Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:55 pm BST

PDB ID	:	5OFA
Title	:	Crystal structure of human MORC2 (residues 1-603) with spinal muscular atrophy mutation T424R
Authors	:	Douse, C.H.; Liu, Y.; Modis, Y.
Deposited on	:	2017-07-10
Resolution	:	2.57 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:

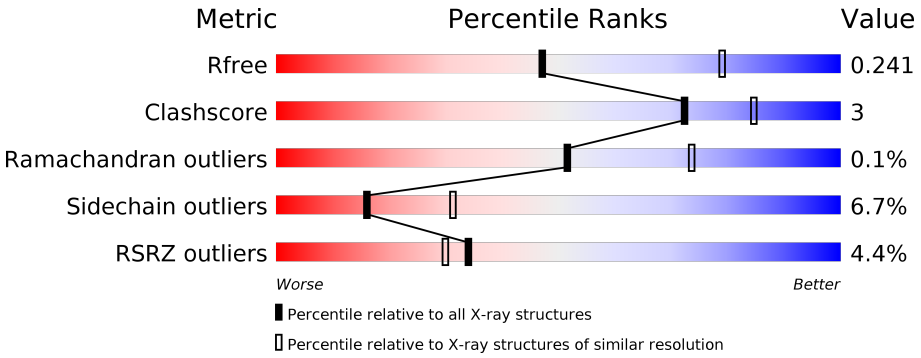
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 <=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	606	3% 73% 11% • 12%
1	B	606	4% 76% 11% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8801 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 MORC family CW-type zinc finger protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	540	Total	C	N	O	S	0	0	0
			4385	2763	780	815	27			
1	A	531	Total	C	N	O	S	0	1	0
			4311	2713	772	799	27			

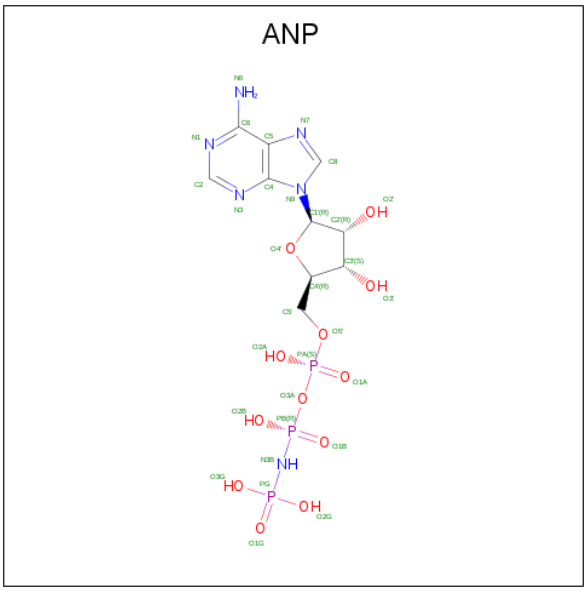
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9Y6X9
B	-1	PRO	-	expression tag	UNP Q9Y6X9
B	0	ARG	-	expression tag	UNP Q9Y6X9
B	424	ARG	THR	engineered mutation	UNP Q9Y6X9
A	-2	GLY	-	expression tag	UNP Q9Y6X9
A	-1	PRO	-	expression tag	UNP Q9Y6X9
A	0	ARG	-	expression tag	UNP Q9Y6X9
A	424	ARG	THR	engineered mutation	UNP Q9Y6X9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 31 10 6 12 3	0	0
3	A	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is water.

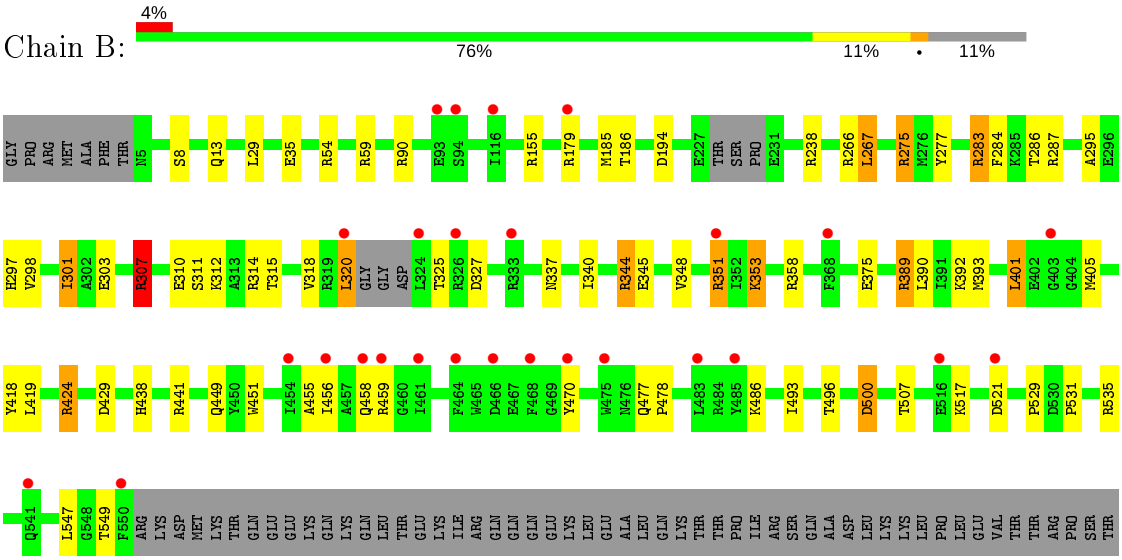
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	A	12	Total O 12 12	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

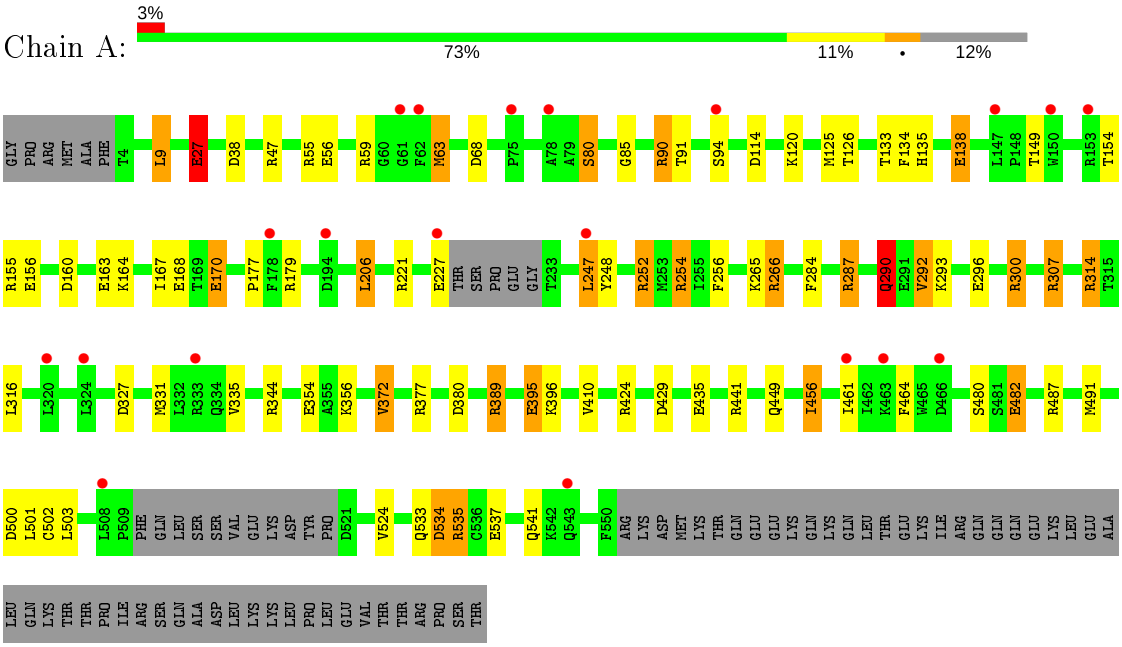
- Molecule 1: MORC family CW-type zinc finger protein 2

Chain B:



- Molecule 1: MORC family CW-type zinc finger protein 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.61Å 125.73Å 81.53Å 90.00° 97.91° 90.00°	Depositor
Resolution (Å)	80.75 – 2.57 80.75 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.6 (80.75-2.57) 99.6 (80.75-2.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.211 , 0.239 0.215 , 0.241	Depositor DCC
R_{free} test set	2154 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8801	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ANP, MG

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	0.72	3/4398 (0.1%)	1.05	42/5919 (0.7%)
1	B	0.76	4/4472 (0.1%)	1.06	30/6020 (0.5%)
All	All	0.74	7/8870 (0.1%)	1.05	72/11939 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	TYR	CE1-CZ	-7.00	1.29	1.38
1	A	372	VAL	CB-CG1	-6.22	1.39	1.52
1	A	435	GLU	CB-CG	-6.19	1.40	1.52
1	B	35	GLU	CD-OE2	5.78	1.32	1.25
1	B	470	TYR	CE2-CZ	-5.72	1.31	1.38
1	B	418	TYR	CD2-CE2	5.09	1.47	1.39
1	A	80	SER	CB-OG	-5.05	1.35	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	LEU	CB-CG-CD2	15.32	137.05	111.00
1	B	314	ARG	NE-CZ-NH2	12.68	126.64	120.30
1	A	377	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	B	500	ASP	CB-CG-OD2	-10.31	109.03	118.30
1	B	267	LEU	CB-CG-CD2	9.84	127.72	111.00
1	B	275	ARG	CG-CD-NE	9.20	131.12	111.80
1	B	314	ARG	NE-CZ-NH1	-8.99	115.81	120.30
1	B	351	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	377	ARG	CB-CG-CD	-8.53	89.42	111.60
1	A	252	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	B	29	LEU	CB-CG-CD1	7.76	124.19	111.00
1	A	287	ARG	NE-CZ-NH1	-7.63	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	B	320	LEU	CB-CG-CD1	7.58	123.88	111.00
1	B	353	LYS	CA-CB-CG	7.57	130.06	113.40
1	A	377	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	47	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	B	54	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	283	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	267	LEU	CB-CG-CD1	-7.33	98.55	111.00
1	A	314	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	500	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	292	VAL	CA-CB-CG2	7.08	121.52	110.90
1	A	482	GLU	CB-CA-C	-6.95	96.50	110.40
1	B	275	ARG	CD-NE-CZ	6.85	133.19	123.60
1	A	168	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	A	221	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	290	GLN	CA-CB-CG	6.80	128.36	113.40
1	B	418	TYR	CB-CG-CD2	6.59	124.95	121.00
1	A	138	GLU	N-CA-C	-6.54	93.35	111.00
1	A	377	ARG	CD-NE-CZ	6.30	132.42	123.60
1	A	534	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	389	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	63	MET	CG-SD-CE	6.21	110.13	100.20
1	A	314	ARG	CA-CB-CG	6.19	127.01	113.40
1	A	307	ARG	CA-CB-CG	6.14	126.90	113.40
1	B	307	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	134	PHE	CB-CG-CD1	6.13	125.09	120.80
1	A	300	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	38	ASP	CB-CG-OD1	6.06	123.76	118.30
1	A	491	MET	CA-CB-CG	5.89	123.31	113.30
1	B	194	ASP	CB-CG-OD1	5.87	123.59	118.30
1	B	547	LEU	CB-CG-CD1	5.84	120.92	111.00
1	B	358	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	389	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	59	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	310	GLU	CG-CD-OE2	5.71	129.72	118.30
1	A	221	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	535	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	138	GLU	CA-C-N	5.64	127.49	116.20
1	B	90	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	206	LEU	CB-CG-CD1	5.58	120.49	111.00
1	A	435	GLU	CG-CD-OE1	5.53	129.36	118.30
1	B	283	ARG	NE-CZ-NH1	5.49	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	401	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	A	500	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	252	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	B	327	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	424	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	266	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	286	THR	CA-CB-CG2	5.34	119.88	112.40
1	B	284	PHE	CB-CG-CD1	5.20	124.44	120.80
1	A	27	GLU	CG-CD-OE2	5.18	128.67	118.30
1	A	395	GLU	CA-CB-CG	5.14	124.71	113.40
1	B	90	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	344	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	254	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	68	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	424	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	9	LEU	CB-CG-CD2	5.06	119.60	111.00
1	A	354	GLU	CG-CD-OE1	5.06	128.41	118.30
1	A	254	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	4311	0	4295	40	0
1	B	4385	0	4360	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	0	0	0
5	B	27	0	0	1	0
All	All	8801	0	8681	60	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 (60) 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:533:GLN:NE2	1:A:541:GLN:OE1	2.00	0.94
1:A:380:ASP:OD1	1:A:396:LYS:NZ	2.06	0.88
1:A:59:ARG:CD	1:A:206:LEU:HD21	2.06	0.85
1:A:59:ARG:CG	1:A:206:LEU:HD21	2.06	0.85
1:A:59:ARG:HD2	1:A:206:LEU:HD21	1.67	0.76
1:A:59:ARG:HG2	1:A:206:LEU:HD21	1.69	0.75
1:B:295:ALA:HA	1:B:298:VAL:HG22	1.72	0.71
1:B:455:ALA:HB1	1:B:458:GLN:HG2	1.73	0.71
1:B:337:ASN:O	1:B:340:ILE:HG13	1.92	0.69
1:A:126:THR:OG1	1:A:149:THR:HG22	1.93	0.69
1:B:477:GLN:OE1	1:B:478:PRO:HD2	1.92	0.68
1:B:424:ARG:NH2	1:A:27:GLU:OE1	2.27	0.67
1:A:85:GLY:O	1:A:90:ARG:NH2	2.27	0.66
1:A:59:ARG:HD2	1:A:206:LEU:CD2	2.26	0.65
1:B:438:HIS:O	1:B:441:ARG:HG2	1.99	0.62
1:A:135:HIS:O	1:A:138:GLU:O	2.20	0.59
1:B:303:GLU:HG3	1:B:307:ARG:HD2	1.85	0.57
1:A:55:ARG:HG3	1:A:63:MET:CE	2.35	0.56
1:A:247:LEU:HD23	1:A:389:ARG:CD	2.36	0.56
1:A:91:THR:O	1:A:94:SER:HB3	2.07	0.55
1:A:59:ARG:CD	1:A:206:LEU:CD2	2.82	0.54
1:B:451:TRP:CH2	1:B:456:ILE:HD12	2.42	0.54
1:A:254:ARG:NH2	1:A:256:PHE:HZ	2.06	0.53
1:B:390:LEU:HD21	1:B:393:MET:CE	2.40	0.52
1:A:114:ASP:OD2	1:A:133:THR:OG1	2.28	0.50
1:A:55:ARG:HG3	1:A:63:MET:HE3	1.94	0.49
1:B:13:GLN:NE2	5:B:801:HOH:O	2.36	0.49
1:B:155:ARG:NE	1:B:185:MET:HE2	2.28	0.49
1:B:295:ALA:HA	1:B:298:VAL:CG2	2.41	0.49
1:A:63:MET:CE	1:A:177:PRO:HB3	2.43	0.49
1:A:331:MET:HA	1:A:331:MET:HE2	1.94	0.49
1:B:155:ARG:CZ	1:B:185:MET:HE2	2.44	0.47
1:B:390:LEU:HD21	1:B:393:MET:HE3	1.97	0.46
1:A:292:VAL:O	1:A:296:GLU:HG3	2.17	0.45
1:A:533:GLN:NE2	1:A:541:GLN:CD	2.68	0.45
1:B:529:PRO:O	1:B:531:PRO:HD3	2.15	0.45
1:B:345:GLU:O	1:B:348:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ALA:HB1	1:B:458:GLN:CG	2.43	0.44
1:A:154:THR:OG1	1:A:156:GLU:HG3	2.17	0.44
1:B:8:SER:O	1:A:164:LYS:HE2	2.18	0.44
1:A:456:ILE:CD1	1:A:464:PHE:CD1	3.02	0.43
1:B:311:SER:O	1:B:315:THR:HG22	2.19	0.43
1:A:120:LYS:HD3	1:A:125:MET:CE	2.48	0.43
1:B:496:THR:HG22	1:B:507:THR:HG22	1.99	0.43
1:A:247:LEU:HD23	1:A:389:ARG:HD3	2.01	0.42
1:A:247:LEU:HD22	1:A:248:TYR:CZ	2.54	0.42
1:A:372:VAL:HG22	1:A:410:VAL:HG22	2.02	0.42
1:A:502:CYS:O	1:A:503:LEU:HB2	2.19	0.42
1:A:167:ILE:O	1:A:170:GLU:HG3	2.20	0.42
1:A:316:LEU:HD23	1:A:335:VAL:HG21	2.00	0.42
1:A:292:VAL:HG12	1:A:356:LYS:HB3	2.02	0.41
1:B:179:ARG:HG3	1:B:179:ARG:O	2.20	0.41
1:A:287:ARG:HA	1:A:290:GLN:HG2	2.02	0.41
1:A:456:ILE:HD13	1:A:456:ILE:HA	1.85	0.41
1:A:456:ILE:HD11	1:A:464:PHE:CE1	2.56	0.41
1:A:480:SER:OG	1:A:482:GLU:HG3	2.21	0.41
1:A:501:LEU:HD12	1:A:524:VAL:HG21	2.02	0.41
1:A:266:ARG:HE	1:A:266:ARG:HB3	1.72	0.40
1:A:63:MET:HE2	1:A:177:PRO:HB3	2.02	0.40
1:B:297:HIS:O	1:B:301:ILE:HG12	2.22	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	526/606 (87%)	510 (97%)	16 (3%)	0	100 100
1	B	534/606 (88%)	519 (97%)	14 (3%)	1 (0%)	47 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1060/1212 (88%)	1029 (97%)	30 (3%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	ASP

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	464/533 (87%)	433 (93%)	31 (7%)	16 31
1	B	473/533 (89%)	441 (93%)	32 (7%)	16 30
All	All	937/1066 (88%)	874 (93%)	63 (7%)	16 31

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	THR
1	B	238	ARG
1	B	266	ARG
1	B	267	LEU
1	B	275	ARG
1	B	283	ARG
1	B	287	ARG
1	B	301	ILE
1	B	307	ARG
1	B	312	LYS
1	B	318	VAL
1	B	320	LEU
1	B	325	THR
1	B	344	ARG
1	B	351	ARG
1	B	353	LYS
1	B	375	GLU

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Mol	Chain	Res	Type
1	B	389	ARG
1	B	392	LYS
1	B	401	LEU
1	B	405	MET
1	B	419	LEU
1	B	424	ARG
1	B	429	ASP
1	B	449	GLN
1	B	459	ARG
1	B	486	LYS
1	B	493	ILE
1	B	500	ASP
1	B	517	LYS
1	B	535	ARG
1	B	549	THR
1	A	9	LEU
1	A	27	GLU
1	A	56	GLU
1	A	80	SER
1	A	90	ARG
1	A	155	ARG
1	A	160	ASP
1	A	163	GLU
1	A	170	GLU
1	A	179	ARG
1	A	227	GLU
1	A	252	ARG
1	A	265	LYS
1	A	284	PHE
1	A	290	GLN
1	A	293	LYS
1	A	300	ARG
1	A	307	ARG
1	A	314	ARG
1	A	327	ASP
1	A	344	ARG
1	A	395	GLU
1	A	429	ASP
1	A	441	ARG
1	A	449	GLN
1	A	456	ILE
1	A	461	ILE

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Mol	Chain	Res	Type
1	A	487	ARG
1	A	534	ASP
1	A	535	ARG
1	A	537	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	ANP	B	702	4	29,33,33	2.23	8 (27%)	31,52,52	2.46	9 (29%)
3	ANP	A	702	4	29,33,33	2.09	9 (31%)	31,52,52	2.37	10 (32%)

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
3	ANP	B	702	4	-	4/14/38/38	0/3/3/3
3	ANP	A	702	4	-	3/14/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ANP	PG-N3B	5.78	1.78	1.63
3	A	702	ANP	PB-O1B	5.02	1.54	1.46
3	B	702	ANP	PB-O1B	4.68	1.53	1.46
3	B	702	ANP	PG-O1G	4.42	1.53	1.46
3	A	702	ANP	PB-O3A	3.80	1.63	1.59
3	A	702	ANP	PB-N3B	3.80	1.73	1.63
3	A	702	ANP	PG-O1G	3.68	1.52	1.46
3	B	702	ANP	PB-O3A	3.61	1.63	1.59
3	A	702	ANP	PG-N3B	3.54	1.72	1.63
3	B	702	ANP	C5-C4	3.05	1.49	1.40
3	A	702	ANP	PB-O2B	-2.96	1.48	1.56
3	A	702	ANP	C5-C4	2.93	1.48	1.40
3	B	702	ANP	PB-N3B	2.73	1.70	1.63
3	B	702	ANP	O4'-C1'	2.60	1.44	1.41
3	B	702	ANP	C2'-C1'	-2.45	1.50	1.53
3	A	702	ANP	O4'-C1'	2.37	1.44	1.41
3	A	702	ANP	PG-O2G	-2.06	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	ANP	O1G-PG-N3B	-9.09	98.39	111.77
3	A	702	ANP	O1B-PB-N3B	-7.77	100.33	111.77
3	A	702	ANP	O2B-PB-O1B	5.64	121.75	109.92
3	B	702	ANP	O3G-PG-O1G	4.76	125.42	113.45
3	A	702	ANP	O1G-PG-N3B	-4.70	104.84	111.77
3	B	702	ANP	PA-O3A-PB	-4.23	117.73	132.62
3	B	702	ANP	C4-C5-N7	-3.98	105.25	109.40
3	B	702	ANP	O1B-PB-N3B	-3.10	107.20	111.77
3	A	702	ANP	PA-O3A-PB	-3.04	121.91	132.62
3	A	702	ANP	N3-C2-N1	-2.94	124.08	128.68
3	A	702	ANP	C2-N1-C6	2.83	123.59	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	ANP	O3G-PG-O2G	2.82	115.16	107.64
3	B	702	ANP	O2B-PB-O1B	2.21	114.56	109.92
3	B	702	ANP	C5-C6-N6	2.19	123.69	120.35
3	B	702	ANP	C3'-C2'-C1'	2.18	104.25	100.98
3	A	702	ANP	C3'-C2'-C1'	2.15	104.22	100.98
3	B	702	ANP	O2A-PA-O1A	2.09	122.58	112.24
3	A	702	ANP	O2'-C2'-C3'	-2.05	105.18	111.82
3	A	702	ANP	C1'-N9-C4	-2.03	123.08	126.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

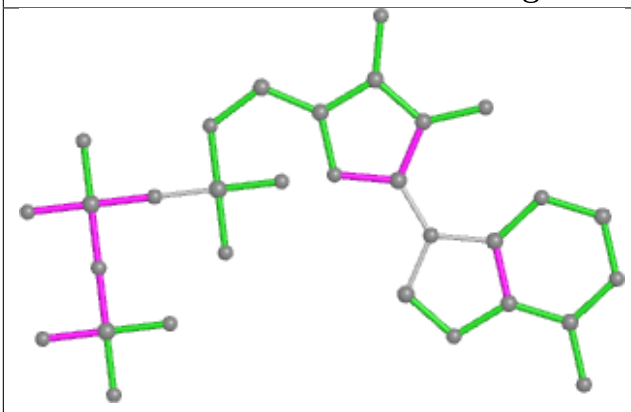
Mol	Chain	Res	Type	Atoms
3	B	702	ANP	PA-O3A-PB-O1B
3	B	702	ANP	PA-O3A-PB-O2B
3	A	702	ANP	PB-N3B-PG-O1G
3	A	702	ANP	PA-O3A-PB-O1B
3	A	702	ANP	PA-O3A-PB-O2B
3	B	702	ANP	C5'-O5'-PA-O3A
3	B	702	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

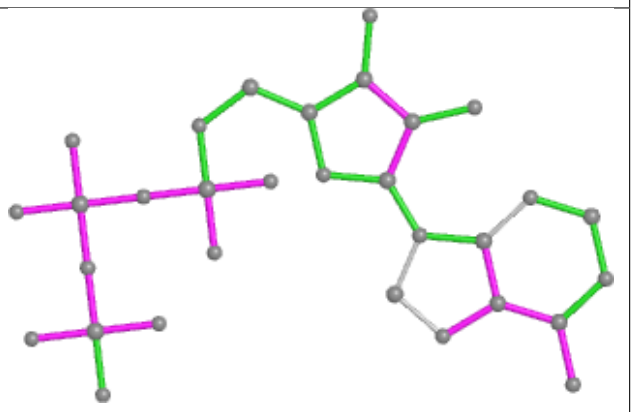
No monomer is involved in short contacts.

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.

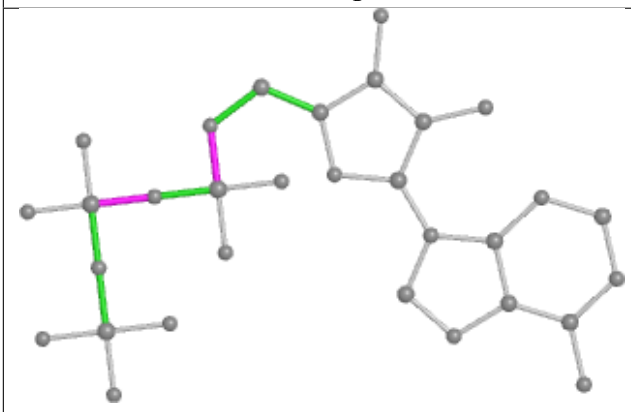
Ligand ANP B 702



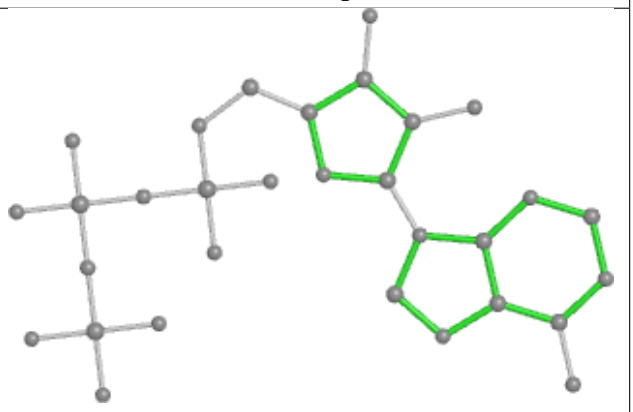
Bond lengths



Bond angles

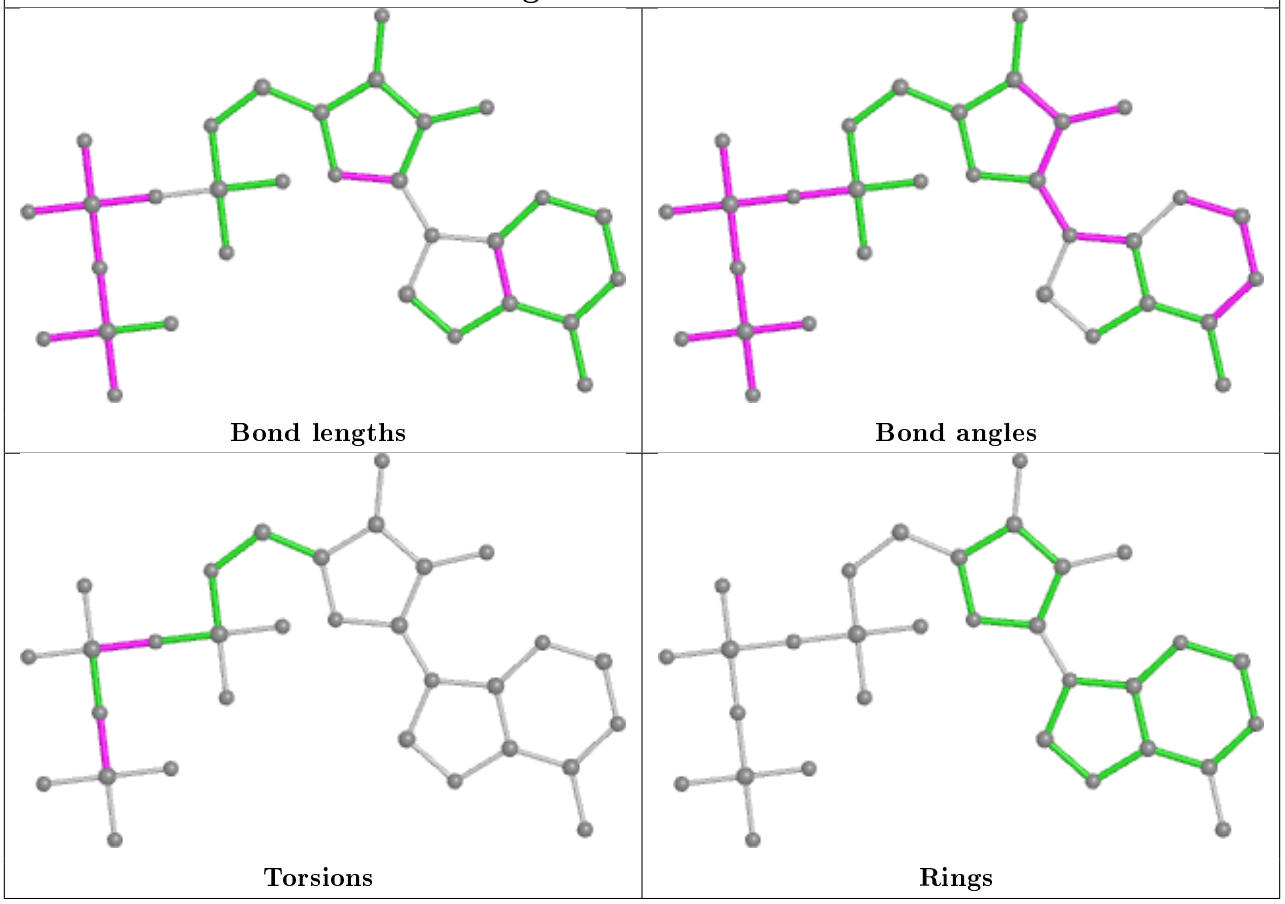


Torsions



Rings

Ligand ANP A 702



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, 95^{th} 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	531/606 (87%)	0.49	20 (3%)	40	36	53, 92, 146, 176	0
1	B	540/606 (89%)	0.52	27 (5%)	28	25	47, 84, 143, 183	0
All	All	1071/1212 (88%)	0.51	47 (4%)	34	30	47, 88, 145, 183	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	LEU	6.4
1	A	150	TRP	6.0
1	B	458	GLN	6.0
1	B	468	PHE	4.7
1	B	521	ASP	3.8
1	B	326	ARG	3.6
1	B	93	GLU	3.5
1	A	463	LYS	3.4
1	A	508	LEU	3.1
1	B	320	LEU	3.1
1	B	483	LEU	3.0
1	B	475	TRP	3.0
1	B	454	ILE	3.0
1	B	94	SER	3.0
1	B	464	PHE	3.0
1	A	61	GLY	2.9
1	B	466	ASP	2.8
1	A	466	ASP	2.8
1	A	543	GLN	2.8
1	A	461	ILE	2.8
1	B	179	ARG	2.7
1	A	194	ASP	2.7
1	A	320	LEU	2.6
1	B	461	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	550	PHE	2.6
1	A	75	PRO	2.5
1	A	247	LEU	2.5
1	B	470	TYR	2.4
1	A	94	SER	2.4
1	B	351	ARG	2.4
1	A	153	ARG	2.4
1	B	116	ILE	2.4
1	B	485	TYR	2.4
1	A	333	ARG	2.3
1	B	333	ARG	2.2
1	B	403	GLY	2.2
1	A	62	PHE	2.2
1	B	324	LEU	2.2
1	A	78	ALA	2.1
1	A	227	GLU	2.1
1	A	147	LEU	2.1
1	B	456	ILE	2.0
1	B	516	GLU	2.0
1	A	178	PHE	2.0
1	B	459	ARG	2.0
1	B	368	PHE	2.0
1	B	541	GLN	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 carbohydrates 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, 95^{th} 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.

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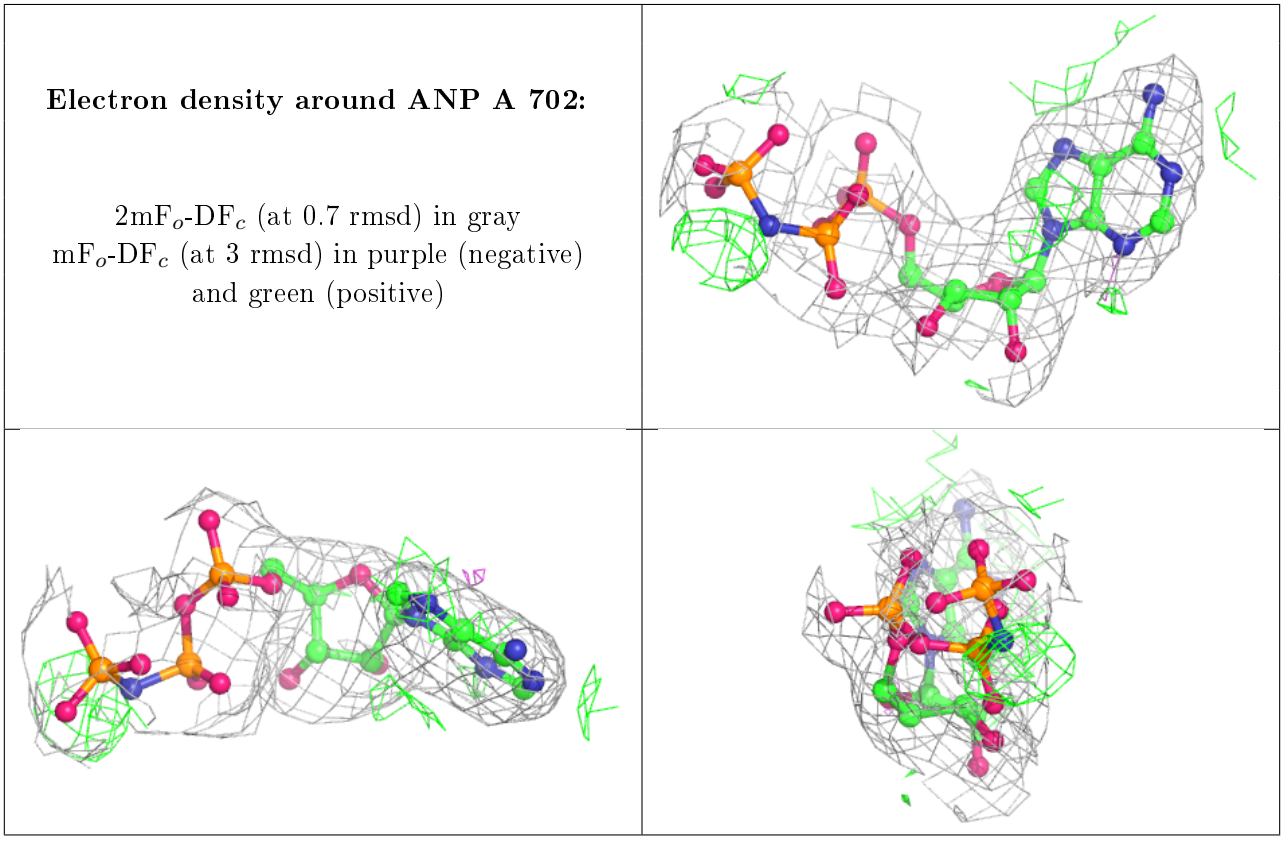
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	701	1/1	0.66	0.15	113,113,113,113	0
2	ZN	B	701	1/1	0.66	0.24	81,81,81,81	0
4	MG	B	703	1/1	0.90	0.19	49,49,49,49	0
4	MG	A	703	1/1	0.97	0.08	49,49,49,49	0
3	ANP	A	702	31/31	0.97	0.16	41,55,66,69	0
3	ANP	B	702	31/31	0.99	0.17	33,43,50,58	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.

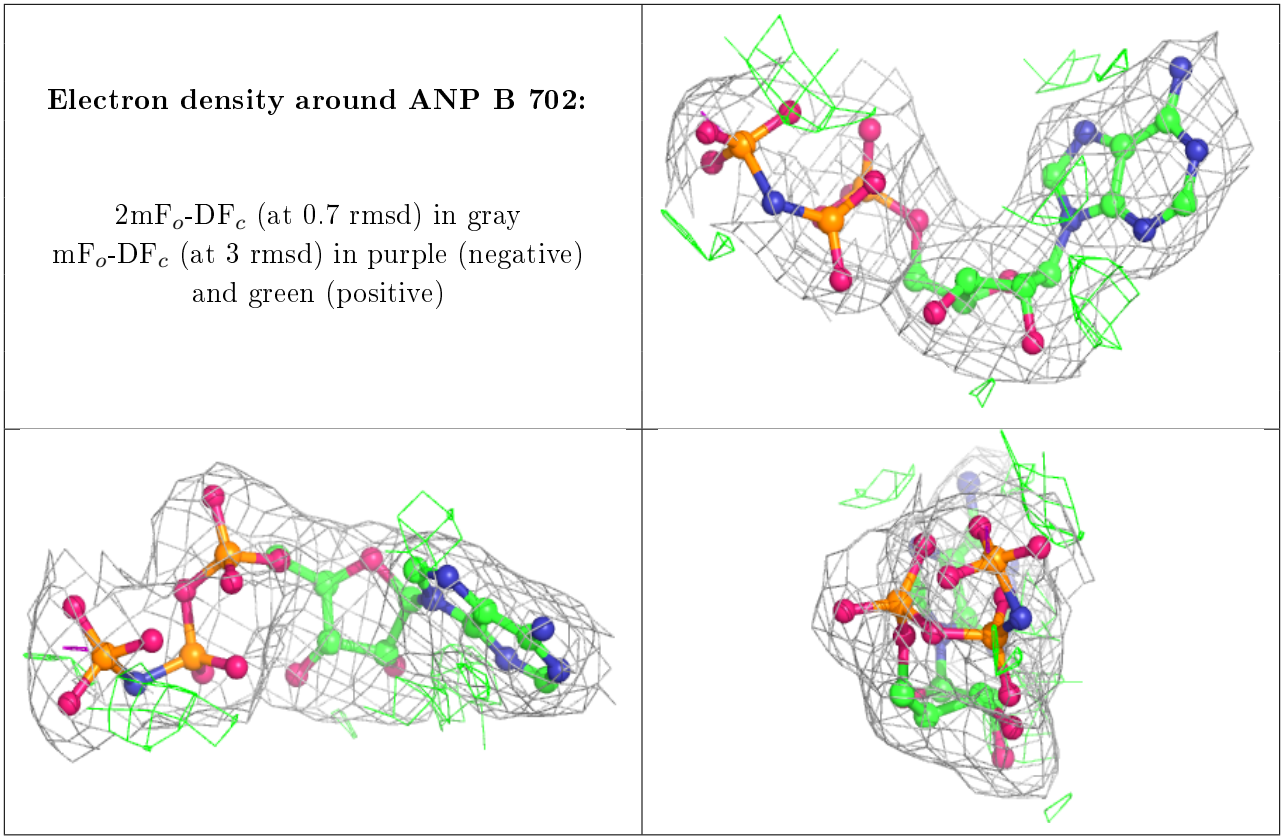
Electron density around ANP A 702:

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



Electron density around ANP B 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

There are no such residues in this entry.