



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 06:05 PM EDT

PDB ID : 7L9H
Title : Crystal structure of human ARH3-D77A bound to magnesium and ADP-ribose
Authors : Pourfarjam, Y.; Kurinov, I.; Moss, J.; Kim, I.K.
Deposited on : 2021-01-04
Resolution : 1.85 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 : 2.18
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) : 2.18

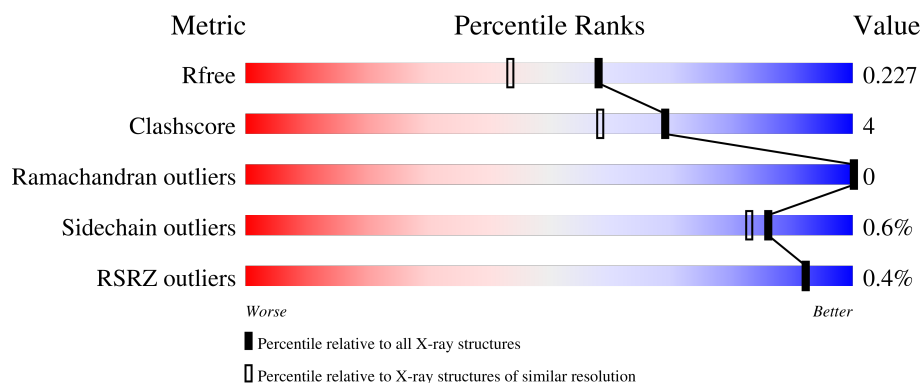
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	366	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 86%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 86% 5% 9% </div> </div>
1	B	366	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 83%, yellow 7%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 83% 7% 10% </div> </div>
1	C	366	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 85%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 7% 8% </div> </div>
1	D	366	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 84%, yellow 6%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 6% 9% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20332 atoms, of which 9430 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.

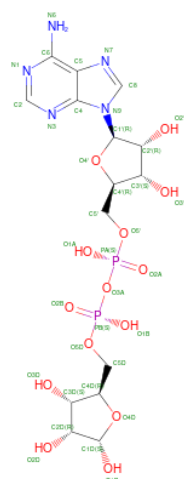
- Molecule 1 is a protein called ADP-ribose glycohydrolase ARH3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	336	Total	C	H	N	O	S	0	0	0
			4907	1567	2408	427	491	14			
1	D	334	Total	C	H	N	O	S	0	0	0
			4831	1557	2353	423	484	14			
1	A	334	Total	C	H	N	O	S	0	0	0
			4767	1540	2317	415	481	14			
1	B	331	Total	C	H	N	O	S	0	0	0
			4690	1522	2272	411	472	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9NX46
C	-1	PRO	-	expression tag	UNP Q9NX46
C	0	HIS	-	expression tag	UNP Q9NX46
C	77	ALA	ASP	engineered mutation	UNP Q9NX46
D	-2	GLY	-	expression tag	UNP Q9NX46
D	-1	PRO	-	expression tag	UNP Q9NX46
D	0	HIS	-	expression tag	UNP Q9NX46
D	77	ALA	ASP	engineered mutation	UNP Q9NX46
A	-2	GLY	-	expression tag	UNP Q9NX46
A	-1	PRO	-	expression tag	UNP Q9NX46
A	0	HIS	-	expression tag	UNP Q9NX46
A	77	ALA	ASP	engineered mutation	UNP Q9NX46
B	-2	GLY	-	expression tag	UNP Q9NX46
B	-1	PRO	-	expression tag	UNP Q9NX46
B	0	HIS	-	expression tag	UNP Q9NX46
B	77	ALA	ASP	engineered mutation	UNP Q9NX46

- 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 depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total 56	C 15	H 20	N 5	O 14	P 2	0	0
2	D	1	Total 56	C 15	H 20	N 5	O 14	P 2	0	0
2	A	1	Total 56	C 15	H 20	N 5	O 14	P 2	0	0
2	B	1	Total 56	C 15	H 20	N 5	O 14	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	257	Total O 257 257	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	261	Total 261	O 261	0	0
4	A	209	Total 209	O 209	0	0
4	B	182	Total 182	O 182	0	0

E137	P138	M155	S165	S185	L200	L216	E220	D221	R240	S243	I271	A272	M288	T317	T320	Q341	Y346	Q361	LYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.70Å 71.61Å 115.93Å 94.24° 94.58° 107.62°	Depositor
Resolution (Å)	61.29 – 1.85 67.89 – 1.67	Depositor EDS
% Data completeness (in resolution range)	89.5 (61.29-1.85) 87.9 (67.89-1.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.180 , 0.227 0.180 , 0.227	Depositor DCC
R_{free} test set	5276 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20332	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.73 % 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 1.9603e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.54	1/2490 (0.0%)	0.66	1/3374 (0.0%)
1	B	0.55	2/2460 (0.1%)	0.69	2/3336 (0.1%)
1	C	0.57	0/2539	0.72	1/3433 (0.0%)
1	D	0.57	1/2522 (0.0%)	0.69	1/3415 (0.0%)
All	All	0.56	4/10011 (0.0%)	0.69	5/13558 (0.0%)

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	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	MET	SD-CE	-9.84	1.22	1.77
1	A	228	SER	CB-OG	7.61	1.52	1.42
1	B	185	SER	CB-OG	5.92	1.50	1.42
1	D	332	MET	CG-SD	-5.72	1.66	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	MET	CG-SD-CE	12.50	120.21	100.20
1	C	288	MET	CG-SD-CE	8.23	113.38	100.20
1	D	332	MET	CG-SD-CE	6.41	110.45	100.20
1	A	316	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	288	MET	CG-SD-CE	5.70	109.32	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	HIS	Sidechain

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	2450	2317	2316	9	0
1	B	2418	2272	2272	21	0
1	C	2499	2408	2408	23	0
1	D	2478	2353	2352	20	0
2	A	36	20	19	0	0
2	B	36	20	19	1	0
2	C	36	20	19	0	0
2	D	36	20	19	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	209	0	0	0	1
4	B	182	0	0	5	1
4	C	257	0	0	4	0
4	D	261	0	0	5	0
All	All	10902	9430	9424	71	1

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 4.

All (71) 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:B:83:ARG:NH2	4:B:502:HOH:O	2.18	0.76
1:A:30:ALA:O	1:A:320:THR:HG23	1.91	0.70
1:B:165:SER:OG	4:B:501:HOH:O	2.12	0.68
1:C:47:ASP:O	1:C:50:SER:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASP:OD2	4:C:501:HOH:O	2.14	0.65
1:D:128:LEU:O	4:D:501:HOH:O	2.15	0.64
1:B:125:LYS:HA	1:B:128:LEU:HD12	1.83	0.61
1:C:260:ARG:HH21	1:C:260:ARG:HG2	1.66	0.61
1:B:271:ILE:HD12	1:B:272:ALA:N	2.16	0.60
1:D:55:VAL:CA	4:D:681:HOH:O	2.49	0.60
1:D:289:GLU:OE2	4:D:502:HOH:O	2.16	0.60
1:D:24:ARG:HB2	1:D:332:MET:HG2	1.85	0.57
1:C:254:ASP:OD2	1:D:97:GLU:OE1	2.23	0.56
1:C:317:THR:O	1:C:320:THR:HG22	2.06	0.56
1:D:271:ILE:HD13	2:D:401:AR6:O4'	2.05	0.56
1:C:260:ARG:HH21	1:C:260:ARG:CG	2.19	0.56
1:C:363:SER:HB3	4:C:671:HOH:O	2.05	0.56
1:C:47:ASP:HB3	1:C:50:SER:OG	2.08	0.54
1:D:247:LYS:HZ2	1:D:247:LYS:HB3	1.73	0.54
1:D:14:ALA:N	4:D:507:HOH:O	2.41	0.54
1:D:317:THR:HA	1:D:320:THR:HG22	1.90	0.53
1:A:32:LEU:HD23	1:A:343:CYS:SG	2.50	0.52
1:A:55:VAL:O	1:A:58:LEU:HB3	2.10	0.52
1:B:200:LEU:HD21	4:B:602:HOH:O	2.10	0.52
1:B:81:MET:HE1	4:B:508:HOH:O	2.09	0.51
1:A:162:LEU:HD23	1:A:202:LEU:HD11	1.92	0.51
1:C:220:GLU:HG2	4:C:505:HOH:O	2.10	0.51
1:D:357:HIS:O	1:D:361:GLN:HB2	2.11	0.50
1:C:260:ARG:CG	1:C:260:ARG:NH2	2.72	0.50
1:B:221:ASP:OD1	4:B:503:HOH:O	2.18	0.49
1:D:186:LEU:N	1:D:186:LEU:HD22	2.29	0.48
1:C:260:ARG:NH2	1:C:310:SER:OG	2.47	0.48
1:C:108:TYR:CZ	1:C:121:VAL:HG13	2.49	0.47
1:C:181:THR:HG1	1:C:182:HIS:CE1	2.29	0.47
1:B:81:MET:HE2	1:B:155:MET:CE	2.44	0.47
1:A:48:LEU:O	1:A:52:LEU:HG	2.16	0.46
1:C:47:ASP:O	1:C:48:LEU:C	2.54	0.46
1:C:32:LEU:HD23	1:C:343:CYS:SG	2.56	0.45
1:B:51:VAL:O	1:B:55:VAL:HG13	2.16	0.45
1:B:271:ILE:HD13	2:B:401:AR6:O4'	2.15	0.45
1:B:317:THR:O	1:B:320:THR:HG22	2.16	0.45
1:C:292:PRO:O	4:C:502:HOH:O	2.21	0.45
1:B:81:MET:CE	1:B:155:MET:CE	2.94	0.45
1:B:271:ILE:HD12	1:B:271:ILE:C	2.37	0.45
1:C:58:LEU:N	1:C:58:LEU:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:ASP:OD1	1:D:50:SER:CB	2.66	0.44
1:C:175:ARG:O	1:C:179:GLN:HG3	2.17	0.44
1:B:216:LEU:O	1:B:220:GLU:HG2	2.18	0.43
1:D:247:LYS:HB3	1:D:247:LYS:NZ	2.34	0.43
1:D:186:LEU:N	1:D:186:LEU:CD2	2.82	0.43
1:A:40:TYR:CD1	1:A:40:TYR:N	2.87	0.42
1:C:48:LEU:HB2	1:C:260:ARG:NH1	2.35	0.42
1:B:40:TYR:CE1	1:B:51:VAL:HA	2.55	0.42
1:D:317:THR:O	1:D:320:THR:HG22	2.19	0.42
1:B:341:GLN:HG2	1:B:346:TYR:CZ	2.54	0.42
1:C:47:ASP:O	1:C:50:SER:CB	2.68	0.42
1:B:137:GLU:N	1:B:138:PRO:CD	2.83	0.42
1:C:186:LEU:HD22	1:C:186:LEU:N	2.34	0.42
1:C:241:PRO:O	1:C:245:ARG:HD2	2.19	0.42
1:A:254:ASP:OD2	1:B:97:GLU:OE1	2.38	0.42
1:D:238:GLU:CB	4:D:727:HOH:O	2.68	0.41
1:D:216:LEU:O	1:D:220:GLU:HG2	2.20	0.41
1:A:300:SER:HB3	1:A:330:TYR:CZ	2.55	0.41
1:B:81:MET:CE	1:B:155:MET:HE1	2.50	0.41
1:A:105:ALA:HB1	1:A:128:LEU:HG	2.02	0.41
1:D:156:ARG:HH11	1:D:156:ARG:HD3	1.70	0.41
1:C:47:ASP:N	1:C:50:SER:OG	2.54	0.41
1:D:162:LEU:HD23	1:D:202:LEU:HD11	2.02	0.41
1:D:350:ASP:O	1:D:354:GLN:HG3	2.20	0.41
1:B:52:LEU:O	1:B:55:VAL:HG22	2.21	0.41
1:B:240:ARG:HB3	1:B:243:SER:HB2	2.03	0.40

All (1) 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)
4:A:647:HOH:O	4:B:644:HOH:O[1_445]	2.09	0.11

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	328/366 (90%)	322 (98%)	6 (2%)	0	100	100
1	B	325/366 (89%)	320 (98%)	5 (2%)	0	100	100
1	C	330/366 (90%)	325 (98%)	5 (2%)	0	100	100
1	D	330/366 (90%)	324 (98%)	6 (2%)	0	100	100
All	All	1313/1464 (90%)	1291 (98%)	22 (2%)	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	240/282 (85%)	238 (99%)	2 (1%)	81	76
1	B	234/282 (83%)	233 (100%)	1 (0%)	91	89
1	C	253/282 (90%)	252 (100%)	1 (0%)	91	89
1	D	245/282 (87%)	243 (99%)	2 (1%)	81	76
All	All	972/1128 (86%)	966 (99%)	6 (1%)	86	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	ASP
1	D	47	ASP
1	D	78	ASP
1	A	78	ASP
1	A	338	SER
1	B	78	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	106	GLN
1	C	171	GLN
1	C	227	GLN
1	A	203	GLN
1	B	171	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
2	AR6	D	401	3	34,39,39	1.00	3 (8%)	40,60,60	1.82	7 (17%)
2	AR6	C	401	3	34,39,39	1.03	3 (8%)	40,60,60	1.80	9 (22%)
2	AR6	A	401	3	34,39,39	1.07	3 (8%)	40,60,60	1.62	7 (17%)
2	AR6	B	401	3	34,39,39	1.10	3 (8%)	40,60,60	1.95	6 (15%)

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	D	401	3	-	2/18/54/54	0/4/4/4
2	AR6	C	401	3	-	2/18/54/54	0/4/4/4
2	AR6	A	401	3	-	2/18/54/54	0/4/4/4
2	AR6	B	401	3	-	3/18/54/54	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	AR6	O4'-C1'	3.65	1.46	1.41
2	A	401	AR6	O4'-C1'	3.09	1.45	1.41
2	C	401	AR6	C2-N3	2.49	1.36	1.32
2	B	401	AR6	C2-N3	2.47	1.36	1.32
2	C	401	AR6	C1D-C2D	2.46	1.55	1.52
2	C	401	AR6	C5-C4	2.41	1.47	1.40
2	D	401	AR6	O4'-C1'	2.38	1.44	1.41
2	B	401	AR6	C5-C4	2.22	1.46	1.40
2	D	401	AR6	C5-C4	2.15	1.46	1.40
2	A	401	AR6	C1D-C2D	2.14	1.55	1.52
2	A	401	AR6	C5-C4	2.09	1.46	1.40
2	D	401	AR6	C2-N3	2.08	1.35	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	AR6	O1D-C1D-O4D	-6.84	102.37	111.13
2	B	401	AR6	O1D-C1D-O4D	-6.20	103.20	111.13
2	C	401	AR6	O1D-C1D-O4D	-5.50	104.09	111.13
2	A	401	AR6	O1D-C1D-O4D	-4.85	104.92	111.13
2	D	401	AR6	N3-C2-N1	-4.75	121.26	128.68
2	B	401	AR6	C3'-C2'-C1'	4.38	107.57	100.98
2	A	401	AR6	N3-C2-N1	-4.18	122.14	128.68
2	C	401	AR6	C3'-C2'-C1'	4.01	107.02	100.98
2	C	401	AR6	N3-C2-N1	-3.95	122.51	128.68
2	C	401	AR6	O4D-C1D-C2D	3.91	109.27	104.46
2	B	401	AR6	N3-C2-N1	-3.88	122.61	128.68
2	B	401	AR6	O4D-C1D-C2D	3.81	109.15	104.46
2	D	401	AR6	O4D-C1D-C2D	3.67	108.98	104.46
2	B	401	AR6	C4-C5-N7	-3.29	105.97	109.40
2	D	401	AR6	C2-N1-C6	3.26	124.33	118.75
2	A	401	AR6	C3'-C2'-C1'	2.98	105.46	100.98
2	A	401	AR6	O4D-C1D-C2D	2.83	107.94	104.46
2	D	401	AR6	C1'-N9-C4	-2.66	121.96	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AR6	C2-N1-C6	2.54	123.11	118.75
2	A	401	AR6	C4-C5-N7	-2.54	106.76	109.40
2	D	401	AR6	C2D-C3D-C4D	2.53	107.55	102.64
2	B	401	AR6	C2-N1-C6	2.39	122.84	118.75
2	A	401	AR6	C2D-C3D-C4D	2.38	107.27	102.64
2	C	401	AR6	C1'-N9-C4	-2.37	122.48	126.64
2	C	401	AR6	C2-N1-C6	2.35	122.78	118.75
2	C	401	AR6	O1B-PB-O2B	2.29	123.59	112.24
2	C	401	AR6	C4-C5-N7	-2.28	107.03	109.40
2	D	401	AR6	N6-C6-N1	2.12	122.97	118.57
2	C	401	AR6	O4'-C1'-C2'	-2.09	103.87	106.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	AR6	PB-O3A-PA-O5'
2	D	401	AR6	PB-O3A-PA-O5'
2	A	401	AR6	PB-O3A-PA-O5'
2	B	401	AR6	PB-O3A-PA-O5'
2	D	401	AR6	PA-O3A-PB-O2B
2	B	401	AR6	PA-O3A-PB-O1B
2	A	401	AR6	PA-O3A-PB-O2B
2	B	401	AR6	PA-O3A-PB-O2B
2	C	401	AR6	C5D-O5D-PB-O2B

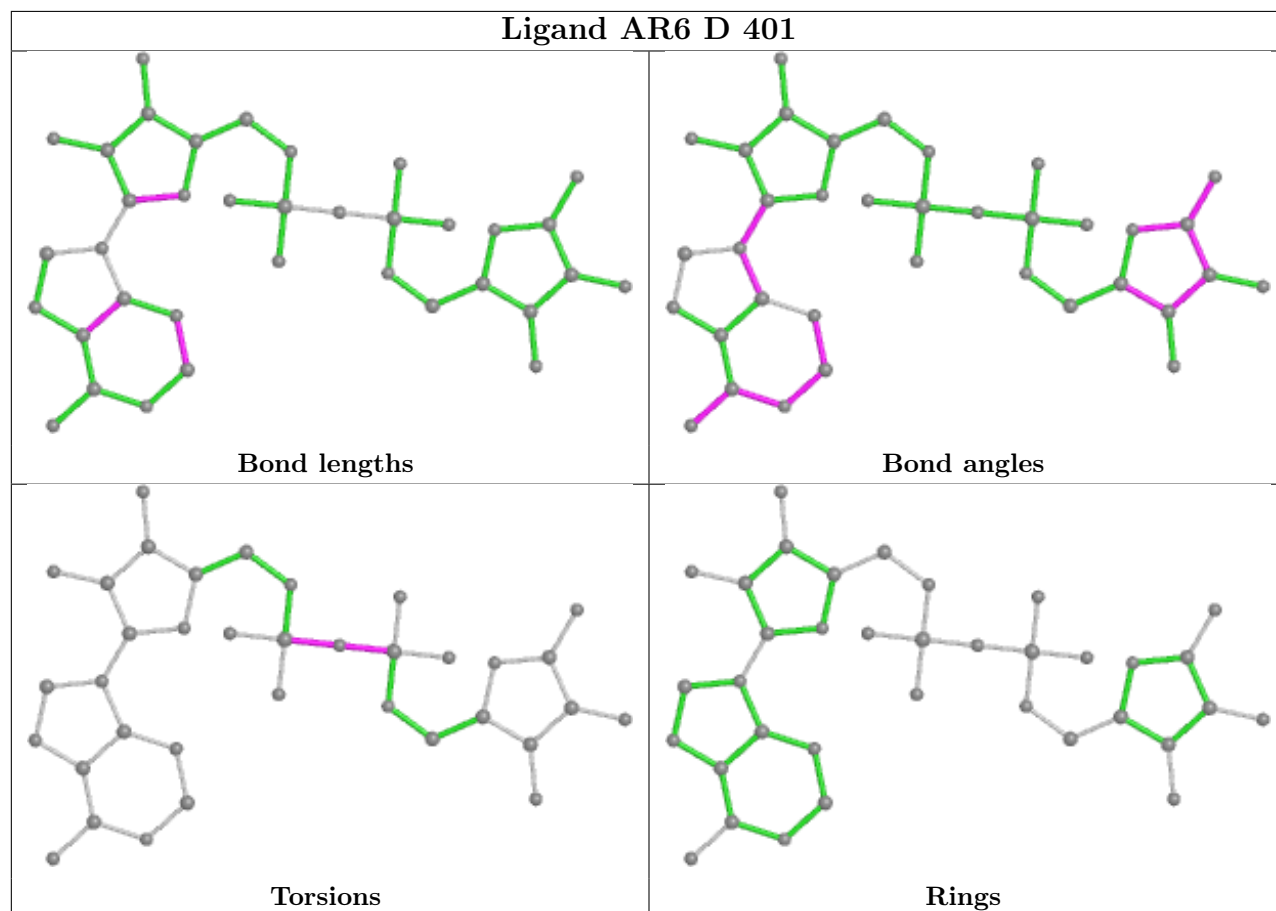
There are no ring outliers.

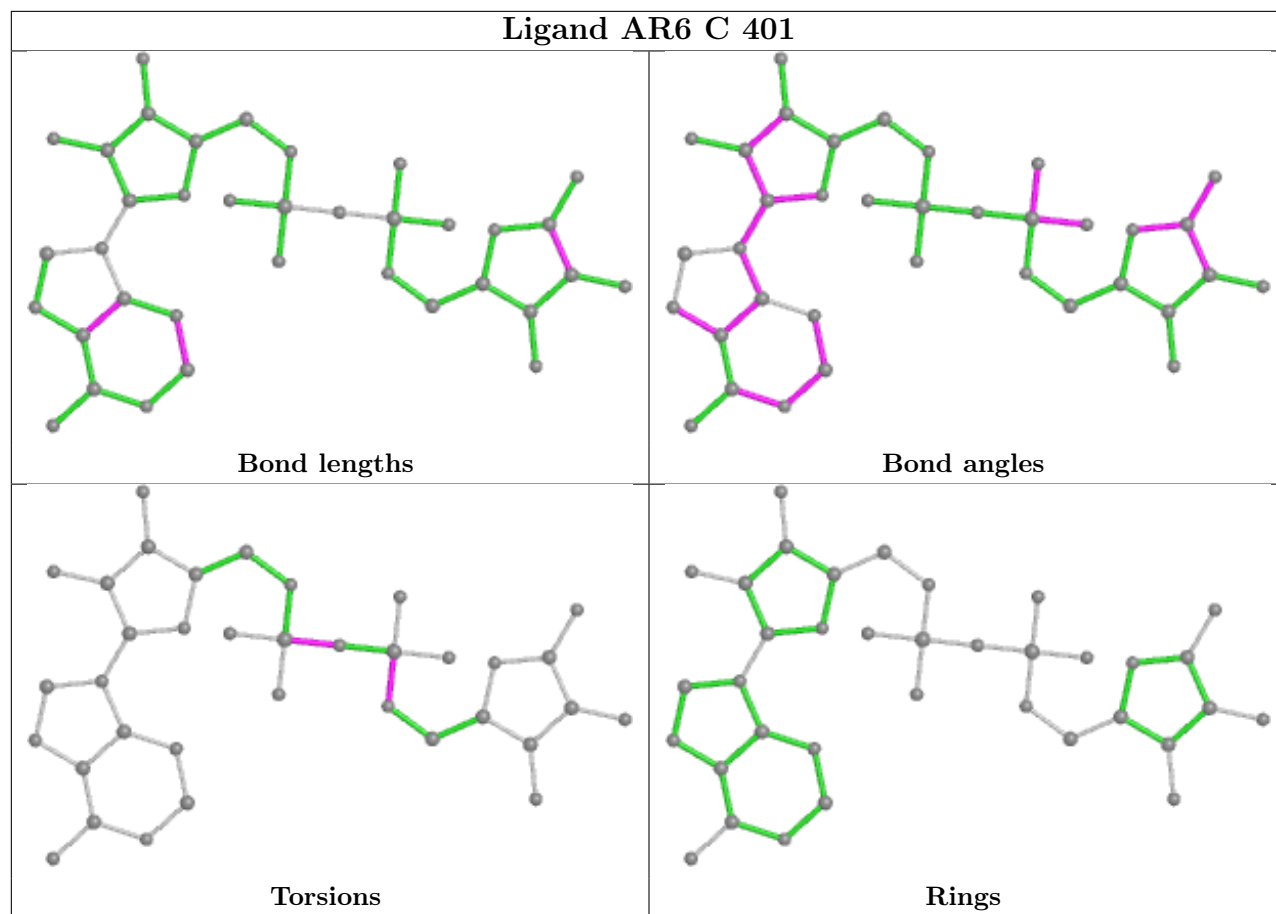
2 monomers are involved in 2 short contacts:

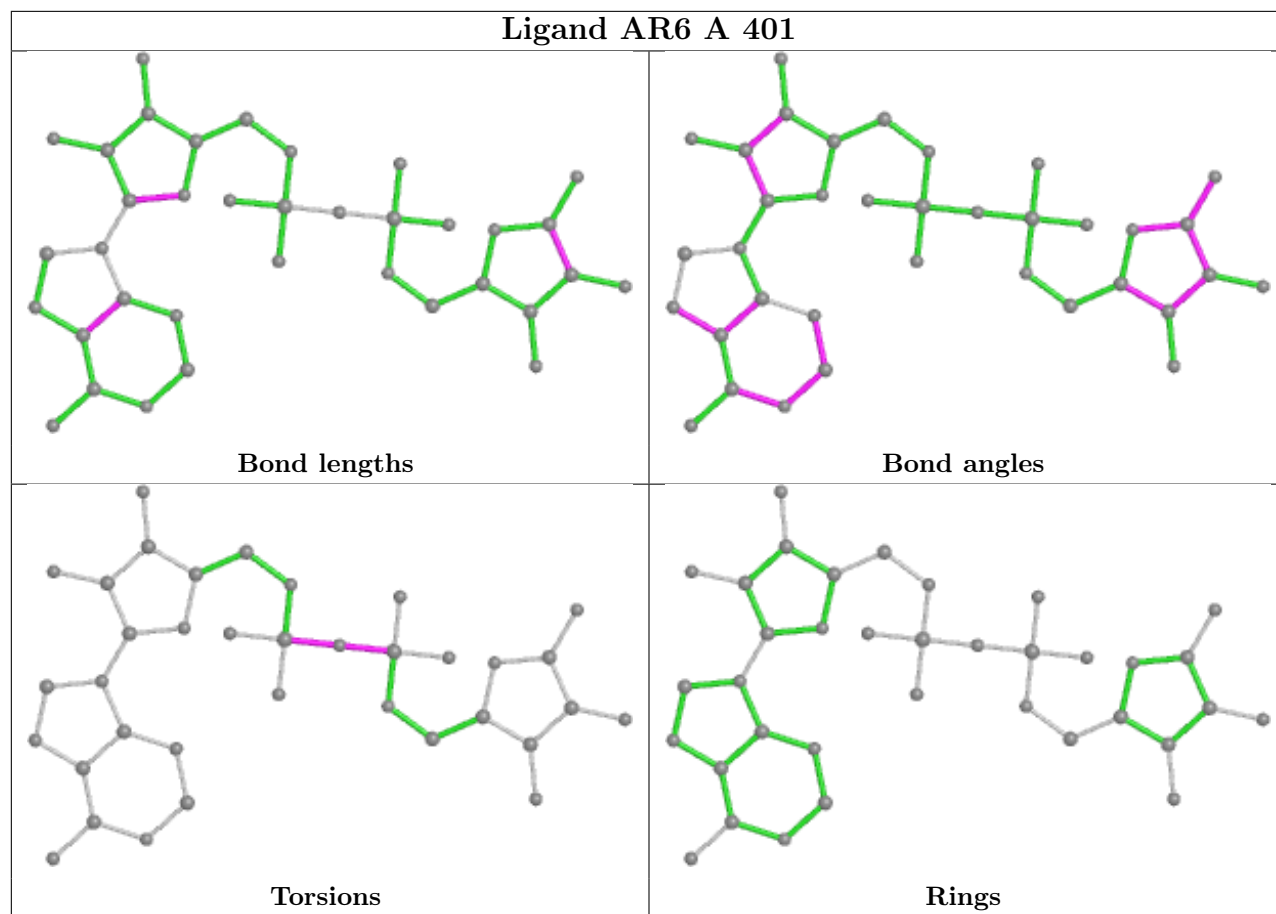
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	AR6	1	0
2	B	401	AR6	1	0

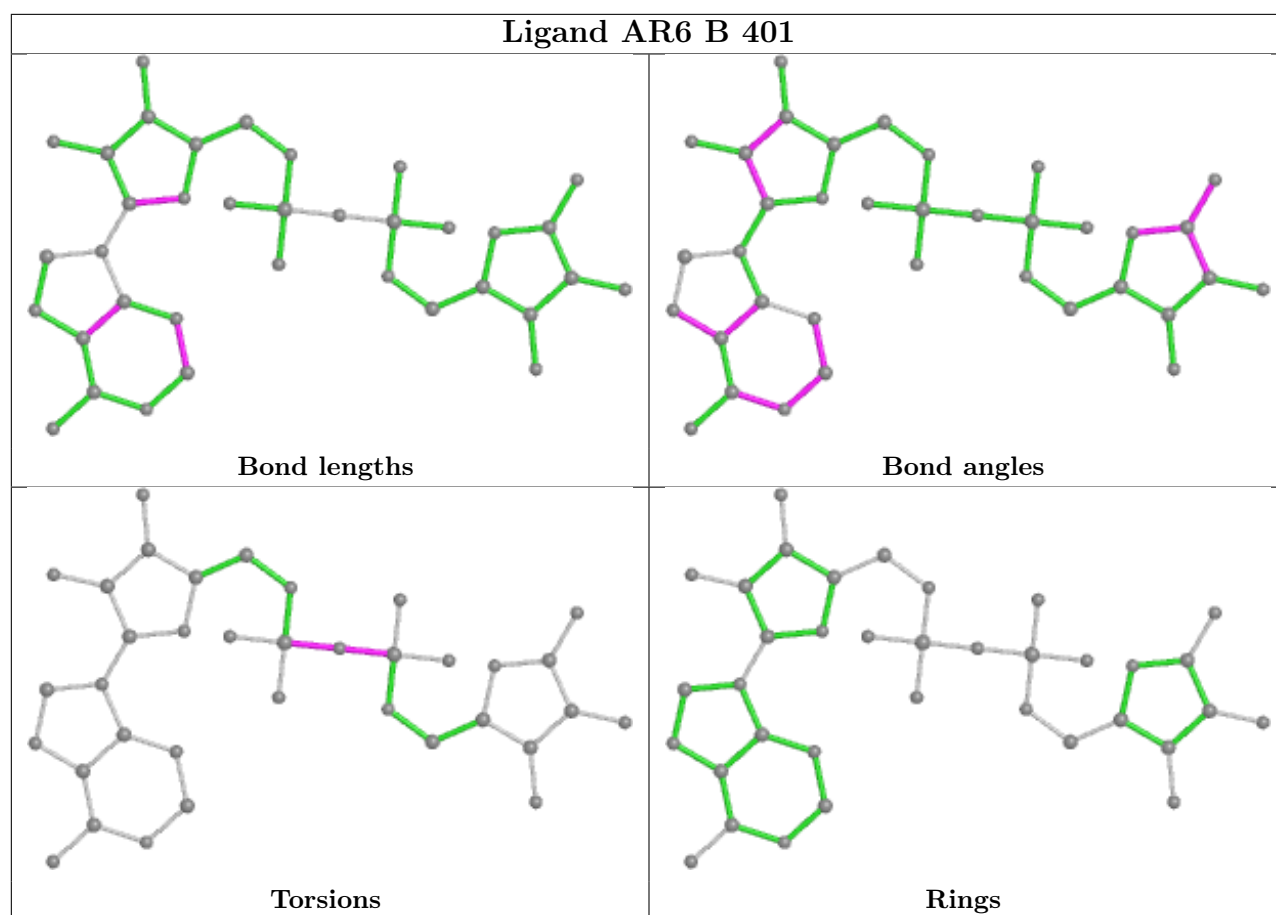
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	A	334/366 (91%)	-0.40	3 (0%) 84 84	12, 22, 50, 71	0
1	B	331/366 (90%)	-0.42	0 100 100	12, 23, 42, 61	0
1	C	336/366 (91%)	-0.48	3 (0%) 84 84	8, 17, 44, 66	0
1	D	334/366 (91%)	-0.56	0 100 100	7, 17, 34, 61	0
All	All	1335/1464 (91%)	-0.47	6 (0%) 92 92	7, 20, 44, 71	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	TYR	5.0
1	C	54	HIS	3.6
1	C	41	GLU	3.1
1	A	41	GLU	2.5
1	C	51	VAL	2.2
1	A	58	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

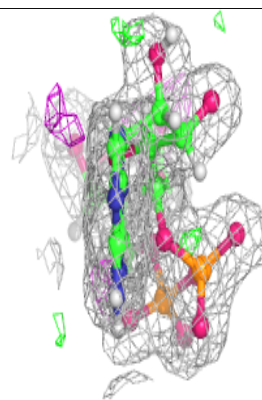
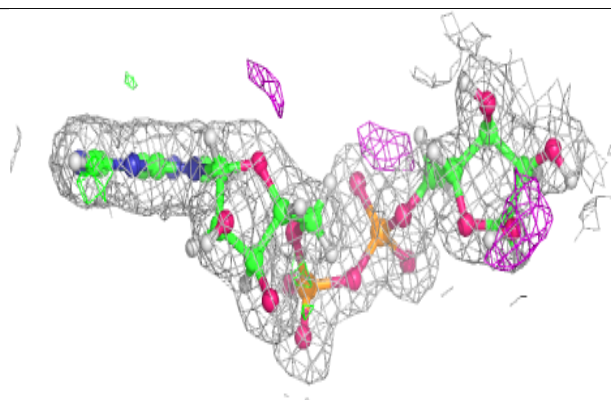
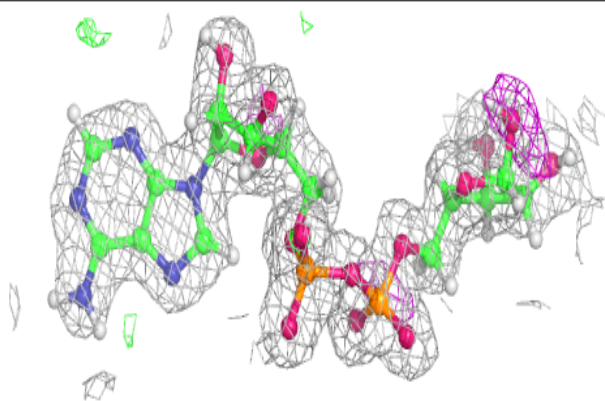
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AR6	C	401	36/36	0.97	0.08	9,16,27,32	0
2	AR6	D	401	36/36	0.97	0.08	10,19,31,37	0
2	AR6	A	401	36/36	0.97	0.08	13,21,35,42	0
2	AR6	B	401	36/36	0.97	0.08	15,27,38,39	0
3	MG	C	402	1/1	0.98	0.05	10,10,10,10	0
3	MG	D	402	1/1	0.99	0.03	12,12,12,12	0
3	MG	A	402	1/1	1.00	0.03	14,14,14,14	0
3	MG	B	402	1/1	1.00	0.04	17,17,17,17	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.

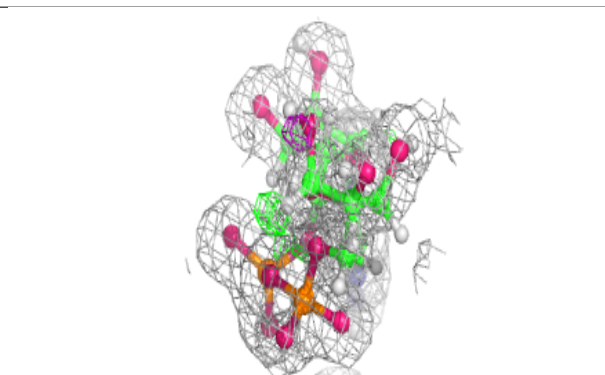
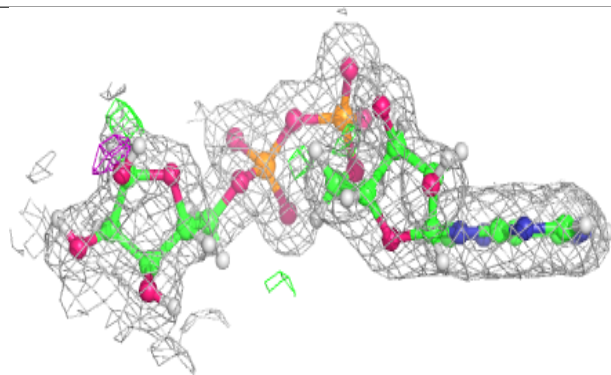
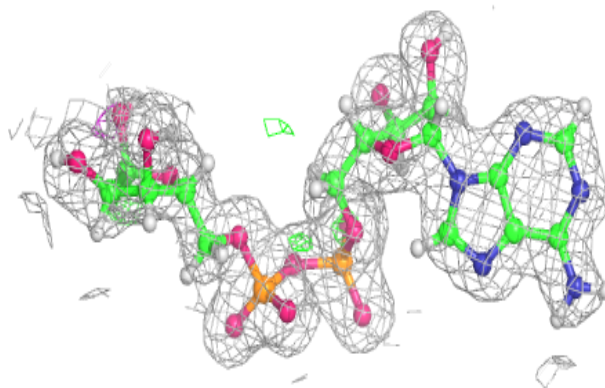
Electron density around AR6 C 401:

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

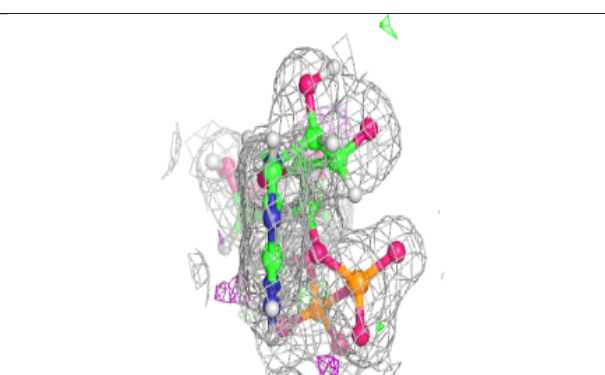
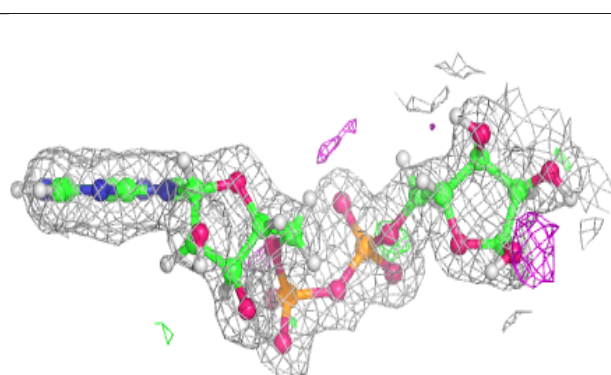
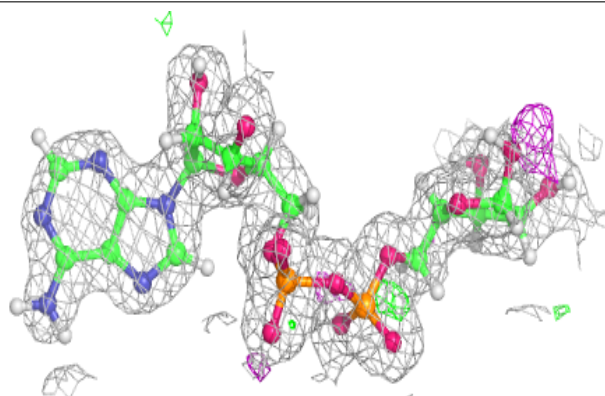


Electron density around AR6 D 401:

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

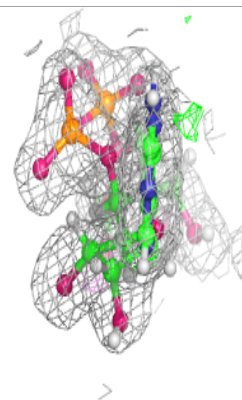
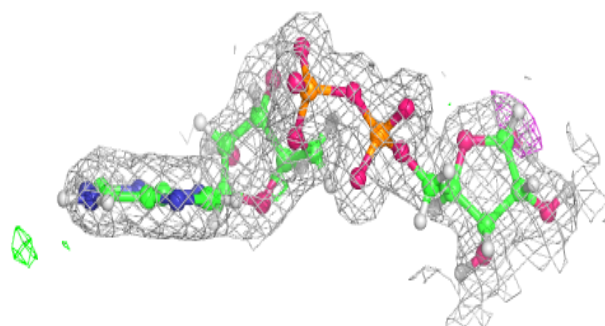
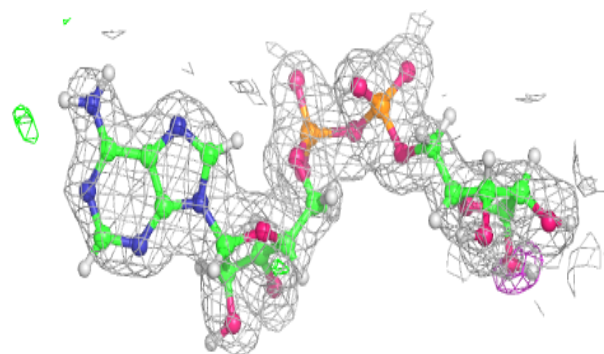
**Electron density around AR6 A 401:**

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



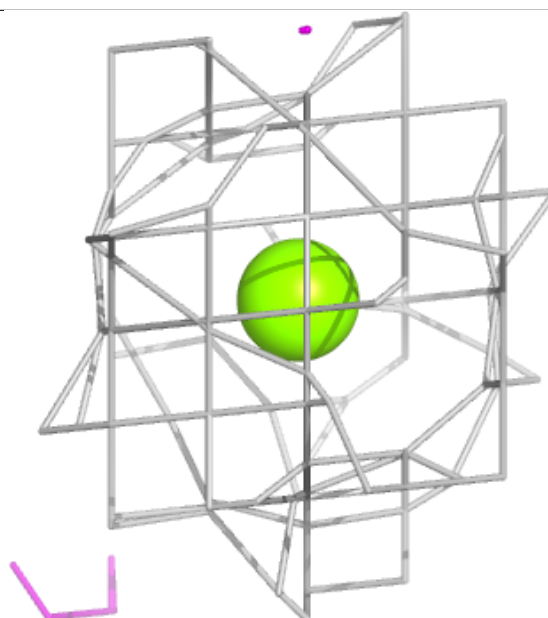
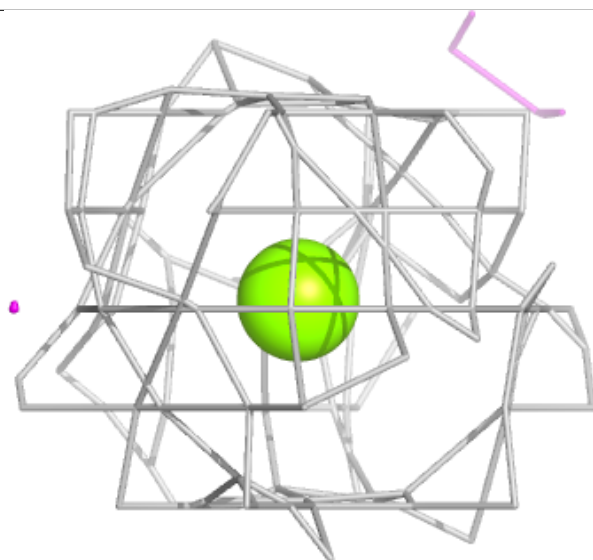
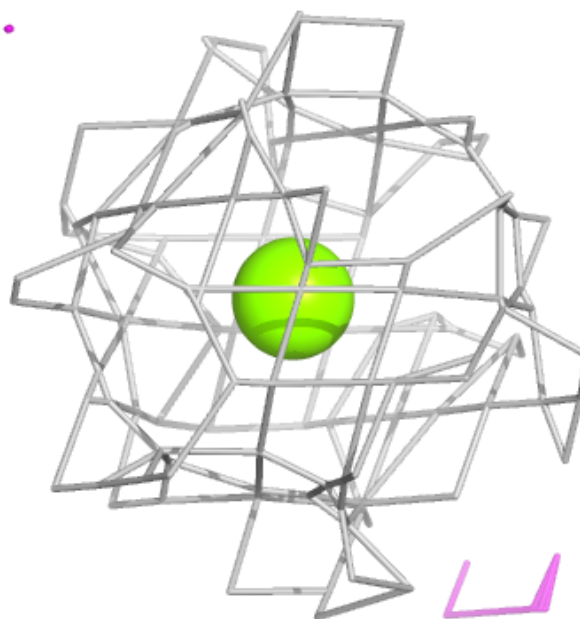
Electron density around AR6 B 401:

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



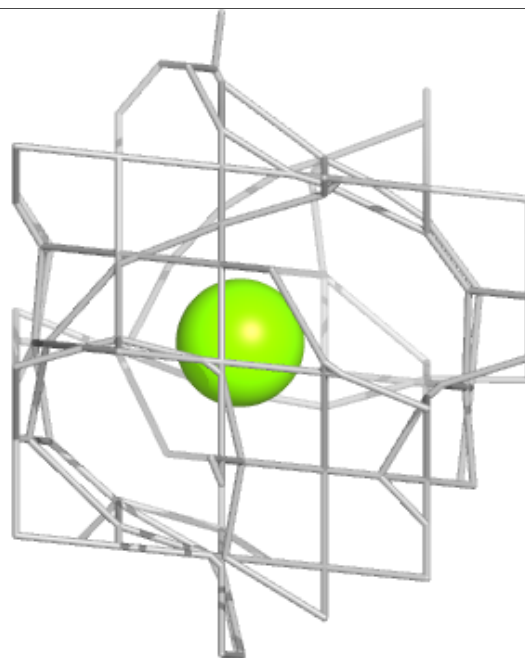
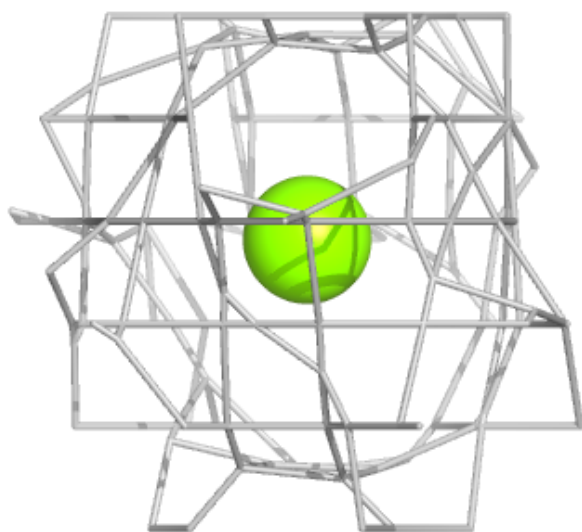
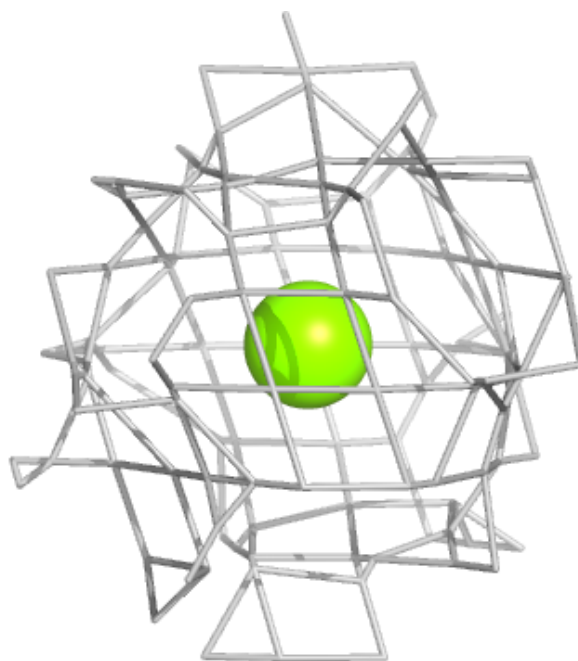
Electron density around MG C 402:

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



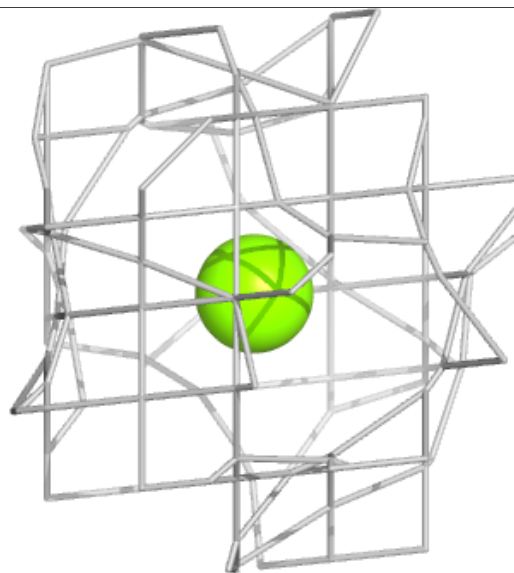
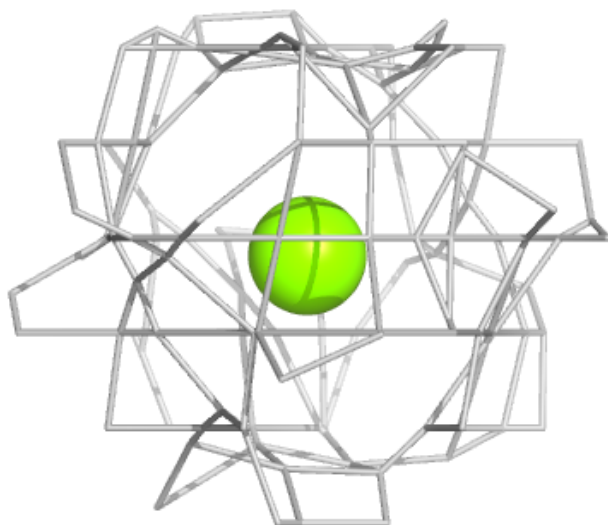
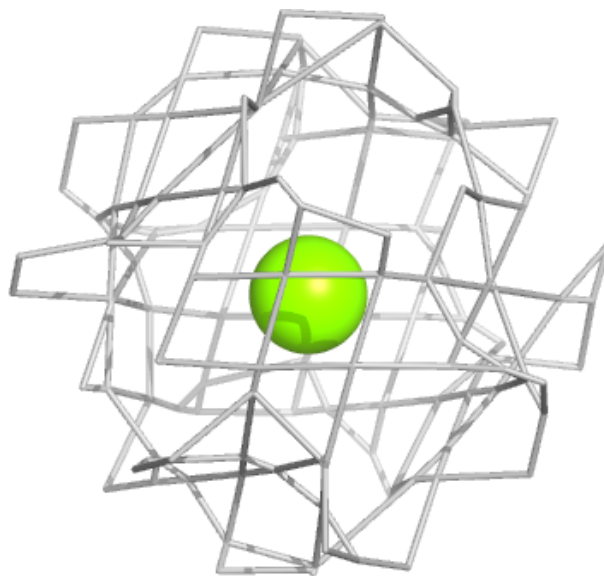
Electron density around MG D 402:

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



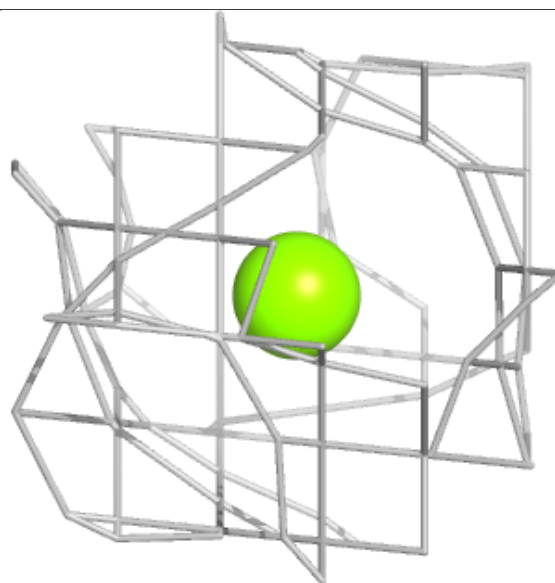
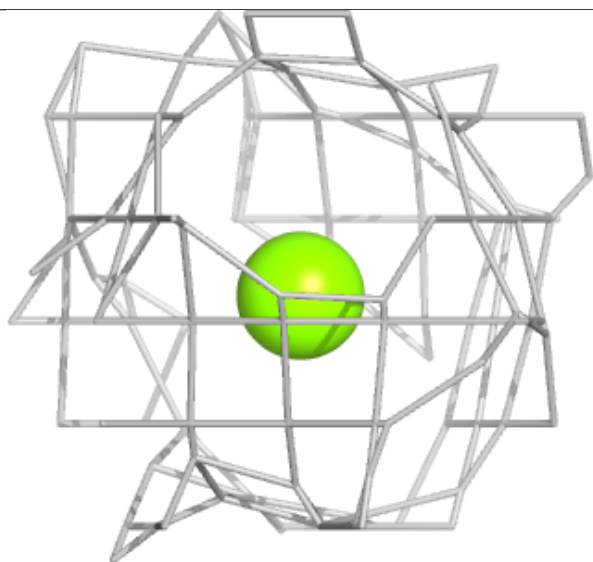
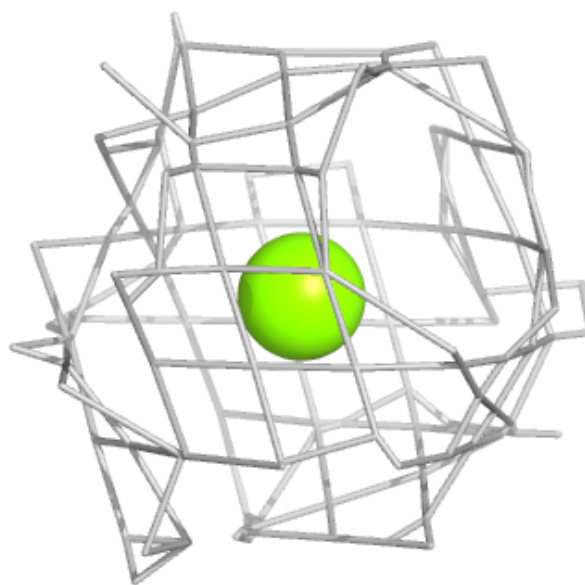
Electron density around MG A 402:

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



Electron density around MG B 402:

$2mF_o-DF_c$ (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.