Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2021 – 05:03 am GMT

PDB ID	:	7ALV
Title	:	Crystal Structure of NLRP3 NACHT domain in complex with a potent inhibitor
Authors	:	Dekker, C.; Hinniger, A.
Deposited on	:	2020-10-07
Resolution	:	2.83 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 (i) symbol.

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

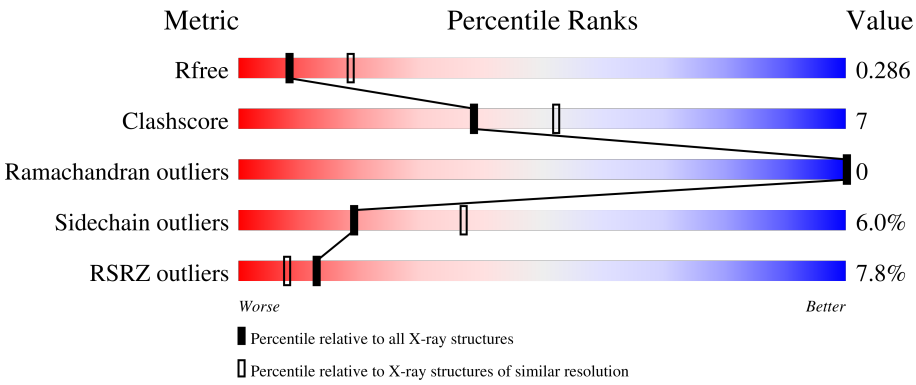
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

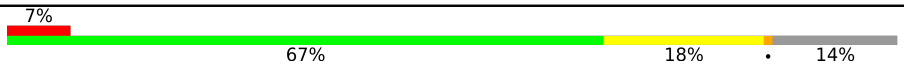
The reported resolution of this entry is 2.83 Å.

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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 <=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	550	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3782 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.

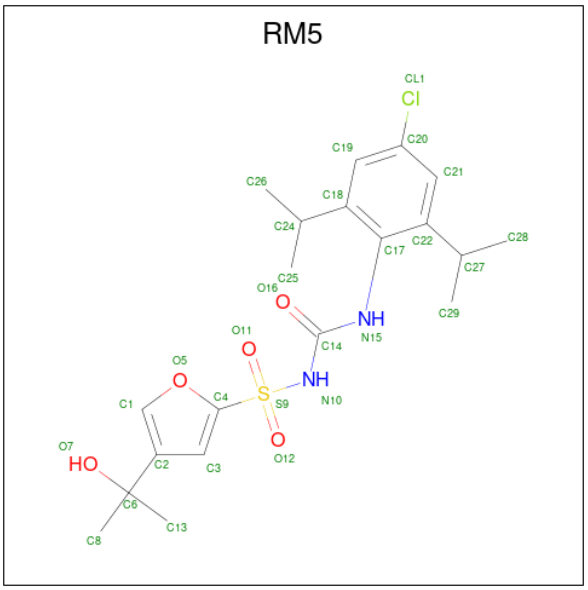
- Molecule 1 is a protein called NACHT, LRR and PYD domains-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3718	2411	623	657	27	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	GLY	-	expression tag	UNP Q96P20

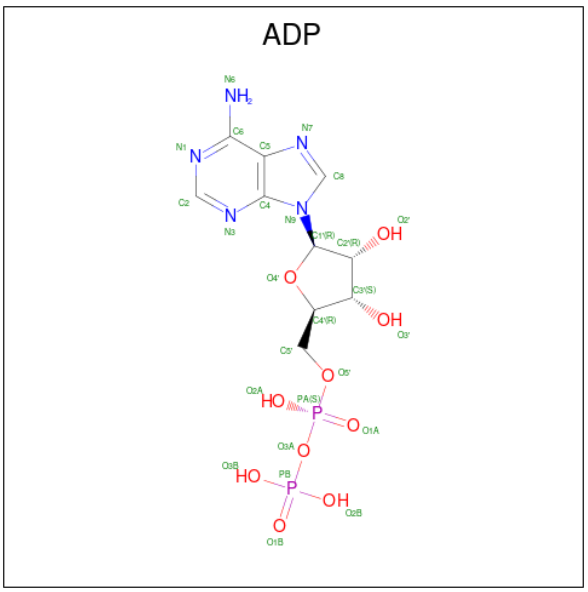
- Molecule 2 is 1-[4-chloranyl-2,6-di(propan-2-yl)phenyl]-3-[4-(2-oxidanylpropan-2-yl)furan-2-yl]sulfonyl-urea (three-letter code: RM5) (formula: $C_{20}H_{27}ClN_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	29	20	1	2	5	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is water.

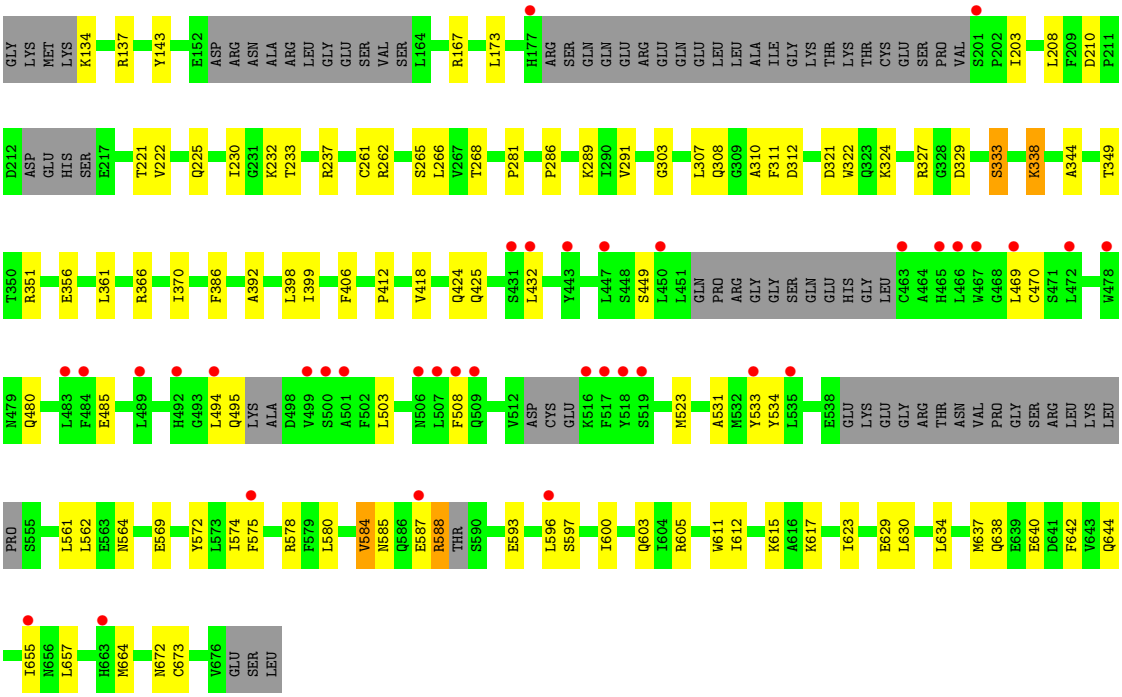
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NACHT, LRR and PYD domains-containing protein 3

Chain A: 7% 67% 18% • 14%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.18Å 96.18Å 262.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.39 – 2.83 79.39 – 2.83	Depositor EDS
% Data completeness (in resolution range)	68.2 (79.39-2.83) 68.1 (79.39-2.83)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.213 , 0.265 0.226 , 0.286	Depositor DCC
R_{free} test set	633 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3782	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, RM5

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	0.44	0/3797	0.61	0/5128

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	3718	0	3579	55	0
2	A	29	0	0	0	0
3	A	27	0	12	0	0
4	A	8	0	0	0	0
All	All	3782	0	3591	55	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 7.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:HD11	1:A:418:VAL:HG11	1.63	0.78
1:A:597:SER:HB3	1:A:600:ILE:HG12	1.65	0.78
1:A:424:GLN:HG3	1:A:449:SER:HB3	1.67	0.75
1:A:562:LEU:HD22	1:A:611:TRP:CE2	2.25	0.71
1:A:611:TRP:NE1	1:A:615:LYS:HE3	2.04	0.71
1:A:321:ASP:HB3	1:A:324:LYS:HB2	1.76	0.67
1:A:572:TYR:HB3	1:A:574:ILE:HD13	1.76	0.65
1:A:233:THR:O	1:A:237:ARG:HG3	1.98	0.64
1:A:338:LYS:HE2	1:A:344:ALA:O	2.00	0.61
1:A:562:LEU:HD22	1:A:611:TRP:CD1	2.35	0.61
1:A:562:LEU:HD22	1:A:611:TRP:NE1	2.16	0.60
1:A:611:TRP:HE1	1:A:615:LYS:HE3	1.66	0.60
1:A:386:PHE:HB2	1:A:392:ALA:HB2	1.85	0.59
1:A:585:ASN:HD21	1:A:638:GLN:H	1.51	0.59
1:A:265:SER:HB3	1:A:268:THR:HB	1.83	0.59
1:A:232:LYS:HG2	1:A:349:THR:HB	1.86	0.57
1:A:134:LYS:HA	1:A:137:ARG:HB2	1.84	0.57
1:A:534:TYR:CE2	1:A:561:LEU:HD11	2.40	0.57
1:A:585:ASN:ND2	1:A:638:GLN:H	2.02	0.57
1:A:600:ILE:HA	1:A:603:GLN:HG2	1.88	0.55
1:A:398:LEU:HD11	1:A:432:LEU:HB3	1.90	0.54
1:A:310:ALA:HB2	1:A:569:GLU:HG3	1.90	0.53
1:A:580:LEU:O	1:A:584:VAL:HB	2.09	0.53
1:A:351:ARG:NH1	1:A:575:PHE:CE2	2.76	0.53
1:A:143:TYR:CD1	1:A:281:PRO:HB3	2.44	0.53
1:A:612:ILE:HG13	1:A:630:LEU:HD22	1.89	0.53
1:A:634:LEU:O	1:A:637:MET:O	2.26	0.53
1:A:593:GLU:HA	1:A:596:LEU:HD12	1.91	0.52
1:A:173:LEU:HB3	1:A:203:ILE:HD11	1.93	0.50
1:A:605:ARG:HH21	1:A:642:PHE:HB2	1.77	0.49
1:A:291:VAL:HG11	1:A:322:TRP:CE2	2.48	0.49
1:A:531:ALA:HB1	1:A:580:LEU:HB3	1.93	0.49
1:A:232:LYS:HG3	1:A:370:ILE:HD12	1.95	0.48
1:A:655:ILE:HG23	1:A:657:LEU:HG	1.94	0.48
1:A:203:ILE:HD13	1:A:208:LEU:HD21	1.96	0.47
1:A:286:PRO:HB2	1:A:289:LYS:HB3	1.96	0.47
1:A:562:LEU:HD22	1:A:611:TRP:CD2	2.49	0.47
1:A:644:GLN:HE21	1:A:672:ASN:HD22	1.62	0.47
1:A:569:GLU:H	1:A:569:GLU:CD	2.16	0.47
1:A:291:VAL:HG11	1:A:322:TRP:NE1	2.31	0.46
1:A:637:MET:HG2	1:A:642:PHE:CD1	2.51	0.46
1:A:308:GLN:HB3	1:A:480:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:CYS:HB2	1:A:303:GLY:O	2.16	0.46
1:A:470:CYS:HB3	1:A:533:TYR:HB2	1.97	0.46
1:A:230:ILE:HA	1:A:412:PRO:HD2	1.98	0.46
1:A:222:VAL:HG22	1:A:366:ARG:HB3	1.97	0.45
1:A:399:ILE:HG23	1:A:406:PHE:HA	1.97	0.45
1:A:494:LEU:O	1:A:495:GLN:O	2.35	0.44
1:A:469:LEU:HD11	1:A:503:LEU:HD22	2.00	0.44
1:A:611:TRP:NE1	1:A:615:LYS:CE	2.79	0.42
1:A:578:ARG:NH2	1:A:629:GLU:OE1	2.44	0.42
1:A:329:ASP:O	1:A:333:SER:HB2	2.20	0.41
1:A:311:PHE:HE1	1:A:361:LEU:HD11	1.86	0.41
1:A:266:LEU:HD11	1:A:307:LEU:HB3	2.03	0.40
1:A:585:ASN:HB3	1:A:588:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	454/550 (82%)	436 (96%)	18 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	382/497 (77%)	359 (94%)	23 (6%)	19 37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	210	ASP
1	A	221	THR
1	A	225	GLN
1	A	262	ARG
1	A	312	ASP
1	A	327	ARG
1	A	333	SER
1	A	338	LYS
1	A	356	GLU
1	A	425	GLN
1	A	485	GLU
1	A	508	PHE
1	A	523	MET
1	A	564	ASN
1	A	584	VAL
1	A	587	GLU
1	A	588	ARG
1	A	617	LYS
1	A	623	ILE
1	A	640	GLU
1	A	664	MET
1	A	673	CYS

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

Mol	Chain	Res	Type
1	A	225	GLN
1	A	250	GLN
1	A	424	GLN
1	A	585	ASN
1	A	672	ASN

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)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

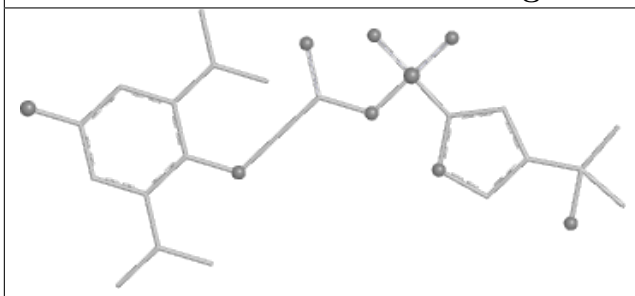
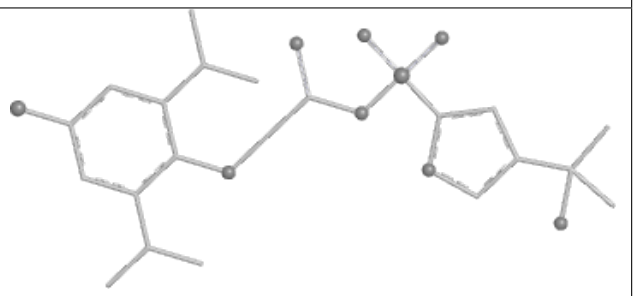
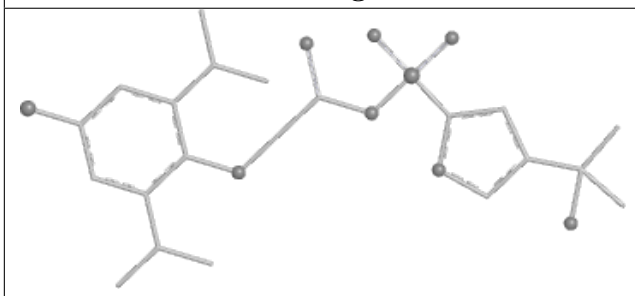
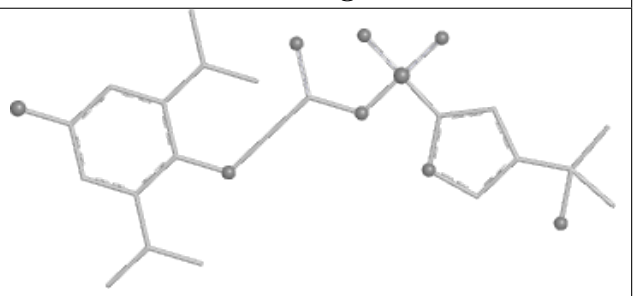
There are no chirality outliers.

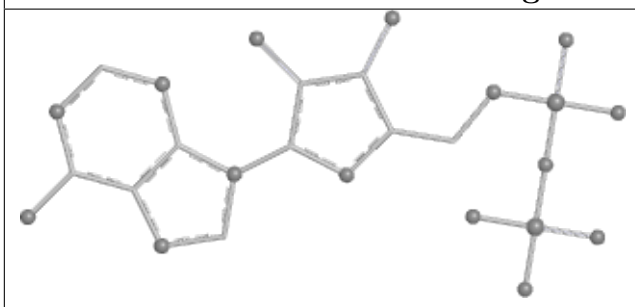
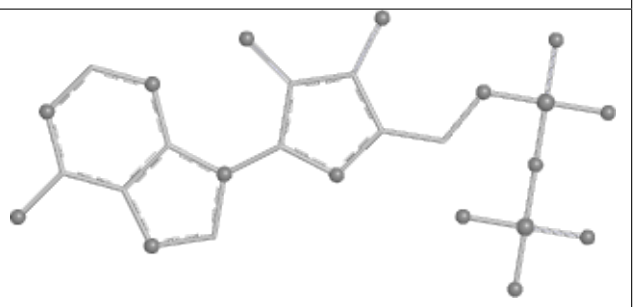
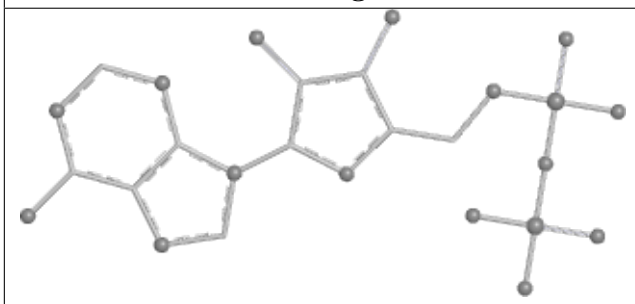
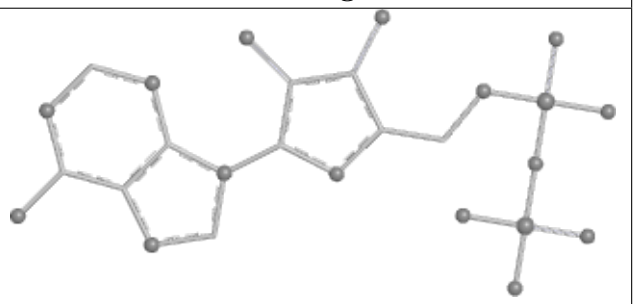
There are no torsion outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand RM5 A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	472/550 (85%)	0.58	37 (7%) 13 8	42, 78, 142, 205	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	587	GLU	4.6
1	A	484	PHE	4.5
1	A	432	LEU	4.4
1	A	500	SER	3.7
1	A	517	PHE	3.6
1	A	494	LEU	3.5
1	A	507	LEU	3.5
1	A	499	VAL	3.3
1	A	483	LEU	3.2
1	A	443	TYR	3.1
1	A	516	LYS	3.1
1	A	533	TYR	3.0
1	A	478	TRP	3.0
1	A	489	LEU	2.9
1	A	467	TRP	2.9
1	A	506	ASN	2.9
1	A	201	SER	2.8
1	A	447	LEU	2.8
1	A	596	LEU	2.7
1	A	492	HIS	2.7
1	A	508	PHE	2.7
1	A	472	LEU	2.6
1	A	177	HIS	2.6
1	A	431	SER	2.6
1	A	655	ILE	2.5
1	A	518	TYR	2.5
1	A	501	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	519	SER	2.3
1	A	450	LEU	2.3
1	A	469	LEU	2.3
1	A	663	HIS	2.3
1	A	463	CYS	2.3
1	A	509	GLN	2.2
1	A	535	LEU	2.2
1	A	466	LEU	2.2
1	A	465	HIS	2.2
1	A	575	PHE	2.1

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)

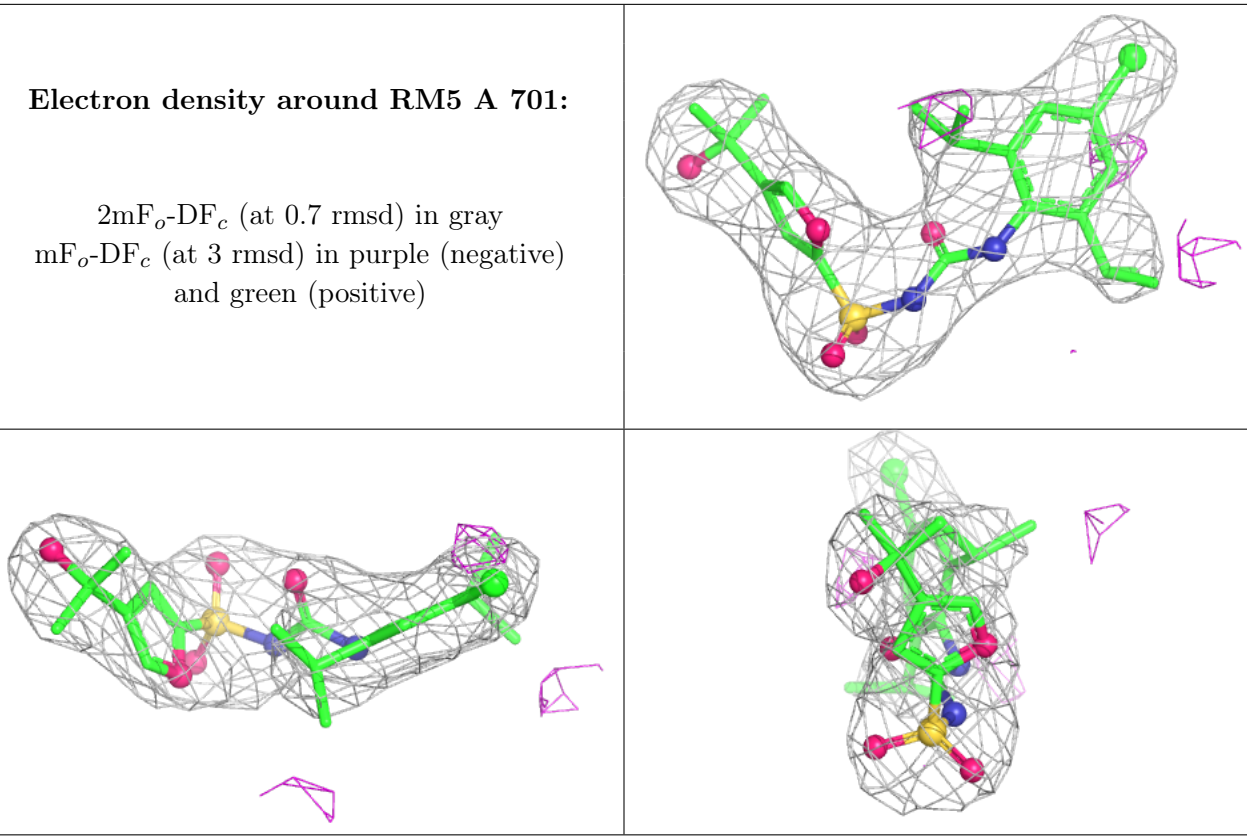
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	RM5	A	701	29/29	0.97	0.33	58,60,62,64	0
3	ADP	A	702	27/27	0.98	0.23	46,49,50,51	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.

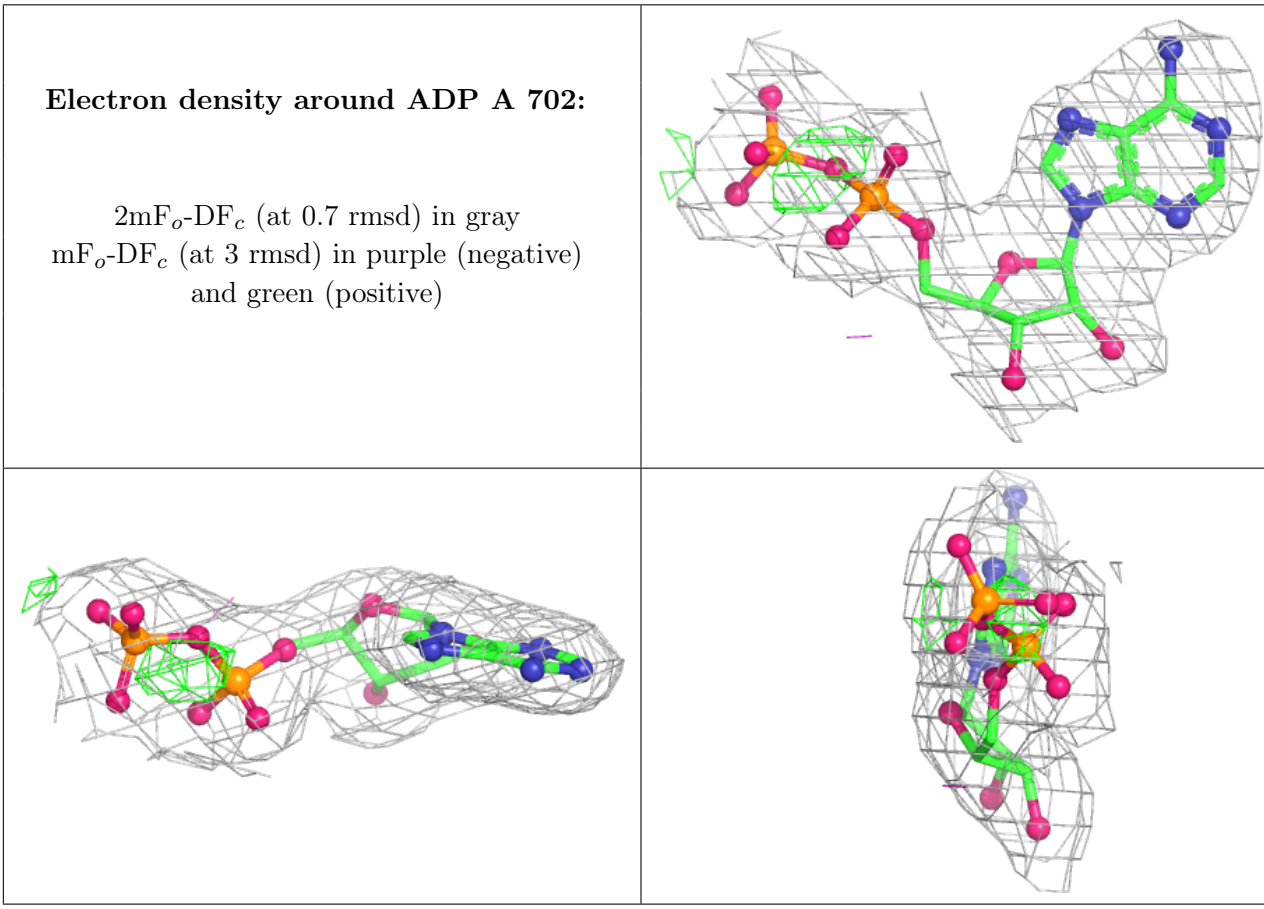
Electron density around RM5 A 701:

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



Electron density around ADP A 702:

$2mF_o$-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.