



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:55 PM UTC

PDB ID : 6N7E / pdb_00006n7e
Title : Crystal structure of the cytosolic domain of human CNNM2 in complex with AMP-PNP and Mg²⁺
Authors : Chen, Y.S.; Gehring, K.
Deposited on : 2018-11-27
Resolution : 3.50 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

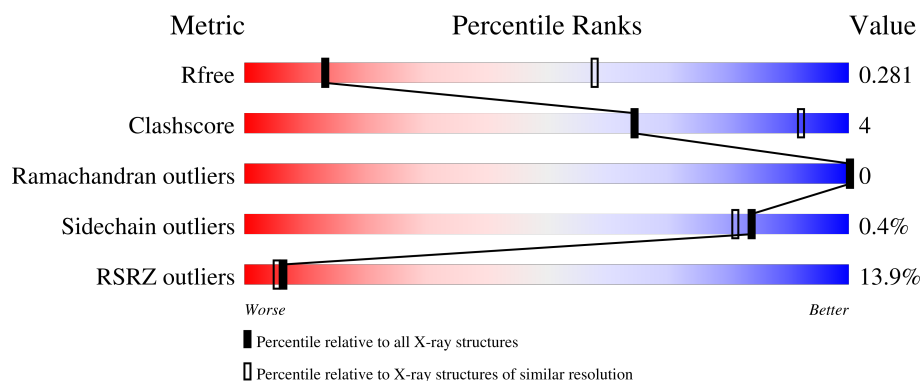
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	354	
1	B	354	
1	C	354	
1	D	354	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18135 atoms, of which 8720 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 Metal transporter CNNM2,Metal transporter CNNM2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	H	N	O	S	0	0	0
			4483	1493	2169	369	439	13			
1	B	300	Total	C	H	N	O	S	0	0	0
			4506	1487	2195	372	439	13			
1	C	302	Total	C	H	N	O	S	0	0	0
			4369	1457	2104	365	432	11			
1	D	319	Total	C	H	N	O	S	0	0	0
			4591	1539	2202	386	453	11			

There are 40 discrepancies between the modelled and reference sequences:

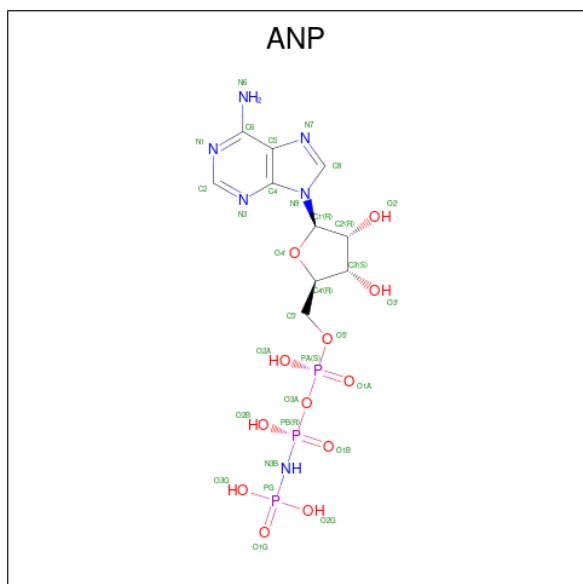
Chain	Residue	Modelled	Actual	Comment	Reference
A	428	MET	-	expression tag	UNP Q9H8M5
A	767	VAL	-	linker	UNP Q9H8M5
A	818	LEU	-	expression tag	UNP Q9H8M5
A	819	GLU	-	expression tag	UNP Q9H8M5
A	820	HIS	-	expression tag	UNP Q9H8M5
A	821	HIS	-	expression tag	UNP Q9H8M5
A	822	HIS	-	expression tag	UNP Q9H8M5
A	823	HIS	-	expression tag	UNP Q9H8M5
A	824	HIS	-	expression tag	UNP Q9H8M5
A	825	HIS	-	expression tag	UNP Q9H8M5
B	428	MET	-	expression tag	UNP Q9H8M5
B	767	VAL	-	linker	UNP Q9H8M5
B	818	LEU	-	expression tag	UNP Q9H8M5
B	819	GLU	-	expression tag	UNP Q9H8M5
B	820	HIS	-	expression tag	UNP Q9H8M5
B	821	HIS	-	expression tag	UNP Q9H8M5
B	822	HIS	-	expression tag	UNP Q9H8M5
B	823	HIS	-	expression tag	UNP Q9H8M5
B	824	HIS	-	expression tag	UNP Q9H8M5
B	825	HIS	-	expression tag	UNP Q9H8M5
C	428	MET	-	expression tag	UNP Q9H8M5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	723	VAL	-	linker	UNP Q9H8M5
C	818	LEU	-	expression tag	UNP Q9H8M5
C	819	GLU	-	expression tag	UNP Q9H8M5
C	820	HIS	-	expression tag	UNP Q9H8M5
C	821	HIS	-	expression tag	UNP Q9H8M5
C	822	HIS	-	expression tag	UNP Q9H8M5
C	823	HIS	-	expression tag	UNP Q9H8M5
C	824	HIS	-	expression tag	UNP Q9H8M5
C	825	HIS	-	expression tag	UNP Q9H8M5
D	428	MET	-	expression tag	UNP Q9H8M5
D	723	VAL	-	linker	UNP Q9H8M5
D	818	LEU	-	expression tag	UNP Q9H8M5
D	819	GLU	-	expression tag	UNP Q9H8M5
D	820	HIS	-	expression tag	UNP Q9H8M5
D	821	HIS	-	expression tag	UNP Q9H8M5
D	822	HIS	-	expression tag	UNP Q9H8M5
D	823	HIS	-	expression tag	UNP Q9H8M5
D	824	HIS	-	expression tag	UNP Q9H8M5
D	825	HIS	-	expression tag	UNP Q9H8M5

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			43	10	12	6	12	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	
			44	10	13	6	12	3	
2	C	1	Total	C	H	N	O	P	
			44	10	13	6	12	3	
2	D	1	Total	C	H	N	O	P	
			43	10	12	6	12	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg		
			2	2	0	0
3	B	3	Total	Mg		
			3	3	0	0
3	C	1	Total	Mg		
			1	1	0	0
3	D	2	Total	Mg		
			2	2	0	0

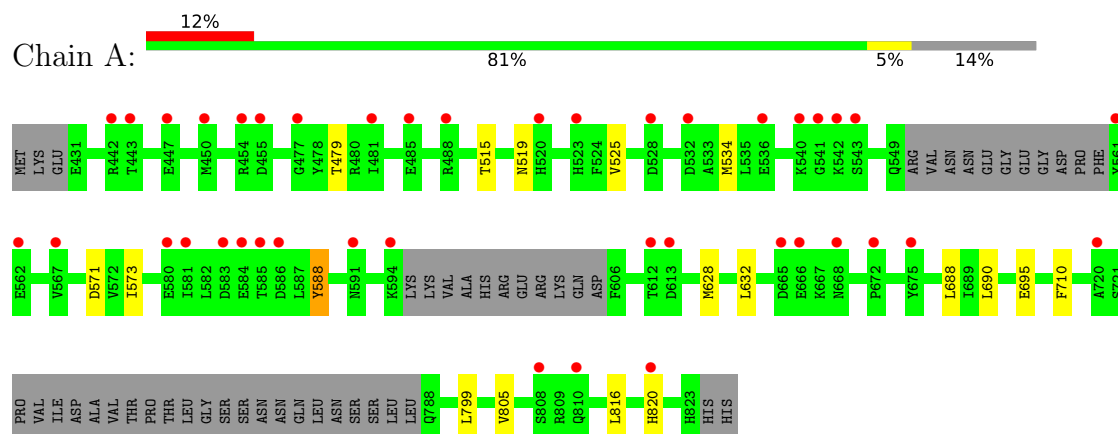
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O		
			2	2	0	0
4	C	1	Total	O		
			1	1	0	0
4	D	1	Total	O		
			1	1	0	0

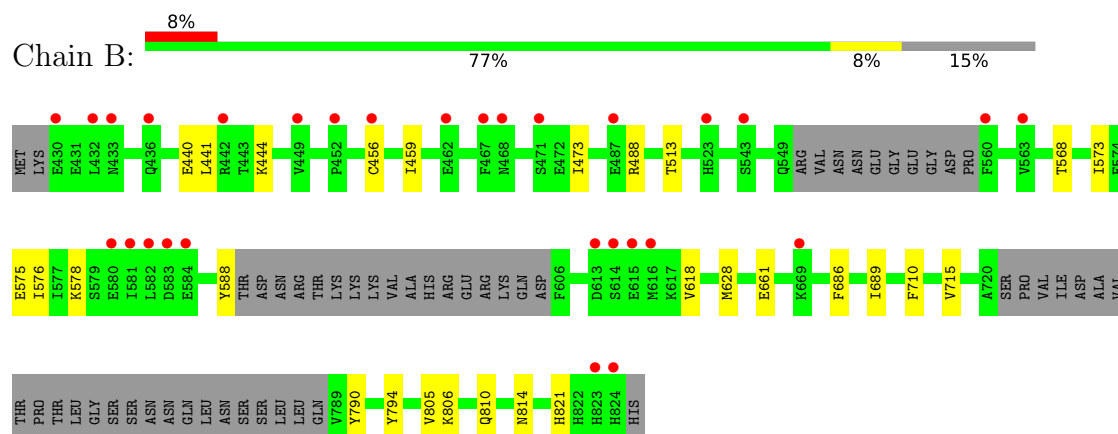
3 Residue-property plots [i](#)

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.

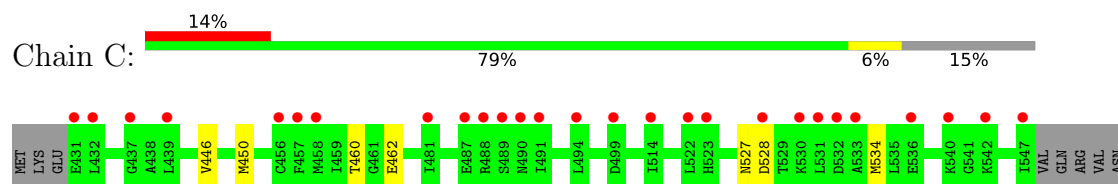
- Molecule 1: Metal transporter CNNM2, Metal transporter CNNM2

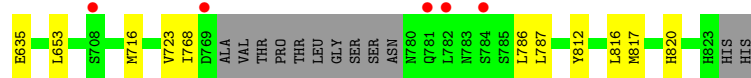


- Molecule 1: Metal transporter CNNM2, Metal transporter CNNM2

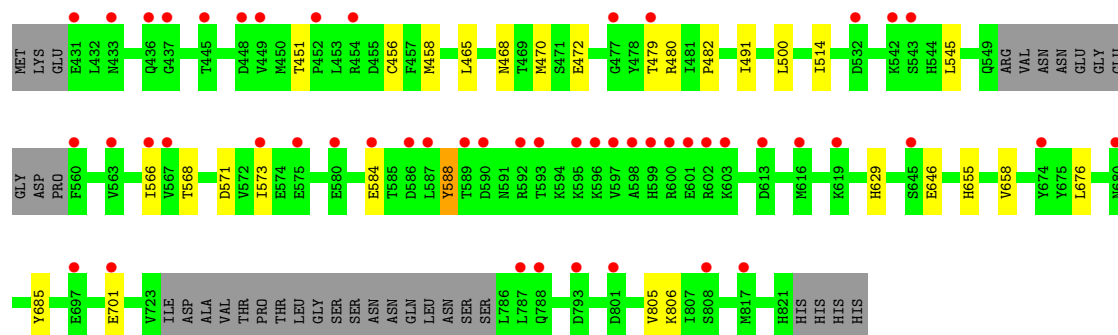


- Molecule 1: Metal transporter CNNM2, Metal transporter CNNM2





Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	290.58Å 111.14Å 103.52Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	48.76 – 3.50 48.76 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.76-3.50) 84.8 (48.76-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.282 , 0.282 0.241 , 0.281	Depositor DCC
R_{free} test set	2000 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	18135	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/2358	0.31	0/3207
1	B	0.10	0/2355	0.26	0/3197
1	C	0.11	0/2307	0.28	0/3141
1	D	0.11	0/2436	0.30	0/3320
All	All	0.11	0/9456	0.29	0/12865

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	2314	2169	2165	18	0
1	B	2311	2195	2195	18	0
1	C	2265	2104	2102	17	0
1	D	2389	2202	2201	22	0
2	A	31	12	13	2	0
2	B	31	13	13	1	0
2	C	31	13	13	0	0
2	D	31	12	13	7	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
All	All	9415	8720	8715	71	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 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:D:676:LEU:O	1:D:685:TYR:OH	2.00	0.79
1:B:573:ILE:HD13	1:C:573:ILE:HG21	1.67	0.77
1:B:441:LEU:HD21	1:B:576:ILE:HD11	1.69	0.75
1:B:444:LYS:NZ	1:B:575:GLU:OE1	2.13	0.72
1:B:513:THR:OG1	1:C:635:GLU:OE2	2.18	0.62
1:B:628:MET:SD	1:B:805:VAL:HG21	2.40	0.62
1:B:810:GLN:O	1:B:814:ASN:ND2	2.32	0.60
1:C:786:LEU:O	1:C:787:LEU:HD12	2.00	0.60
1:A:628:MET:HE2	1:A:690:LEU:HD22	1.86	0.58
1:B:686:PHE:CE1	1:B:715:VAL:HG22	2.39	0.57
1:C:723:VAL:HG21	1:C:786:LEU:HA	1.85	0.57
1:D:451:THR:HG21	2:D:901:ANP:O2'	2.05	0.56
1:C:583:ASP:OD1	1:C:584:GLU:N	2.38	0.56
1:A:628:MET:SD	1:A:710:PHE:CE1	2.98	0.56
1:D:568:THR:HG21	2:D:901:ANP:O1A	2.06	0.55
1:A:628:MET:HE2	1:A:690:LEU:CD2	2.38	0.53
1:A:628:MET:HE3	1:A:628:MET:HA	1.91	0.53
1:C:723:VAL:CG2	1:C:786:LEU:C	2.81	0.53
1:B:456:CYS:O	1:B:488:ARG:NH1	2.42	0.52
1:A:515:THR:O	1:A:519:ASN:N	2.41	0.51
1:A:571:ASP:OD2	2:A:901:ANP:O2'	2.16	0.51
1:D:701:GLU:OE1	4:D:1001:HOH:O	2.19	0.51
1:B:686:PHE:HE1	1:B:715:VAL:HG22	1.74	0.51
1:A:573:ILE:HD13	1:D:573:ILE:HG21	1.92	0.50
1:B:441:LEU:CD2	1:B:576:ILE:HD11	2.38	0.50
1:C:446:VAL:O	1:C:450:MET:N	2.44	0.49
1:B:790:TYR:HH	1:B:794:TYR:HH	1.59	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:MET:SD	1:A:690:LEU:HD22	2.53	0.48
1:A:588:TYR:CD2	1:A:588:TYR:N	2.82	0.48
1:C:723:VAL:O	1:C:723:VAL:HG12	2.14	0.48
1:D:456:CYS:SG	1:D:566:ILE:HD12	2.55	0.47
1:C:446:VAL:HG11	1:C:534:MET:CE	2.45	0.47
1:D:480:ARG:HH12	2:D:901:ANP:HNB1	1.62	0.47
1:C:716:MET:HE1	1:D:701:GLU:HG3	1.96	0.47
1:D:588:TYR:CD2	1:D:588:TYR:C	2.93	0.46
1:C:527:ASN:OD1	1:C:528:ASP:N	2.48	0.46
1:B:440:GLU:OE1	1:B:578:LYS:NZ	2.48	0.46
1:A:628:MET:CE	1:A:690:LEU:HD22	2.46	0.46
1:D:479:THR:OG1	2:D:901:ANP:O1B	2.22	0.46
1:D:465:LEU:HD12	1:D:514:ILE:HD12	1.98	0.45
1:B:459:ILE:CD1	1:B:473:ILE:HD11	2.47	0.45
1:B:568:THR:HG21	2:B:901:ANP:O2A	2.16	0.45
1:C:723:VAL:HG22	1:C:787:LEU:N	2.32	0.45
1:A:816:LEU:O	1:A:820:HIS:ND1	2.44	0.44
1:B:689:ILE:O	1:B:710:PHE:N	2.41	0.44
1:D:571:ASP:OD1	2:D:901:ANP:O3'	2.24	0.44
1:A:632:LEU:HD21	1:A:688:LEU:HD22	1.99	0.44
1:D:655:HIS:O	1:D:658:VAL:HG22	2.18	0.44
1:D:584:GLU:OE2	2:D:901:ANP:O2A	2.36	0.44
1:A:710:PHE:CD1	1:A:710:PHE:N	2.86	0.43
1:A:695:GLU:N	1:A:799:LEU:HD11	2.33	0.43
1:D:482:PRO:HG2	1:D:566:ILE:HD11	1.99	0.43
1:B:459:ILE:HD12	1:B:473:ILE:HD11	2.00	0.43
1:C:723:VAL:O	1:C:768:ILE:C	2.61	0.43
1:D:584:GLU:OE2	2:D:901:ANP:O2B	2.36	0.42
1:C:817:MET:O	1:C:820:HIS:ND1	2.48	0.42
1:D:629:HIS:NE2	1:D:646:GLU:HG3	2.34	0.42
1:C:812:TYR:CE2	1:C:816:LEU:HD11	2.54	0.42
1:D:470:MET:HE3	1:D:500:LEU:HD13	2.01	0.42
1:C:628:MET:HE3	1:C:653:LEU:HD22	2.02	0.42
1:D:458:MET:HE1	1:D:491:ILE:HD11	2.01	0.41
1:D:545:LEU:C	1:D:545:LEU:HD23	2.45	0.41
1:A:688:LEU:HD11	1:A:710:PHE:HA	2.02	0.41
1:A:690:LEU:HD21	1:A:805:VAL:HG23	2.01	0.41
1:C:460:THR:HG22	1:C:462:GLU:H	1.85	0.41
1:D:468:ASN:O	1:D:472:GLU:HG3	2.20	0.41
1:B:618:VAL:HG11	1:B:661:GLU:HG3	2.02	0.41
1:B:686:PHE:O	1:B:806:LYS:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:805:VAL:HG12	1:D:806:LYS:N	2.35	0.41
1:A:479:THR:OG1	2:A:901:ANP:O2G	2.36	0.41
1:A:525:VAL:HG21	1:A:534:MET:HE1	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	297/354 (84%)	285 (96%)	12 (4%)	0	100	100
1	B	292/354 (82%)	276 (94%)	16 (6%)	0	100	100
1	C	294/354 (83%)	281 (96%)	13 (4%)	0	100	100
1	D	313/354 (88%)	295 (94%)	18 (6%)	0	100	100
All	All	1196/1416 (84%)	1137 (95%)	59 (5%)	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	234/322 (73%)	233 (100%)	1 (0%)	84	81
1	B	240/322 (74%)	238 (99%)	2 (1%)	73	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	227/322 (70%)	227 (100%)	0	100	100
1	D	235/322 (73%)	234 (100%)	1 (0%)	84	81
All	All	936/1288 (73%)	932 (100%)	4 (0%)	84	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	TYR
1	B	588	TYR
1	B	821	HIS
1	D	588	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	660	GLN
1	D	544	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 12 ligands modelled in this entry, 8 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	ANP	B	901	3	33,33,33	0.96	4 (12%)	45,52,52	0.55	0
2	ANP	C	901	3	33,33,33	0.95	4 (12%)	45,52,52	0.57	0
2	ANP	D	901	3	33,33,33	0.94	4 (12%)	45,52,52	0.75	1 (2%)
2	ANP	A	901	3	33,33,33	0.93	4 (12%)	45,52,52	0.58	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	ANP	B	901	3	-	9/18/38/38	0/3/3/3
2	ANP	C	901	3	-	6/18/38/38	0/3/3/3
2	ANP	D	901	3	-	7/18/38/38	0/3/3/3
2	ANP	A	901	3	-	2/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ANP	PG-O1G	2.64	1.50	1.46
2	C	901	ANP	PG-O1G	2.62	1.50	1.46
2	A	901	ANP	PG-O1G	2.60	1.50	1.46
2	D	901	ANP	PG-O1G	2.59	1.50	1.46
2	B	901	ANP	PB-O3A	-2.52	1.55	1.59
2	C	901	ANP	PB-O1B	2.47	1.49	1.46
2	D	901	ANP	PG-N3B	2.44	1.69	1.63
2	A	901	ANP	PB-O1B	2.44	1.49	1.46
2	A	901	ANP	PG-N3B	2.43	1.69	1.63
2	D	901	ANP	PB-O3A	-2.43	1.56	1.59
2	B	901	ANP	PB-O1B	2.41	1.49	1.46
2	C	901	ANP	PG-N3B	2.39	1.69	1.63
2	B	901	ANP	PG-N3B	2.38	1.69	1.63
2	C	901	ANP	PB-O3A	-2.36	1.56	1.59
2	D	901	ANP	PB-O1B	2.29	1.49	1.46
2	A	901	ANP	PB-O3A	-2.24	1.56	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	ANP	C3'-C2'-C1'	2.21	105.64	101.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PB-N3B-PG-O1G
2	B	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PA-O3A-PB-O2B
2	B	901	ANP	C5'-O5'-PA-O3A
2	B	901	ANP	O4'-C4'-C5'-O5'
2	C	901	ANP	PB-N3B-PG-O1G
2	C	901	ANP	C5'-O5'-PA-O2A
2	C	901	ANP	C5'-O5'-PA-O3A
2	C	901	ANP	O4'-C4'-C5'-O5'
2	D	901	ANP	PB-N3B-PG-O1G
2	D	901	ANP	PG-N3B-PB-O1B
2	D	901	ANP	C5'-O5'-PA-O2A
2	B	901	ANP	C3'-C4'-C5'-O5'
2	C	901	ANP	C3'-C4'-C5'-O5'
2	D	901	ANP	O4'-C4'-C5'-O5'
2	D	901	ANP	C3'-C4'-C5'-O5'
2	B	901	ANP	C5'-O5'-PA-O1A
2	D	901	ANP	C5'-O5'-PA-O1A
2	D	901	ANP	C5'-O5'-PA-O3A
2	B	901	ANP	PB-O3A-PA-O2A
2	B	901	ANP	PA-O3A-PB-O1B
2	A	901	ANP	PB-N3B-PG-O1G
2	C	901	ANP	PB-O3A-PA-O1A

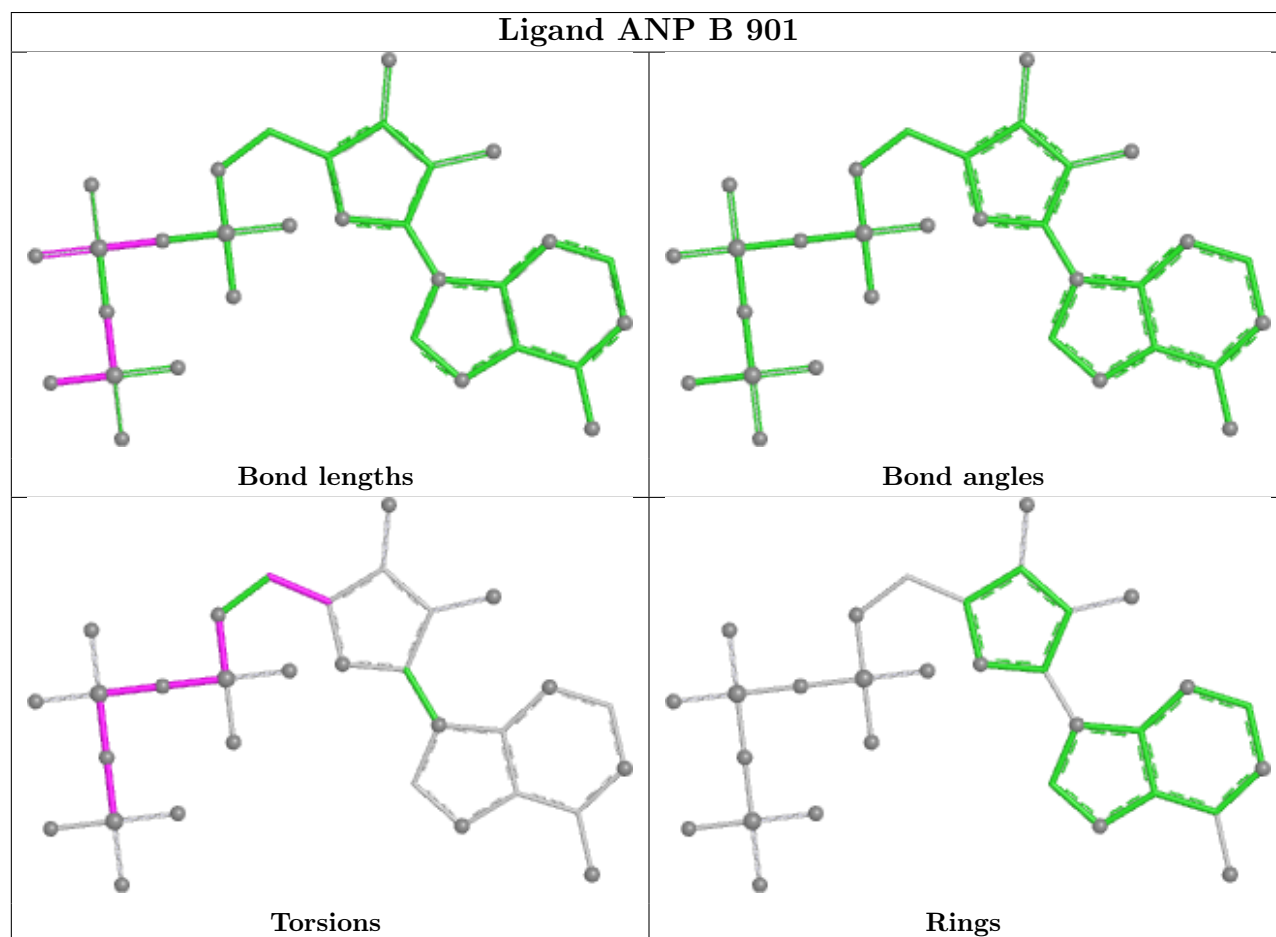
There are no ring outliers.

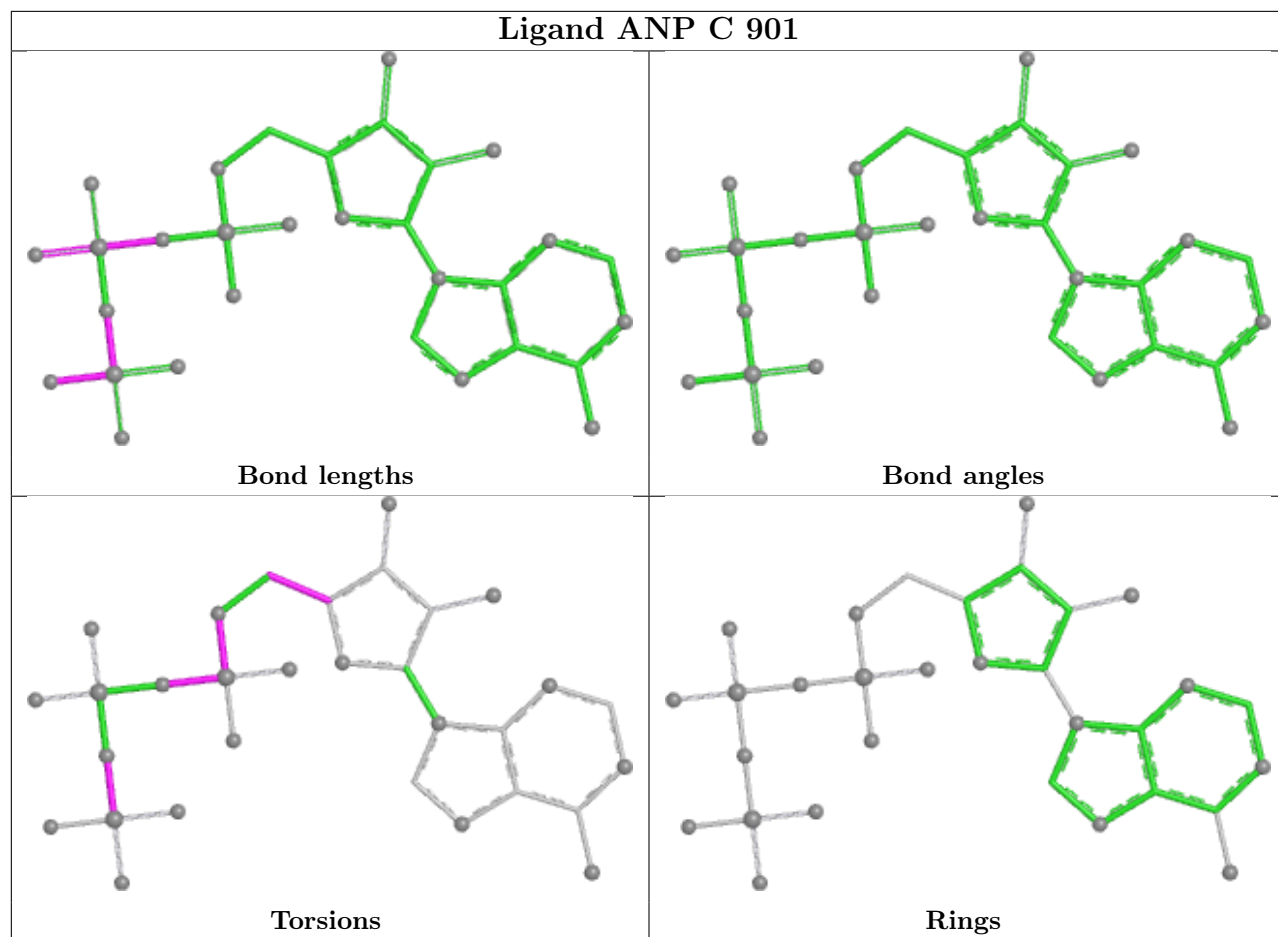
3 monomers are involved in 10 short contacts:

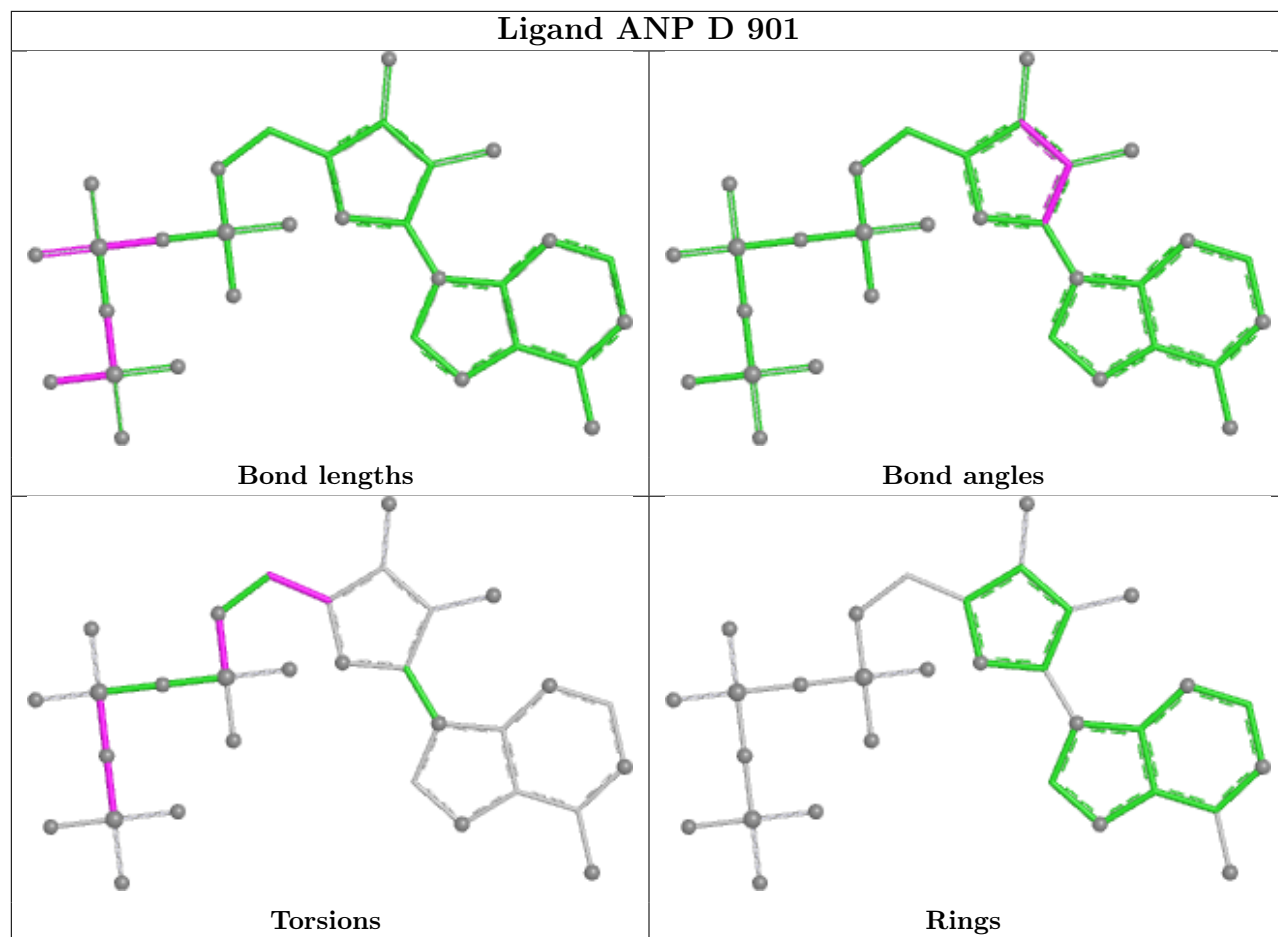
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ANP	1	0
2	D	901	ANP	7	0
2	A	901	ANP	2	0

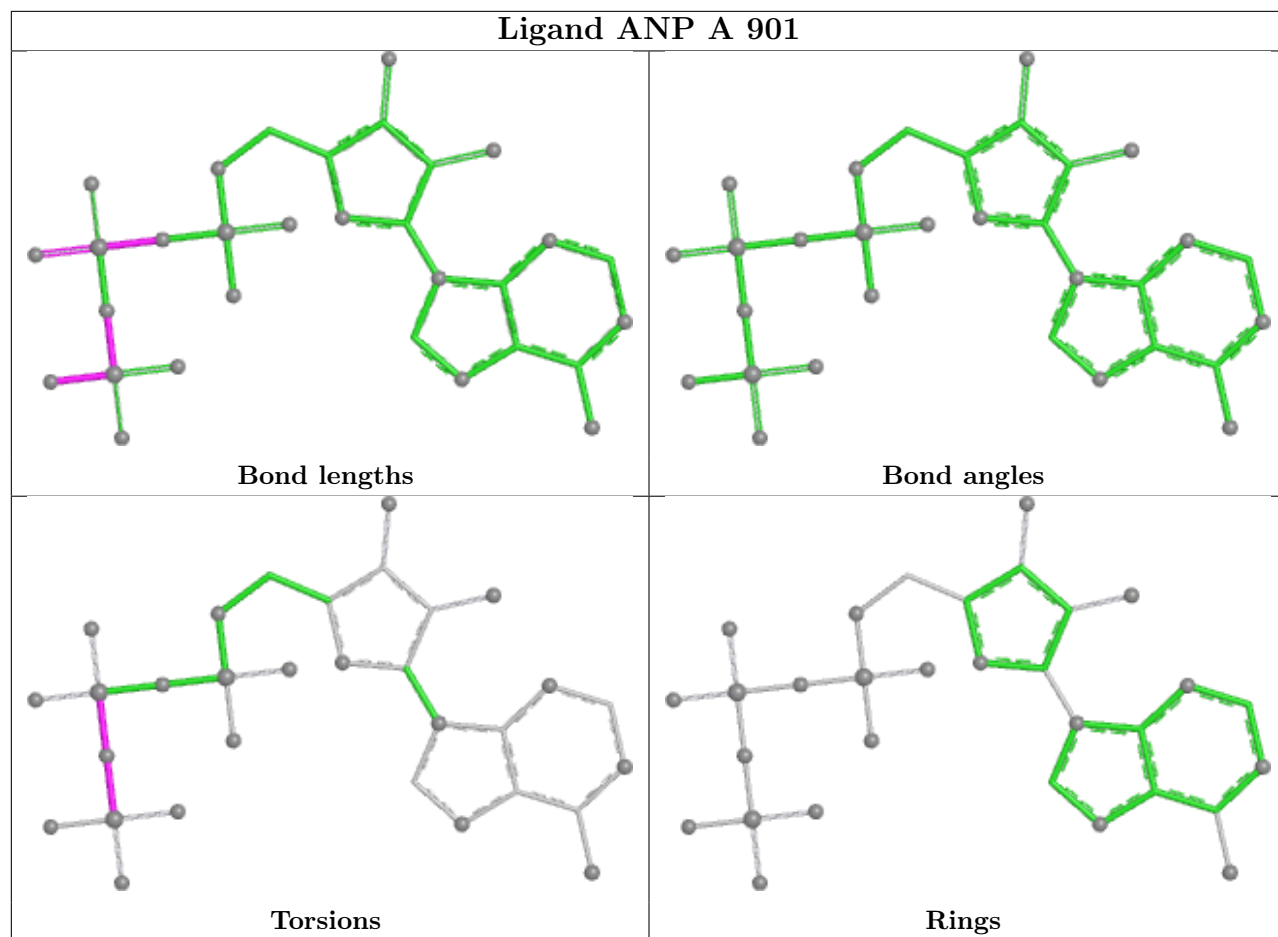
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/354 (86%)	0.96	41 (13%) 7 6	12, 75, 139, 205	0
1	B	300/354 (84%)	0.61	29 (9%) 13 9	6, 65, 124, 168	0
1	C	302/354 (85%)	0.95	49 (16%) 4 4	7, 79, 145, 270	0
1	D	319/354 (90%)	1.06	51 (15%) 5 4	6, 71, 142, 243	0
All	All	1226/1416 (86%)	0.90	170 (13%) 6 5	6, 72, 139, 270	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	613	ASP	8.0
1	C	523	HIS	7.9
1	C	612	THR	6.3
1	A	613	ASP	6.0
1	C	431	GLU	5.8
1	A	562	GLU	5.7
1	A	454	ARG	5.2
1	C	489	SER	5.2
1	A	528	ASP	5.1
1	C	528	ASP	4.8
1	D	448	ASP	4.6
1	C	615	GLU	4.5
1	D	598	ALA	4.5
1	C	579	SER	4.5
1	B	823	HIS	4.5
1	D	616	MET	4.4
1	D	449	VAL	4.4
1	C	532	ASP	4.4
1	D	601	GLU	4.3
1	C	488	ARG	4.3
1	D	597	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	523	HIS	4.2
1	B	584	GLU	4.1
1	D	613	ASP	4.0
1	A	542	LYS	4.0
1	A	720	ALA	4.0
1	B	560	PHE	3.9
1	A	488	ARG	3.9
1	A	584	GLU	3.8
1	D	584	GLU	3.8
1	D	599	HIS	3.8
1	A	540	LYS	3.7
1	B	462	GLU	3.7
1	C	586	ASP	3.7
1	B	543	SER	3.7
1	D	600	ARG	3.7
1	B	616	MET	3.6
1	C	588	TYR	3.6
1	A	581	ILE	3.6
1	D	595	LYS	3.6
1	B	467	PHE	3.5
1	D	589	THR	3.5
1	C	614	SER	3.5
1	C	490	ASN	3.5
1	C	530	LYS	3.5
1	C	547	ILE	3.4
1	A	586	ASP	3.4
1	B	449	VAL	3.4
1	D	596	LYS	3.4
1	D	436	GLN	3.3
1	B	436	GLN	3.3
1	D	477	GLY	3.3
1	B	580	GLU	3.3
1	C	608	ALA	3.3
1	D	592	ARG	3.3
1	B	824	HIS	3.3
1	B	442	ARG	3.2
1	D	580	GLU	3.2
1	A	561	TYR	3.2
1	C	494	LEU	3.2
1	A	447	GLU	3.1
1	D	787	LEU	3.1
1	B	452	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	614	SER	3.1
1	A	580	GLU	3.1
1	A	668	ASN	3.1
1	D	479	THR	3.1
1	D	590	ASP	3.1
1	B	456	CYS	3.0
1	B	468	ASN	3.0
1	D	566	ILE	3.0
1	C	542	LYS	3.0
1	A	585	THR	2.9
1	D	543	SER	2.9
1	D	532	ASP	2.9
1	D	808	SER	2.8
1	B	581	ILE	2.8
1	D	817	MET	2.8
1	D	793	ASP	2.8
1	A	591	ASN	2.8
1	C	583	ASP	2.8
1	A	541	GLY	2.8
1	D	680	ASN	2.8
1	A	450	MET	2.7
1	C	540	LYS	2.7
1	C	536	GLU	2.7
1	A	523	HIS	2.7
1	A	594	LYS	2.7
1	A	477	GLY	2.7
1	D	445	THR	2.7
1	D	801	ASP	2.7
1	C	781	GLN	2.6
1	D	587	LEU	2.6
1	D	573	ILE	2.6
1	A	612	THR	2.6
1	C	522	LEU	2.6
1	C	616	MET	2.6
1	A	455	ASP	2.6
1	C	533	ALA	2.6
1	A	665	ASP	2.6
1	D	602	ARG	2.6
1	A	583	ASP	2.6
1	C	487	GLU	2.5
1	C	531	LEU	2.5
1	D	593	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	458	MET	2.5
1	A	532	ASP	2.5
1	C	708	SER	2.5
1	B	432	LEU	2.5
1	B	487	GLU	2.4
1	B	669	LYS	2.4
1	C	574	GLU	2.4
1	A	810	GLN	2.4
1	C	514	ILE	2.4
1	A	543	SER	2.4
1	C	456	CYS	2.4
1	D	697	GLU	2.4
1	D	452	PRO	2.4
1	B	582	LEU	2.4
1	C	782	LEU	2.4
1	C	610	LYS	2.4
1	A	442	ARG	2.3
1	C	437	GLY	2.3
1	C	481	ILE	2.3
1	A	443	THR	2.3
1	A	675	TYR	2.3
1	B	613	ASP	2.3
1	D	437	GLY	2.3
1	B	433	ASN	2.3
1	C	572	VAL	2.3
1	B	583	ASP	2.3
1	C	439	LEU	2.3
1	C	784	SER	2.3
1	D	560	PHE	2.2
1	D	788	GLN	2.2
1	D	431	GLU	2.2
1	C	769	ASP	2.2
1	A	485	GLU	2.2
1	A	567	VAL	2.2
1	B	563	VAL	2.2
1	D	454	ARG	2.2
1	D	619	LYS	2.2
1	A	672	PRO	2.2
1	B	430	GLU	2.2
1	C	499	ASP	2.2
1	D	575	GLU	2.2
1	D	433	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	520	HIS	2.1
1	B	471	SER	2.1
1	C	611	GLN	2.1
1	A	481	ILE	2.1
1	D	563	VAL	2.1
1	D	603	LYS	2.1
1	A	536	GLU	2.1
1	D	701	GLU	2.1
1	D	645	SER	2.1
1	C	457	PHE	2.1
1	D	586	ASP	2.1
1	A	808	SER	2.1
1	D	542	LYS	2.1
1	C	617	LYS	2.1
1	D	674	TYR	2.1
1	B	615	GLU	2.1
1	C	491	ILE	2.1
1	C	573	ILE	2.0
1	C	432	LEU	2.0
1	A	820	HIS	2.0
1	A	666	GLU	2.0
1	C	582	LEU	2.0
1	D	567	VAL	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](#)

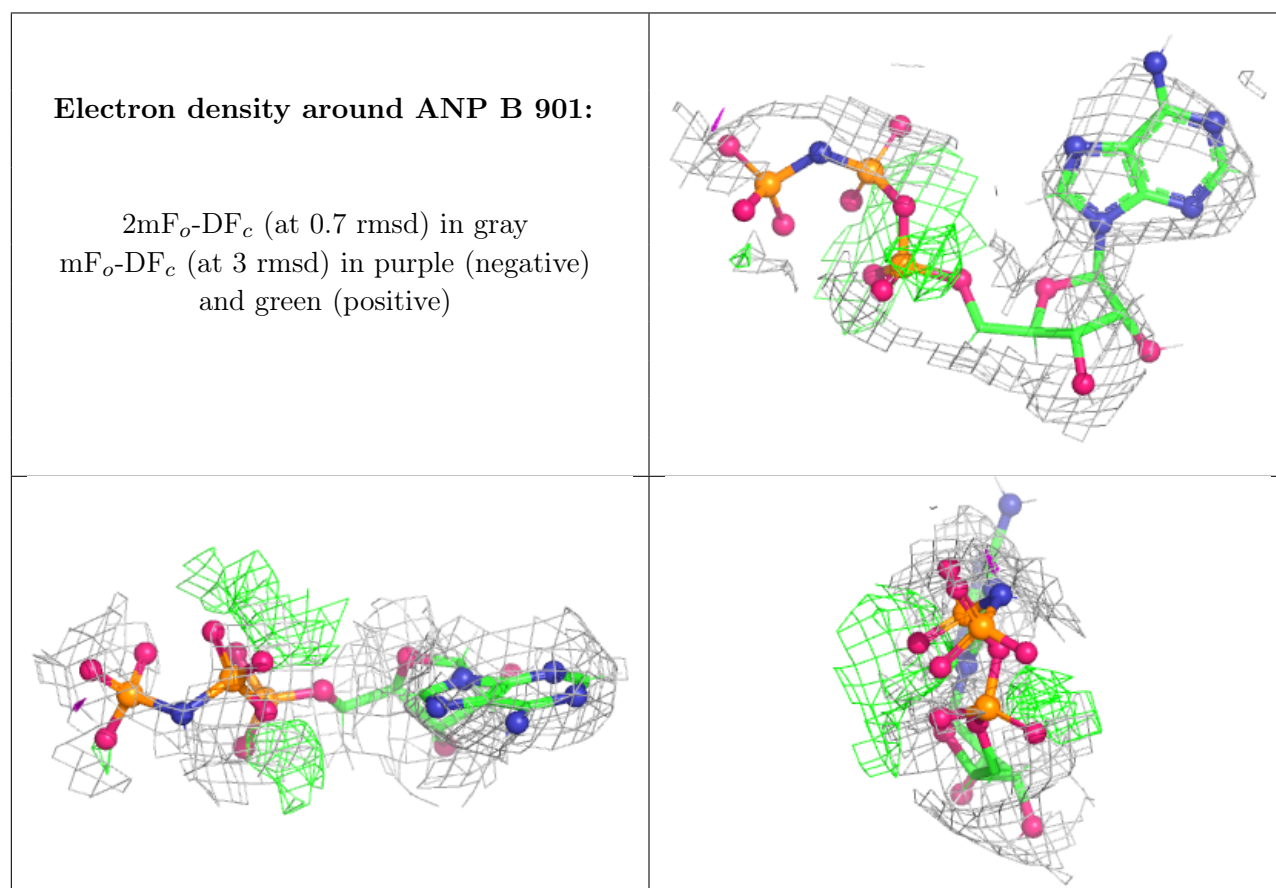
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Continued on next page...

Continued from previous page...

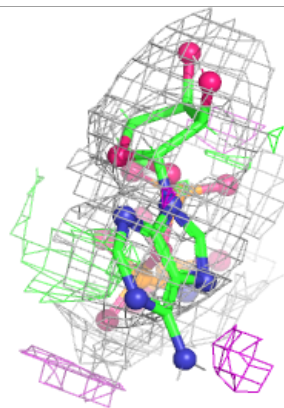
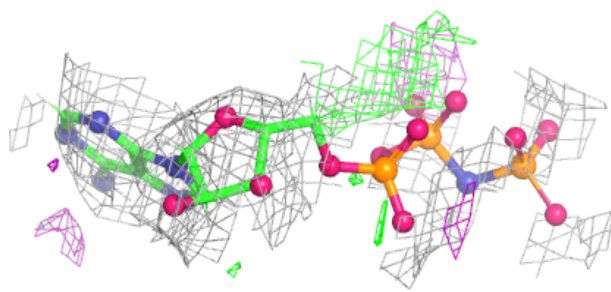
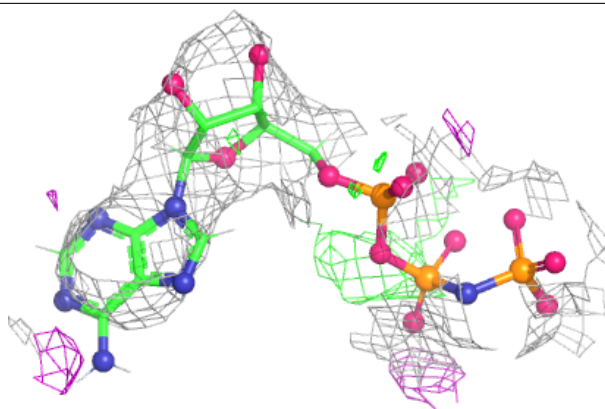
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	902	1/1	0.13	0.27	108,108,108,108	0
3	MG	D	902	1/1	0.47	0.18	99,99,99,99	0
3	MG	B	903	1/1	0.83	0.16	20,20,20,20	0
2	ANP	B	901	31/31	0.89	0.17	76,106,174,200	0
3	MG	A	902	1/1	0.90	0.17	71,71,71,71	0
3	MG	B	904	1/1	0.90	0.28	22,22,22,22	0
2	ANP	D	901	31/31	0.90	0.16	42,92,152,200	0
3	MG	D	903	1/1	0.90	0.23	26,26,26,26	0
3	MG	A	903	1/1	0.92	0.26	24,24,24,24	0
3	MG	C	902	1/1	0.92	0.11	57,57,57,57	0
2	ANP	A	901	31/31	0.93	0.12	48,61,82,99	0
2	ANP	C	901	31/31	0.94	0.11	45,78,133,170	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.



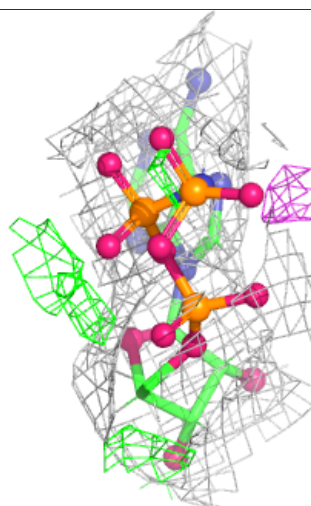
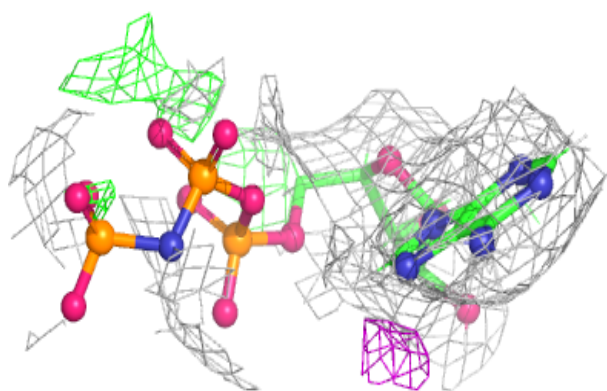
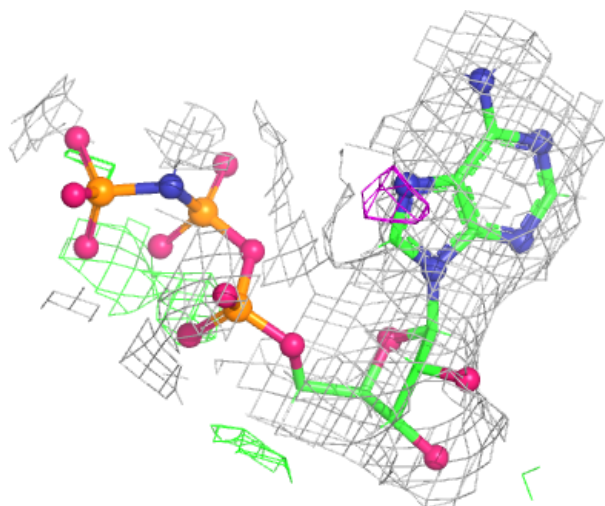
Electron density around ANP D 901:

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



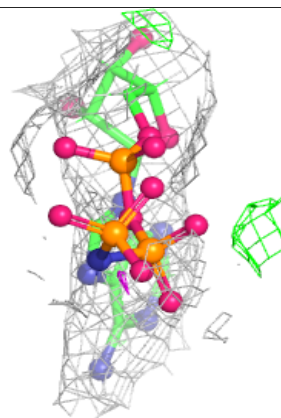
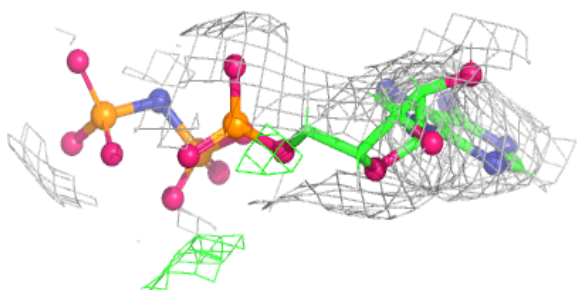
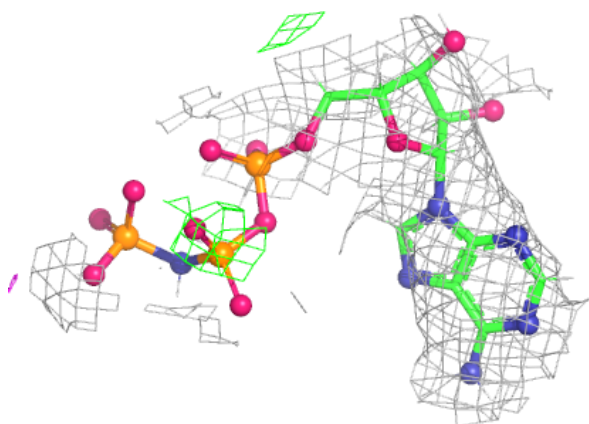
Electron density around ANP A 901:

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



Electron density around ANP C 901:

$2mF_o-DF_c$ (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.