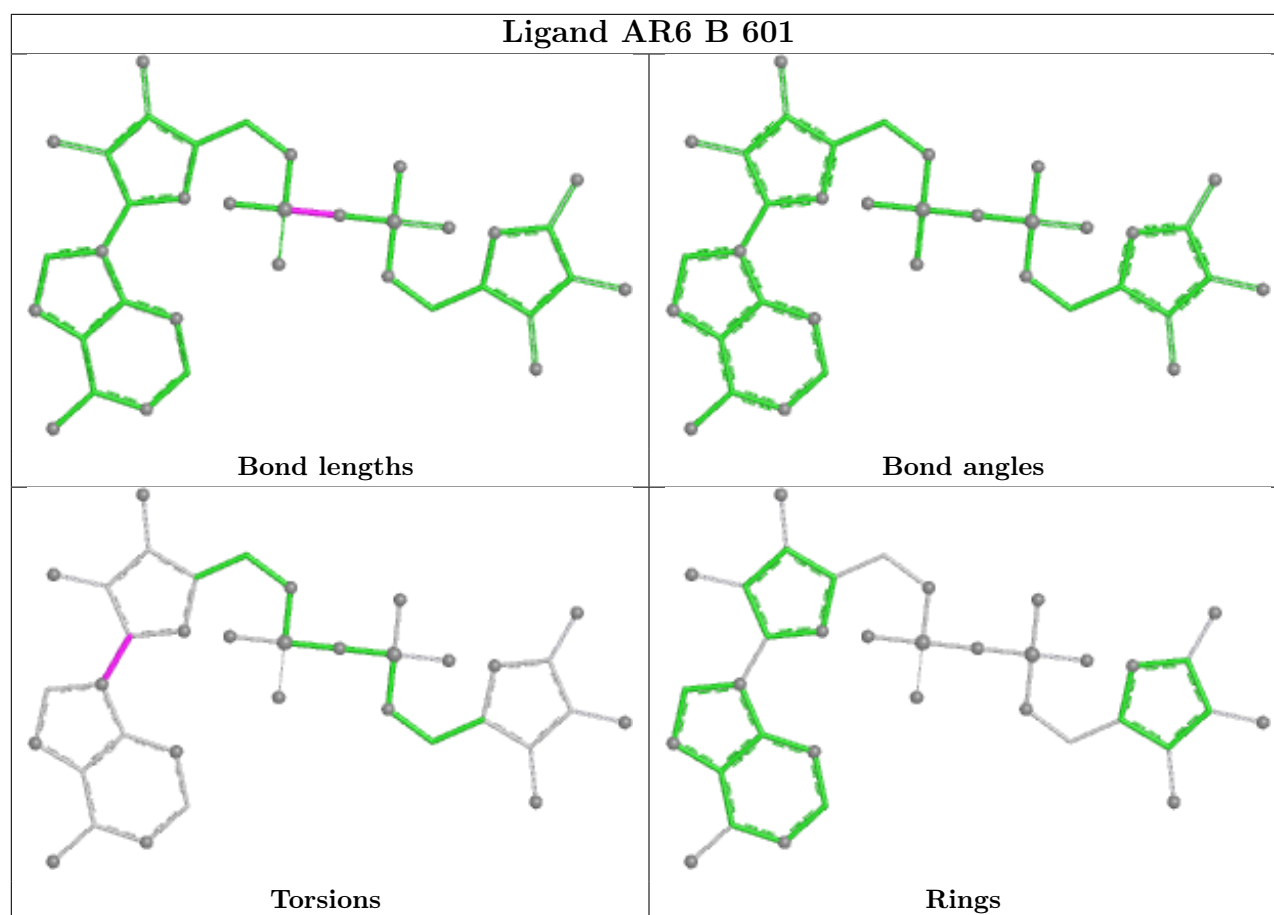
There are no ring outliers.

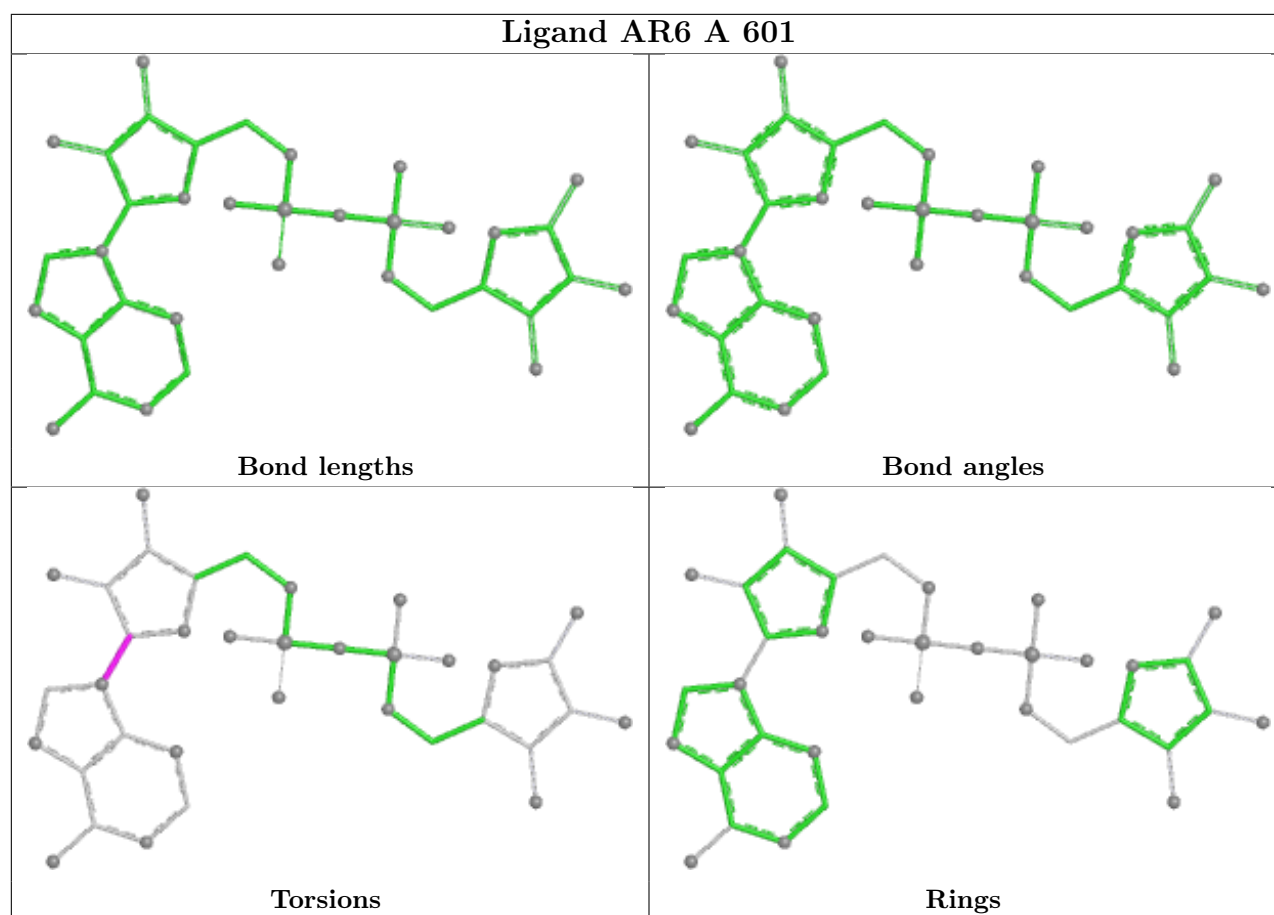
No monomer is involved in short contacts.

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	476/489 (97%)	0.08	19 (3%)	42 41	17, 27, 44, 86	0
1	B	476/489 (97%)	0.21	34 (7%)	22 20	17, 27, 45, 66	0
1	C	474/489 (96%)	0.98	85 (17%)	3 3	21, 36, 62, 94	1 (0%)
1	D	475/489 (97%)	0.95	72 (15%)	5 5	20, 32, 50, 96	0
All	All	1901/1956 (97%)	0.56	210 (11%)	10 9	17, 30, 52, 96	1 (0%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	11.5
1	D	33	PRO	8.3
1	C	54	SER	7.2
1	D	32	LEU	7.1
1	C	262	PHE	7.0
1	C	55	VAL	6.9
1	C	52	ASP	6.8
1	B	507	ILE	6.7
1	C	507	ILE	6.6
1	D	31	ASN	5.8
1	C	270	GLU	5.7
1	C	33	PRO	5.4
1	A	261	GLY	5.3
1	D	271	THR	5.2
1	A	269	SER	5.0
1	D	30	THR	4.9
1	A	262	PHE	4.9
1	D	262	PHE	4.8
1	C	271	THR	4.7
1	B	32	LEU	4.6
1	C	73	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	456	ILE	4.5
1	A	271	THR	4.3
1	D	452	ALA	4.3
1	D	261	GLY	4.3
1	B	31	ASN	4.2
1	C	261	GLY	4.1
1	C	29	ARG	4.0
1	D	72	GLY	4.0
1	B	270	GLU	4.0
1	C	63	ILE	4.0
1	C	34	GLU	3.9
1	C	217	GLN	3.9
1	B	271	THR	3.8
1	A	301	THR	3.8
1	C	218	ASN	3.7
1	D	53	ALA	3.7
1	C	454	MET	3.7
1	A	270	GLU	3.7
1	C	452	ALA	3.7
1	C	506	LEU	3.7
1	A	32	LEU	3.6
1	D	177	PRO	3.6
1	B	431	ASP	3.6
1	A	53	ALA	3.6
1	B	53	ALA	3.6
1	D	162	GLY	3.6
1	D	128	LYS	3.6
1	D	48	MET	3.6
1	C	49	ALA	3.6
1	D	68	PRO	3.6
1	D	126	ILE	3.6
1	C	28	LYS	3.6
1	C	210	VAL	3.5
1	C	51	PRO	3.5
1	D	506	LEU	3.5
1	B	49	ALA	3.5
1	C	37	PHE	3.5
1	C	62	ALA	3.5
1	C	48	MET	3.5
1	B	501	ASP	3.4
1	C	59	ASN	3.4
1	B	301	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	3.4
1	C	56	ASP	3.4
1	D	293	ILE	3.3
1	B	47	GLN	3.3
1	B	30	THR	3.3
1	A	54	SER	3.2
1	C	220	ASP	3.2
1	D	450	PHE	3.2
1	C	35	ASN	3.2
1	A	272	VAL	3.1
1	C	216	LEU	3.1
1	C	256	GLU	3.1
1	D	214	GLU	3.1
1	A	30	THR	3.1
1	D	158	GLN	3.1
1	C	457	SER	3.1
1	C	46	GLY	3.0
1	B	48	MET	3.0
1	C	272	VAL	3.0
1	D	455	LEU	3.0
1	B	54	SER	3.0
1	C	455	LEU	2.9
1	B	409	LYS	2.9
1	C	50	LYS	2.9
1	C	57	LEU	2.9
1	C	66	GLN	2.9
1	B	68	PRO	2.9
1	B	262	PHE	2.9
1	C	67	SER	2.9
1	D	451	TRP	2.9
1	C	39	GLN	2.8
1	C	429	THR	2.8
1	C	450	PHE	2.8
1	D	150	ALA	2.8
1	A	506	LEU	2.8
1	A	256	GLU	2.8
1	B	291	ASP	2.8
1	D	456	ILE	2.8
1	D	240	ASP	2.8
1	D	161	ILE	2.8
1	C	462	ALA	2.7
1	C	41	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	175	LYS	2.7
1	D	40	ARG	2.7
1	D	172	PRO	2.7
1	C	65	GLU	2.7
1	B	50	LYS	2.7
1	B	506	LEU	2.7
1	C	87	ASP	2.7
1	C	42	LEU	2.6
1	C	58	ASP	2.6
1	D	244	TYR	2.6
1	C	465	CYS	2.6
1	B	418	ARG	2.6
1	D	257	ALA	2.6
1	D	151	ASN	2.6
1	D	132	VAL	2.6
1	C	76	CYS	2.6
1	D	252	THR	2.6
1	B	408	ASP	2.6
1	B	29	ARG	2.5
1	D	291	ASP	2.5
1	D	168	ALA	2.5
1	C	158	GLN	2.5
1	D	43	GLN	2.5
1	D	173	ALA	2.5
1	D	57	LEU	2.5
1	D	178	LEU	2.5
1	D	454	MET	2.5
1	C	27	GLY	2.5
1	D	294	TYR	2.4
1	C	151	ASN	2.4
1	D	306	GLU	2.4
1	B	429	THR	2.4
1	C	221	THR	2.4
1	B	416	ARG	2.4
1	C	290	ARG	2.4
1	D	29	ARG	2.4
1	D	427	LYS	2.4
1	A	299	TYR	2.4
1	B	340	GLY	2.4
1	D	292	PHE	2.4
1	C	208[A]	SER	2.4
1	A	48	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	280	ARG	2.3
1	D	71	PHE	2.3
1	B	417	ILE	2.3
1	C	214	GLU	2.3
1	A	43	GLN	2.3
1	A	31	ASN	2.3
1	C	116	LEU	2.3
1	A	430	GLU	2.3
1	D	176	GLU	2.3
1	C	38	THR	2.3
1	C	458	THR	2.3
1	D	181	THR	2.3
1	C	215	VAL	2.3
1	D	170	GLY	2.3
1	D	42	LEU	2.3
1	D	153	TYR	2.3
1	B	214	GLU	2.2
1	D	120	SER	2.2
1	C	212	GLY	2.2
1	D	310	GLY	2.2
1	D	282	TRP	2.2
1	D	166	PHE	2.2
1	C	68	PRO	2.2
1	D	255	THR	2.2
1	D	356	LYS	2.2
1	B	84	ASP	2.2
1	D	55	VAL	2.2
1	D	215	VAL	2.2
1	C	36	ALA	2.2
1	C	45	CYS	2.2
1	C	451	TRP	2.2
1	C	109	ILE	2.1
1	C	161	ILE	2.1
1	C	281	ILE	2.1
1	D	34	GLU	2.1
1	D	183	VAL	2.1
1	C	43	GLN	2.1
1	C	392	HIS	2.1
1	B	66	GLN	2.1
1	C	60	PHE	2.1
1	B	505	ARG	2.1
1	D	458	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	459	GLY	2.1
1	C	71	PHE	2.1
1	C	390	TRP	2.1
1	C	61	LYS	2.1
1	B	339	ALA	2.1
1	C	428	LEU	2.1
1	B	218	ASN	2.1
1	D	453	ASN	2.1
1	B	220	ASP	2.1
1	D	296	ASP	2.1
1	D	353	GLY	2.1
1	C	211	ASN	2.0
1	C	426	ASP	2.0
1	D	58	ASP	2.0
1	D	430	GLU	2.0
1	A	257	ALA	2.0
1	D	309	GLN	2.0
1	D	52	ASP	2.0
1	D	392	HIS	2.0
1	C	213	GLY	2.0
1	C	153	TYR	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
4	SO4	D	603	5/5	0.82	0.15	45,48,59,64	0
4	SO4	C	603	5/5	0.88	0.11	47,49,55,61	0

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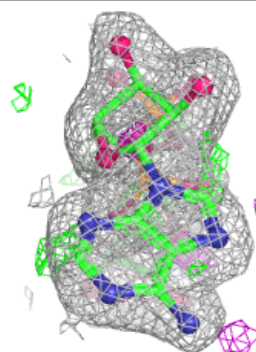
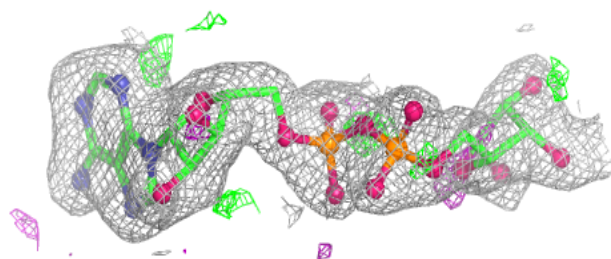
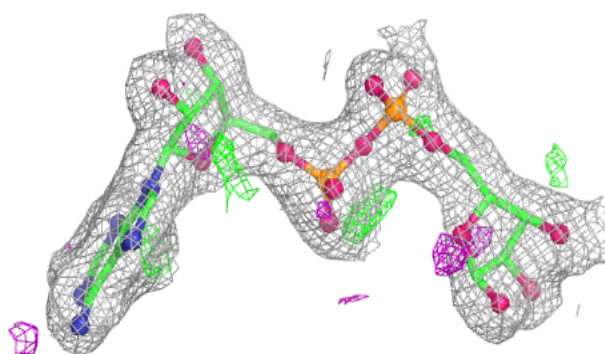
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	604	5/5	0.91	0.07	50,52,62,68	0
4	SO4	B	605	5/5	0.91	0.18	44,48,50,55	0
4	SO4	A	603	5/5	0.91	0.07	53,57,63,68	0
4	SO4	B	603	5/5	0.91	0.24	34,42,49,50	0
4	SO4	A	605	5/5	0.92	0.14	36,41,46,47	0
5	CL	B	607	1/1	0.93	0.14	39,39,39,39	0
5	CL	B	608	1/1	0.93	0.09	52,52,52,52	0
2	AR6	D	601	36/36	0.94	0.10	26,31,33,37	0
4	SO4	A	604	5/5	0.95	0.17	32,39,48,50	0
2	AR6	C	601	36/36	0.95	0.09	29,33,42,42	0
4	SO4	D	602	5/5	0.95	0.13	30,32,36,41	0
5	CL	B	606	1/1	0.96	0.09	53,53,53,53	0
4	SO4	C	602	5/5	0.96	0.16	32,35,37,41	0
5	CL	A	607	1/1	0.96	0.17	55,55,55,55	0
5	CL	A	606	1/1	0.97	0.12	53,53,53,53	0
5	CL	D	604	1/1	0.97	0.15	55,55,55,55	0
2	AR6	A	601	36/36	0.98	0.05	19,23,27,28	0
2	AR6	B	601	36/36	0.98	0.05	19,22,29,30	0
3	NI	A	602	1/1	0.99	0.03	29,29,29,29	0
3	NI	B	602	1/1	0.99	0.05	24,24,24,24	0

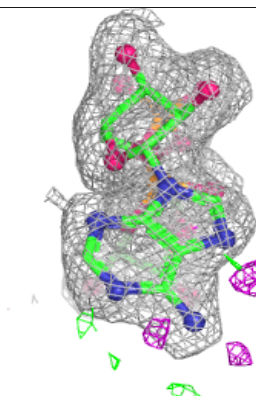
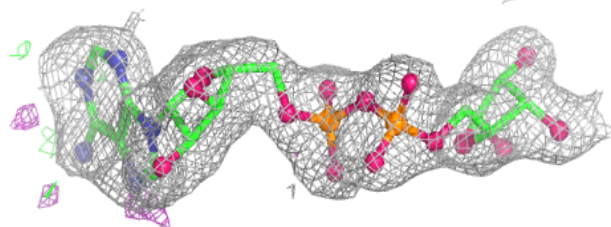
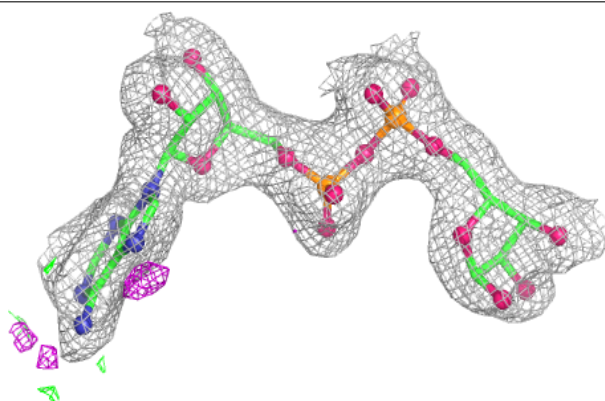
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AR6 D 601:

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

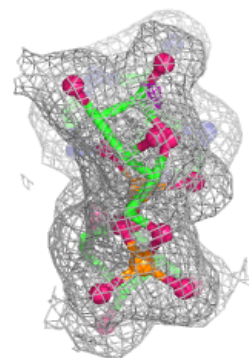
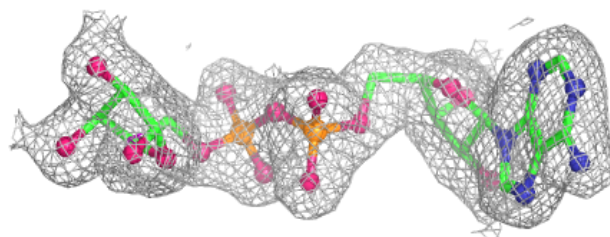
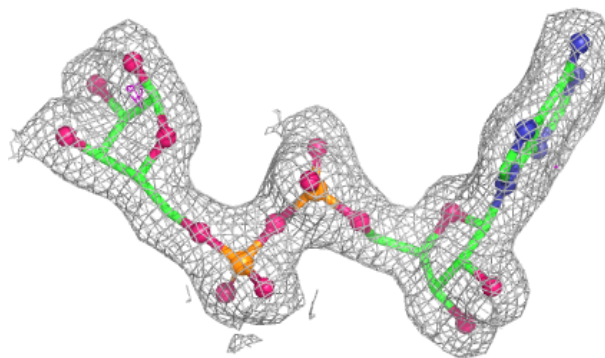
**Electron density around AR6 C 601:**

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

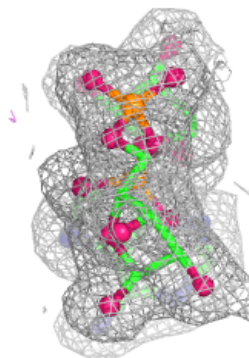
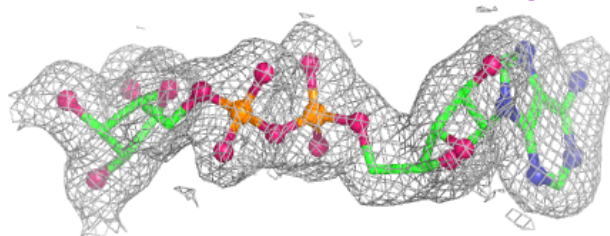
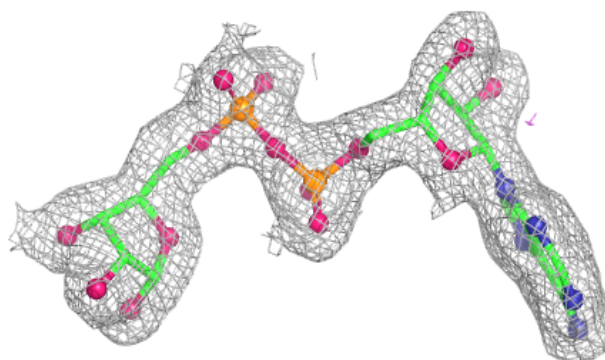


Electron density around AR6 A 601:

$2mF_o-DF_c$ (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.