



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:57 AM UTC

PDB ID : 8PX9 / pdb_00008px9
Title : Structure of the antibacterial peptide ABC transporter McjD, solved at wavelength 2.75 Å
Authors : El Omari, K.; Duman, R.; Mykhaylyk, V.; Orr, C.; Bountra, K.; Beis, K.; Wagner, A.
Deposited on : 2023-07-22
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

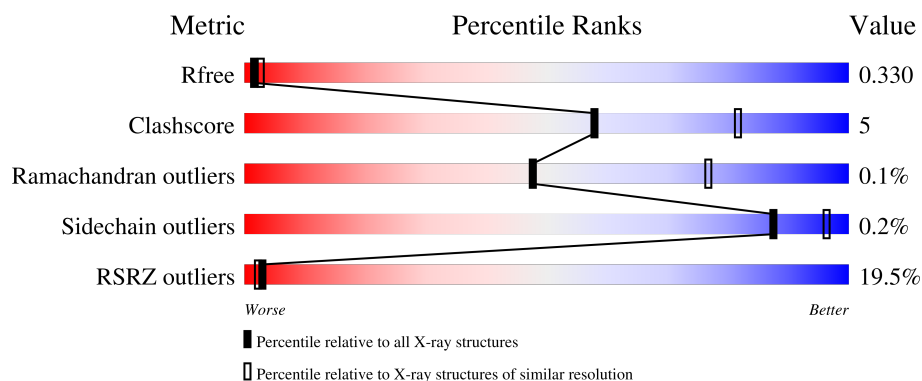
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	580	18% 83% 13% .
1	B	580	20% 90% 8% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8977 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.

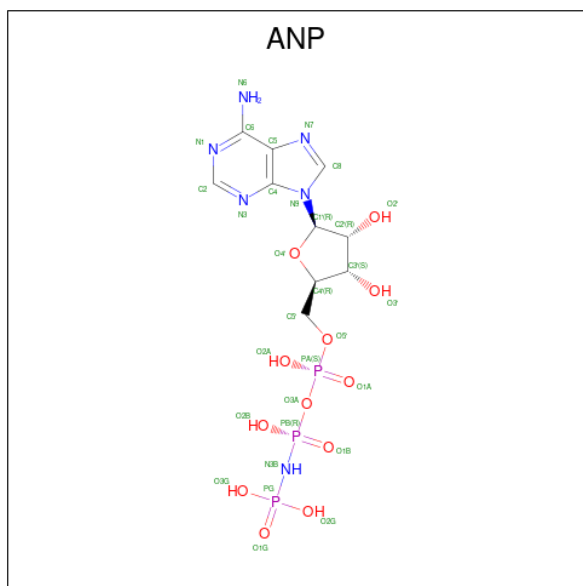
- Molecule 1 is a protein called Microcin-J25 export ATP-binding/permease protein McjD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4415	2849	719	830	17			
1	B	567	Total	C	N	O	S	0	0	0
			4498	2903	733	844	18			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

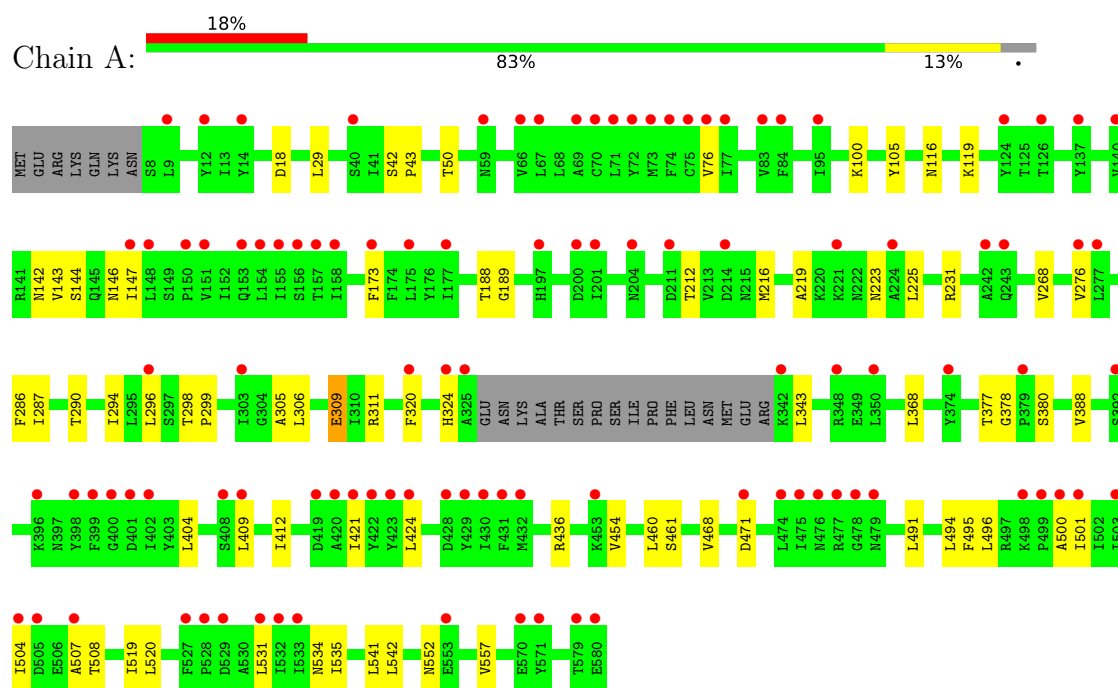


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

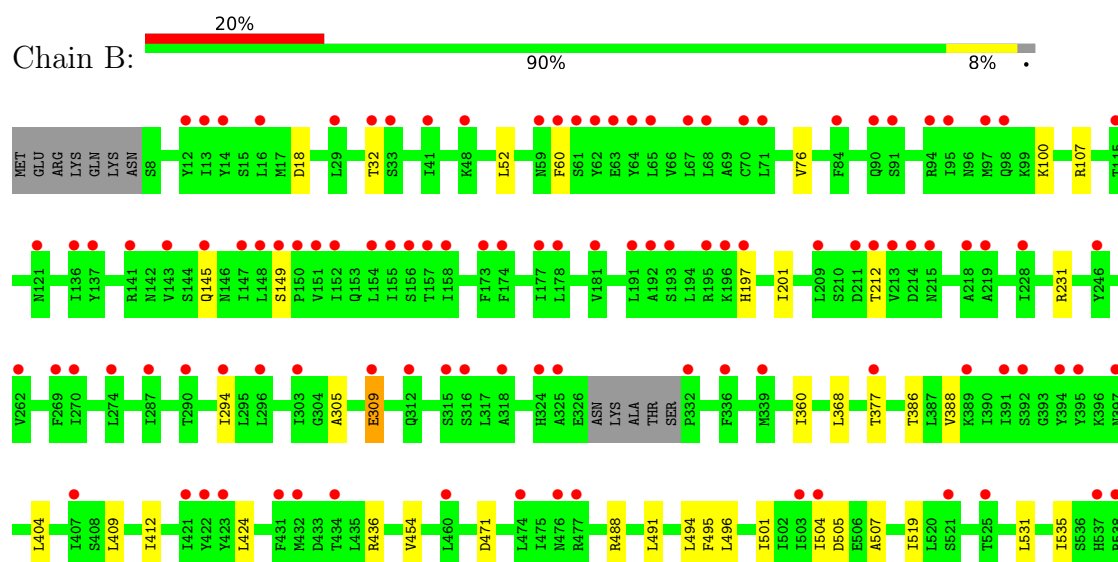
3 Residue-property plots

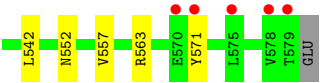
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD



- Molecule 1: Microcin-J25 export ATP-binding/permease protein McjD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 109.32Å 233.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.67 – 2.80 54.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.67-2.80) 99.7 (54.67-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.292 , 0.330 0.297 , 0.330	Depositor DCC
R_{free} test set	2580 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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	0.65	0/4487	1.16	1/6075 (0.0%)
1	B	0.63	0/4573	1.26	2/6191 (0.0%)
All	All	0.64	0/9060	1.21	3/12266 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	309	GLU	CB-CG-CD	6.45	123.56	112.60
1	A	309	GLU	CB-CG-CD	5.16	121.36	112.60
1	B	505	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	563	ARG	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	4415	0	4522	57	0
1	B	4498	0	4607	29	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
All	All	8977	0	9155	82	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 5.

All (82) 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:343:LEU:HD12	1:A:500:ALA:HB3	1.41	1.01
1:A:142:ASN:HD21	1:A:309:GLU:HB2	1.44	0.83
1:A:142:ASN:ND2	1:A:309:GLU:HB2	2.00	0.77
1:A:294:ILE:HD12	1:B:76:VAL:HG11	1.68	0.76
1:A:343:LEU:CD1	1:A:500:ALA:HB3	2.18	0.70
1:B:32:THR:HG22	1:B:149:SER:HB2	1.75	0.68
1:B:377:THR:HG22	1:B:571:TYR:HE2	1.58	0.68
1:A:76:VAL:HG11	1:B:294:ILE:HD12	1.76	0.67
1:A:388:VAL:HG11	1:A:535:ILE:HD11	1.78	0.66
1:A:298:THR:OG1	1:A:299:PRO:HD3	1.96	0.66
1:A:105:TYR:HE1	1:A:324:HIS:CE1	2.14	0.65
1:A:343:LEU:HD12	1:A:500:ALA:CB	2.23	0.64
1:A:142:ASN:HD21	1:A:309:GLU:CB	2.08	0.64
1:B:377:THR:HG22	1:B:571:TYR:CE2	2.32	0.64
1:A:188:THR:HG23	1:A:311:ARG:CD	2.29	0.61
1:A:552:ASN:HB3	1:A:557:VAL:HG21	1.81	0.60
1:A:29:LEU:HD13	1:A:144:SER:HA	1.82	0.60
1:A:212:THR:HG23	1:A:231:ARG:HH21	1.68	0.58
1:B:388:VAL:HG11	1:B:535:ILE:HD11	1.85	0.58
1:B:552:ASN:HB3	1:B:557:VAL:HG21	1.86	0.58
1:A:146:ASN:O	1:A:306:LEU:HD22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:HD12	1:A:412:ILE:HD13	1.87	0.56
1:A:212:THR:CG2	1:A:231:ARG:HH21	2.18	0.56
1:A:368:LEU:HB3	1:A:531:LEU:HD11	1.89	0.55
1:A:188:THR:HG23	1:A:311:ARG:HD3	1.89	0.54
1:B:404:LEU:HD12	1:B:412:ILE:HD13	1.90	0.53
1:B:212:THR:HG23	1:B:231:ARG:HH21	1.73	0.53
1:A:18:ASP:HB3	1:A:100:LYS:HE2	1.92	0.52
1:B:368:LEU:HB3	1:B:531:LEU:HD11	1.91	0.52
1:A:436:ARG:NH2	1:A:471:ASP:OD1	2.44	0.51
1:A:454:VAL:HG13	1:A:495:PHE:HB2	1.93	0.51
1:A:305:ALA:O	1:A:309:GLU:HG2	2.10	0.51
1:B:305:ALA:O	1:B:309:GLU:HG3	2.12	0.50
1:A:377:THR:HG22	1:A:378:GLY:N	2.27	0.50
1:A:225:LEU:HD11	1:B:107:ARG:HG2	1.92	0.49
1:B:436:ARG:NH2	1:B:471:ASP:OD1	2.45	0.48
1:B:32:THR:HG21	1:B:145:GLN:HA	1.96	0.48
1:A:534:ASN:ND2	1:A:541:LEU:HB3	2.28	0.48
1:A:298:THR:HG1	1:A:299:PRO:HD3	1.77	0.48
1:A:534:ASN:HD21	1:A:541:LEU:HB3	1.79	0.47
1:A:377:THR:OG1	1:A:542:LEU:HD21	2.15	0.47
1:A:460:LEU:O	1:A:468:VAL:HG11	2.15	0.47
1:B:212:THR:CG2	1:B:231:ARG:HH21	2.27	0.47
1:A:421:ILE:HG12	1:A:501:ILE:HB	1.97	0.47
1:B:52:LEU:HG	1:B:60:PHE:HB2	1.97	0.46
1:A:424:LEU:HD11	1:A:494:LEU:HD22	1.97	0.46
1:A:409:LEU:HA	1:A:412:ILE:HD12	1.98	0.45
1:A:189:GLY:HA2	1:A:311:ARG:HE	1.80	0.45
1:A:320:PHE:CZ	1:A:324:HIS:NE2	2.84	0.45
1:B:409:LEU:HA	1:B:412:ILE:HD12	1.98	0.45
1:B:424:LEU:HD11	1:B:494:LEU:HD22	1.99	0.45
1:B:360:ILE:CG2	1:B:386:THR:HG21	2.47	0.45
1:A:534:ASN:HD21	1:A:541:LEU:HD13	1.82	0.44
1:A:188:THR:HG23	1:A:311:ARG:HD2	1.99	0.44
1:A:116:ASN:HA	1:A:119:LYS:HE3	1.99	0.44
1:A:491:LEU:HD11	1:A:508:THR:HG22	1.99	0.43
1:A:286:PHE:O	1:A:290:THR:HG23	2.18	0.43
1:B:377:THR:OG1	1:B:542:LEU:HD21	2.18	0.43
1:B:454:VAL:HG13	1:B:495:PHE:HB2	1.99	0.43
1:A:105:TYR:CE1	1:A:324:HIS:CE1	3.00	0.43
1:B:491:LEU:HD13	1:B:519:ILE:HG21	2.01	0.43
1:A:454:VAL:HG21	1:A:496:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ILE:HG23	1:B:507:ALA:HB3	1.99	0.43
1:A:380:SER:HB2	1:B:488:ARG:NH2	2.34	0.43
1:A:173:PHE:CZ	1:A:268:VAL:HG11	2.53	0.43
1:B:18:ASP:HB3	1:B:100:LYS:HE2	2.00	0.43
1:A:296:LEU:C	1:A:299:PRO:HD2	2.45	0.42
1:A:504:ILE:HG23	1:A:507:ALA:HB3	2.02	0.42
1:A:105:TYR:HE1	1:A:324:HIS:NE2	2.17	0.42
1:A:219:ALA:O	1:A:223:ASN:O	2.38	0.42
1:A:50:THR:HG21	1:A:287:ILE:HG13	2.01	0.41
1:B:377:THR:CG2	1:B:571:TYR:HE2	2.28	0.41
1:A:343:LEU:CD1	1:A:500:ALA:CB	2.92	0.41
1:A:216:MET:HE3	1:A:219:ALA:HB3	2.03	0.41
1:A:461:SER:O	1:A:468:VAL:HG12	2.21	0.41
1:A:42:SER:OG	1:A:43:PRO:HD3	2.20	0.41
1:A:491:LEU:HD13	1:A:519:ILE:HG21	2.03	0.41
1:B:454:VAL:HG21	1:B:496:LEU:HG	2.02	0.41
1:B:197:HIS:CE1	1:B:201:ILE:HD11	2.56	0.41
1:A:105:TYR:CE1	1:A:324:HIS:NE2	2.89	0.40
1:B:501:ILE:HG12	1:B:531:LEU:HD23	2.03	0.40
1:A:520:LEU:CD1	1:A:541:LEU:HD21	2.51	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	553/580 (95%)	543 (98%)	9 (2%)	1 (0%)	43	72
1	B	563/580 (97%)	555 (99%)	8 (1%)	0	100	100
All	All	1116/1160 (96%)	1098 (98%)	17 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	VAL

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	507/529 (96%)	505 (100%)	2 (0%)	84	94
1	B	517/529 (98%)	517 (100%)	0	100	100
All	All	1024/1058 (97%)	1022 (100%)	2 (0%)	87	96

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

Mol	Chain	Res	Type
1	A	147	ILE
1	A	276	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	98	GLN
1	A	131	GLN
1	A	142	ASN
1	A	146	ASN
1	A	215	ASN
1	A	222	ASN
1	A	464	ASN
1	A	465	ASN
1	A	526	HIS
1	A	534	ASN
1	A	552	ASN
1	B	96	ASN
1	B	131	GLN
1	B	145	GLN
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	197	HIS
1	B	240	ASN
1	B	243	GLN
1	B	257	ASN
1	B	397	ASN
1	B	465	ASN
1	B	485	GLN
1	B	534	ASN
1	B	540	ASN
1	B	552	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	600	2	33,33,33	1.06	3 (9%)	45,52,52	1.34	5 (11%)
3	ANP	A	602	2	33,33,33	1.18	6 (18%)	45,52,52	1.22	3 (6%)

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	600	2	-	2/18/38/38	0/3/3/3
3	ANP	A	602	2	-	2/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ANP	PB-O1B	3.33	1.51	1.46
3	A	602	ANP	PG-O3G	-3.06	1.48	1.56
3	A	602	ANP	PB-O1B	3.05	1.50	1.46
3	A	602	ANP	PG-O1G	2.53	1.50	1.46
3	B	600	ANP	PG-O1G	2.23	1.49	1.46
3	A	602	ANP	PB-O2B	-2.19	1.51	1.56
3	A	602	ANP	PB-O3A	2.06	1.61	1.59
3	B	600	ANP	PB-O2B	-2.05	1.51	1.56
3	A	602	ANP	PG-O2G	-2.04	1.51	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	ANP	O2B-PB-O1B	5.16	120.93	109.87
3	A	602	ANP	O2B-PB-O1B	4.94	120.47	109.87
3	A	602	ANP	O1G-PG-N3B	4.08	117.78	111.77
3	A	602	ANP	O3G-PG-O1G	-3.86	103.77	113.45
3	B	600	ANP	O1G-PG-N3B	3.67	117.17	111.77
3	B	600	ANP	O3G-PG-O1G	-3.51	104.66	113.45
3	B	600	ANP	O2A-PA-O3A	-2.26	101.17	107.27
3	B	600	ANP	O2G-PG-O1G	-2.15	108.05	113.45

There are no chirality outliers.

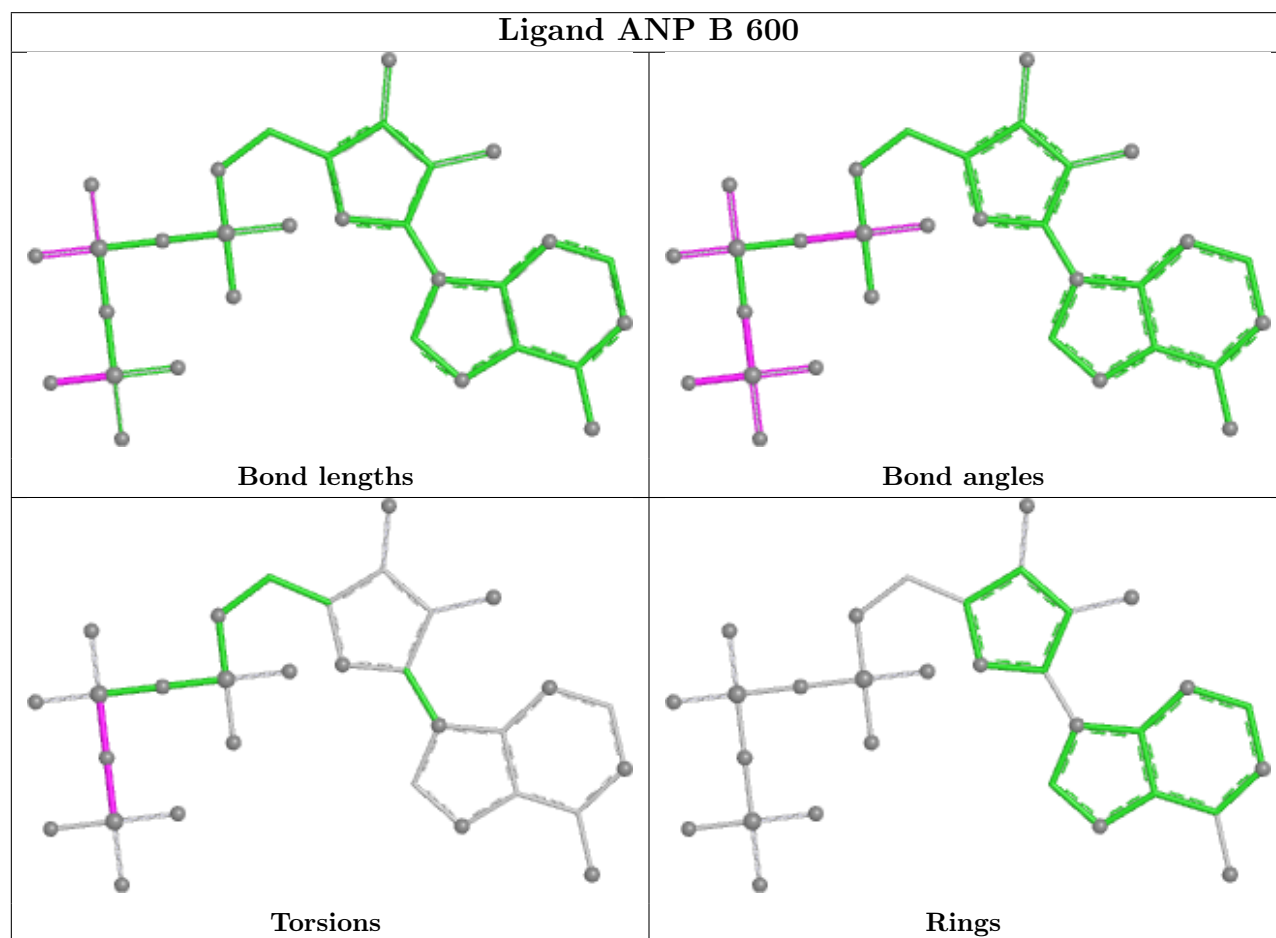
All (4) torsion outliers are listed below:

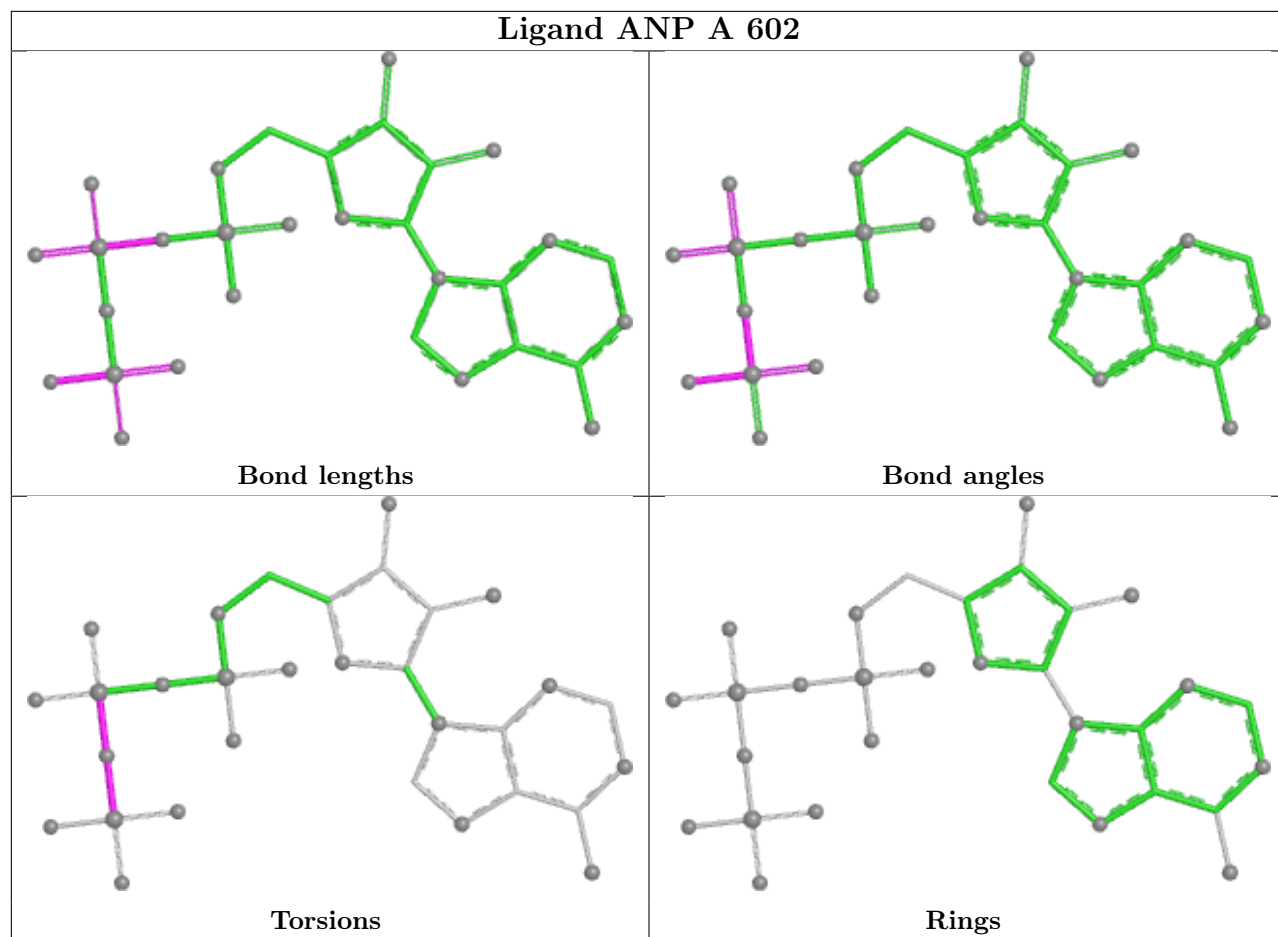
Mol	Chain	Res	Type	Atoms
3	A	602	ANP	PB-N3B-PG-O1G
3	A	602	ANP	PG-N3B-PB-O1B
3	B	600	ANP	PB-N3B-PG-O1G
3	B	600	ANP	PG-N3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	557/580 (96%)	0.94	105 (18%) 3 2	128, 162, 205, 249	0
1	B	567/580 (97%)	1.02	114 (20%) 3 2	122, 158, 205, 244	0
All	All	1124/1160 (96%)	0.98	219 (19%) 3 2	122, 160, 205, 249	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	529	ASP	13.2
1	B	64	TYR	12.8
1	A	476	ASN	11.5
1	A	477	ARG	9.9
1	B	61	SER	9.2
1	B	67	LEU	8.8
1	B	59	ASN	8.2
1	A	204	ASN	7.9
1	A	77	ILE	7.9
1	B	246	TYR	7.1
1	B	137	TYR	6.9
1	A	430	ILE	6.9
1	B	392	SER	6.9
1	B	60	PHE	6.6
1	B	62	TYR	6.5
1	A	72	TYR	6.5
1	A	342	LYS	6.5
1	B	147	ILE	6.5
1	B	394	TYR	6.4
1	A	431	PHE	6.4
1	A	74	PHE	6.3
1	B	196	LYS	6.1
1	B	63	GLU	6.0
1	A	420	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	155	ILE	6.0
1	A	73	MET	6.0
1	A	419	ASP	5.9
1	A	500	ALA	5.9
1	A	70	CYS	5.9
1	B	214	ASP	5.9
1	A	499	PRO	5.7
1	B	476	ASN	5.7
1	B	422	TYR	5.6
1	B	151	VAL	5.4
1	B	154	LEU	5.4
1	B	12	TYR	5.1
1	A	503	ILE	5.0
1	B	215	ASN	5.0
1	B	16	LEU	5.0
1	B	315	SER	4.9
1	A	71	LEU	4.8
1	B	158	ILE	4.8
1	B	193	SER	4.8
1	B	157	THR	4.8
1	B	148	LEU	4.7
1	A	154	LEU	4.5
1	A	475	ILE	4.5
1	B	211	ASP	4.5
1	A	501	ILE	4.4
1	B	503	ILE	4.4
1	B	177	ILE	4.4
1	A	474	LEU	4.4
1	B	141	ARG	4.4
1	B	537	HIS	4.4
1	B	579	THR	4.3
1	A	424	LEU	4.2
1	A	421	ILE	4.2
1	A	498	LYS	4.1
1	B	218	ALA	4.1
1	A	533	ILE	4.1
1	A	157	THR	4.1
1	A	200	ASP	4.1
1	A	531	LEU	4.1
1	A	296	LEU	4.0
1	A	83	VAL	4.0
1	B	143	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLN	3.9
1	A	214	ASP	3.9
1	B	575	LEU	3.9
1	A	69	ALA	3.9
1	B	71	LEU	3.9
1	A	392	SER	3.9
1	B	262	VAL	3.8
1	B	332	PRO	3.8
1	A	478	GLY	3.8
1	A	177	ILE	3.8
1	B	121	ASN	3.8
1	A	242	ALA	3.7
1	B	191	LEU	3.7
1	B	336	PHE	3.7
1	B	296	LEU	3.6
1	B	70	CYS	3.6
1	A	320	PHE	3.6
1	A	429	TYR	3.6
1	B	41	ILE	3.5
1	A	224	ALA	3.5
1	B	174	PHE	3.5
1	A	148	LEU	3.4
1	B	274	LEU	3.4
1	A	84	PHE	3.4
1	B	68	LEU	3.4
1	B	423	TYR	3.4
1	B	173	PHE	3.4
1	A	400	GLY	3.4
1	B	150	PRO	3.4
1	B	149	SER	3.4
1	A	505	ASP	3.4
1	A	67	LEU	3.3
1	A	173	PHE	3.3
1	A	409	LEU	3.3
1	A	155	ILE	3.3
1	B	91	SER	3.3
1	B	477	ARG	3.2
1	B	312	GLN	3.2
1	B	13	ILE	3.2
1	B	294	ILE	3.2
1	A	325	ALA	3.1
1	A	75	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	507	ALA	3.1
1	B	197	HIS	3.1
1	B	181	VAL	3.1
1	A	158	ILE	3.1
1	B	94	ARG	3.0
1	B	325	ALA	3.0
1	A	197	HIS	3.0
1	B	33	SER	3.0
1	B	474	LEU	3.0
1	A	40	SER	3.0
1	B	391	ILE	3.0
1	A	528	PRO	3.0
1	B	309	GLU	3.0
1	B	570	GLU	2.9
1	A	66	VAL	2.9
1	B	95	ILE	2.9
1	A	432	MET	2.9
1	A	402	ILE	2.9
1	A	137	TYR	2.8
1	A	374	TYR	2.8
1	B	178	LEU	2.8
1	B	145	GLN	2.8
1	B	397	ASN	2.8
1	A	580	GLU	2.7
1	A	243	GLN	2.7
1	A	277	LEU	2.7
1	A	156	SER	2.7
1	A	201	ILE	2.7
1	A	350	LEU	2.7
1	A	571	TYR	2.7
1	B	339	MET	2.7
1	A	153	GLN	2.7
1	B	538	ARG	2.7
1	B	434	THR	2.7
1	A	396	LYS	2.6
1	A	428	ASP	2.6
1	A	504	ILE	2.6
1	B	431	PHE	2.6
1	A	221	LYS	2.6
1	A	76	VAL	2.6
1	B	303	ILE	2.6
1	A	140	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	65	LEU	2.6
1	B	136	ILE	2.6
1	A	59	ASN	2.6
1	A	479	ASN	2.6
1	B	316	SER	2.6
1	B	97	MET	2.6
1	B	525	THR	2.6
1	B	84	PHE	2.6
1	A	14	TYR	2.5
1	B	32	THR	2.5
1	B	504	ILE	2.5
1	A	579	THR	2.5
1	B	377	THR	2.5
1	B	29	LEU	2.5
1	A	147	ILE	2.5
1	B	212	THR	2.5
1	A	175	LEU	2.4
1	B	115	THR	2.4
1	A	399	PHE	2.4
1	B	318	ALA	2.4
1	B	571	TYR	2.4
1	B	421	ILE	2.4
1	B	192	ALA	2.4
1	A	124	TYR	2.4
1	A	422	TYR	2.4
1	A	423	TYR	2.4
1	A	324	HIS	2.4
1	B	269	PHE	2.3
1	A	408	SER	2.3
1	A	398	TYR	2.3
1	B	324	HIS	2.3
1	B	395	TYR	2.3
1	B	389	LYS	2.3
1	B	213	VAL	2.3
1	B	578	VAL	2.3
1	B	219	ALA	2.3
1	A	401	ASP	2.3
1	A	471	ASP	2.3
1	B	209	LEU	2.2
1	A	95	ILE	2.2
1	B	407	ILE	2.2
1	A	9	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	532	ILE	2.2
1	A	348	ARG	2.2
1	B	290	THR	2.2
1	B	98	GLN	2.2
1	B	152	ILE	2.2
1	A	150	PRO	2.2
1	B	156	SER	2.2
1	B	521	SER	2.2
1	A	303	ILE	2.1
1	B	460	LEU	2.1
1	A	276	VAL	2.1
1	A	527	PHE	2.1
1	B	14	TYR	2.1
1	B	195	ARG	2.1
1	A	553	GLU	2.1
1	A	570	GLU	2.1
1	A	453	LYS	2.1
1	B	48	LYS	2.1
1	A	151	VAL	2.0
1	A	379	PRO	2.0
1	A	126	THR	2.0
1	B	228	ILE	2.0
1	A	12	TYR	2.0
1	B	270	ILE	2.0
1	B	287	ILE	2.0
1	A	211	ASP	2.0
1	B	432	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

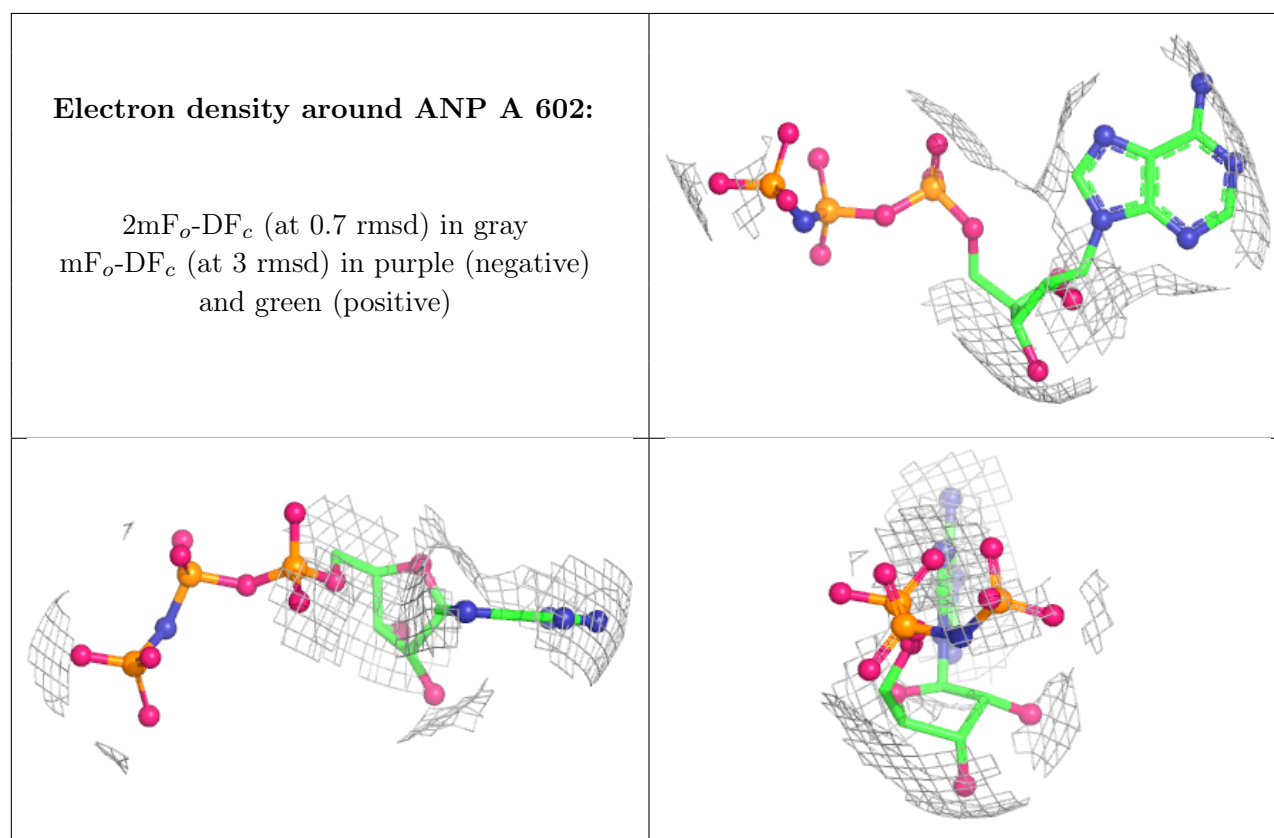
6.4 Ligands [i](#)

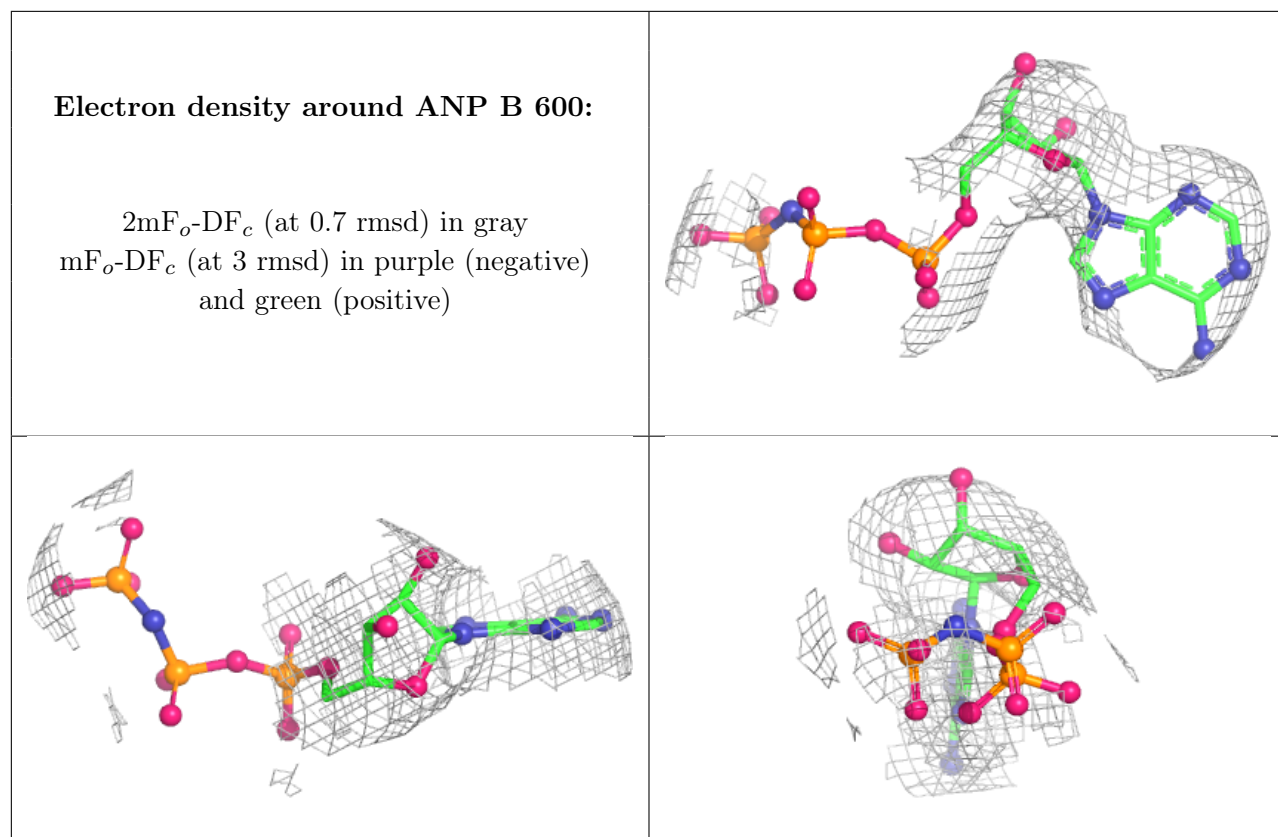
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	601	1/1	0.95	0.10	148,148,148,148	0
2	MG	B	601	1/1	0.95	0.08	142,142,142,142	0
3	ANP	A	602	31/31	0.96	0.06	139,157,174,179	0
3	ANP	B	600	31/31	0.96	0.06	126,147,156,168	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.