



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2022 – 02:13 PM JST

PDB ID : 7E1G
Title : Structure of MreB3 from Spiroplasma eriocheiris
Authors : Takahashi, D.; Miyata, M.; Imada, K.
Deposited on : 2021-02-01
Resolution : 1.75 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 : 2.26
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) : 2.26

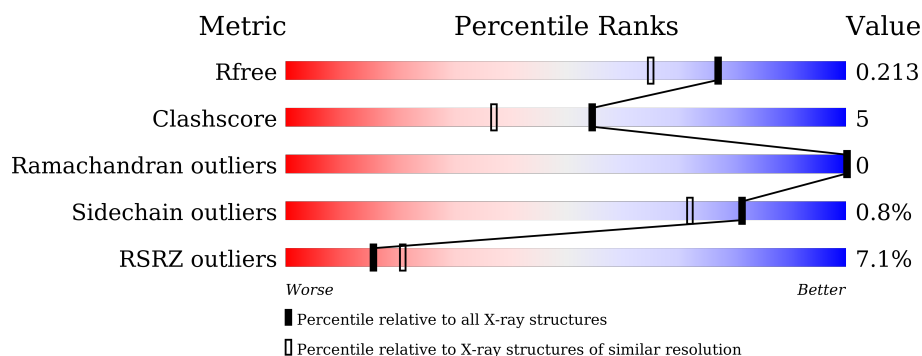
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	355	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	355	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5997 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 Cell shape-determining protein MreB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	4	0
			2590	1667	429	483	11			
1	B	330	Total	C	N	O	S	0	5	0
			2580	1661	429	479	11			

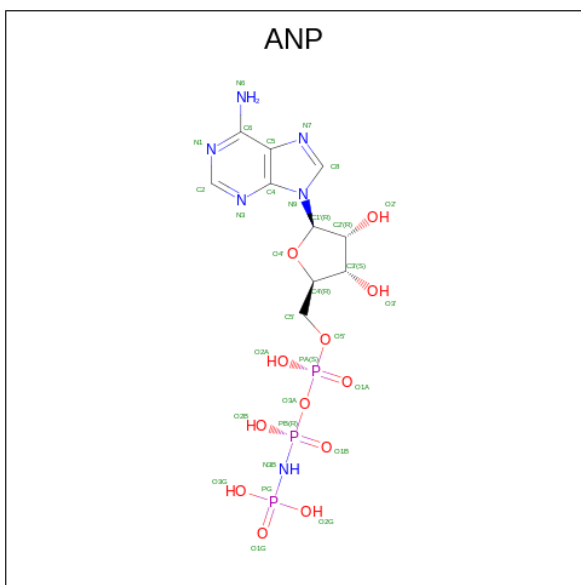
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0H3XJK5
A	-1	SER	-	expression tag	UNP A0A0H3XJK5
A	0	HIS	-	expression tag	UNP A0A0H3XJK5
B	-2	GLY	-	expression tag	UNP A0A0H3XJK5
B	-1	SER	-	expression tag	UNP A0A0H3XJK5
B	0	HIS	-	expression tag	UNP A0A0H3XJK5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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 (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

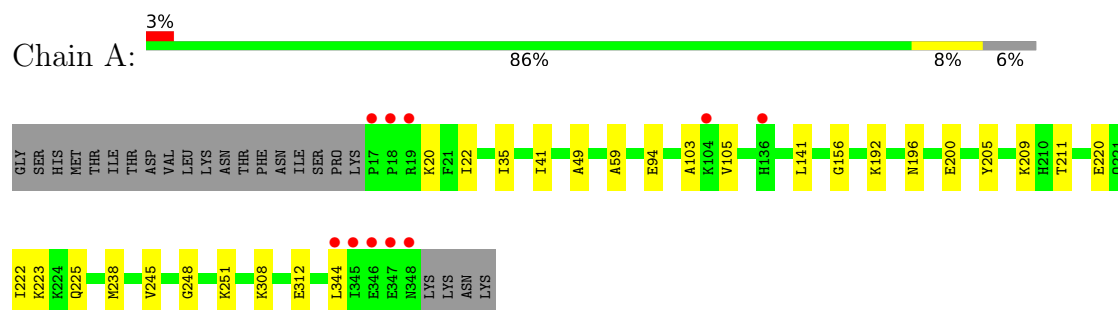
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	463	Total O 463 463	0	0
4	B	300	Total O 300 300	0	0

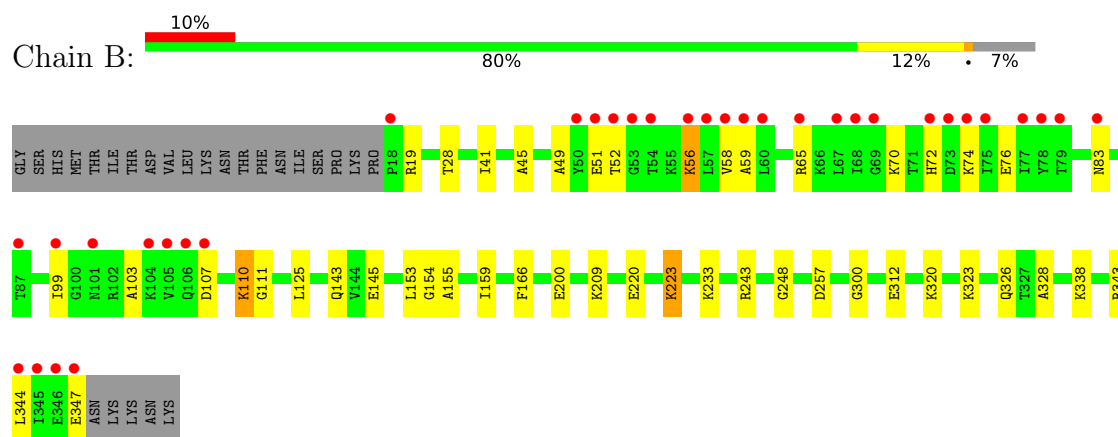
3 Residue-property plots [i](#)

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: Cell shape-determining protein MreB



- Molecule 1: Cell shape-determining protein MreB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.29Å 56.27Å 120.53Å 90.00° 90.56° 90.00°	Depositor
Resolution (Å)	50.99 – 1.75 50.99 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.99-1.75) 96.8 (50.99-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.174 , 0.213 0.174 , 0.213	Depositor DCC
R_{free} test set	2006 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5997	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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

5.1 Standard geometry

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

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	0.34	0/2403	0.53	0/3259
1	B	0.34	0/2394	0.52	0/3245
All	All	0.34	0/4797	0.52	0/6504

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

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	2590	0	2727	25	0
1	B	2580	0	2732	31	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	13	1	0
4	A	463	0	0	10	6
4	B	300	0	0	7	0
All	All	5997	0	5484	56	7

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:HB3	1:B:110:LYS:HG3	1.48	0.96
1:B:220:GLU:HG3	1:B:223:MLY:HH11	1.63	0.78
1:B:52:THR:HG21	1:B:74:LYS:HE3	1.71	0.72
1:B:83:ASN:OD1	4:B:601:HOH:O	2.11	0.69
1:A:245:VAL:O	4:A:601:HOH:O	2.10	0.68
1:B:200[B]:GLU:OE1	4:B:602:HOH:O	2.12	0.66
1:A:200[B]:GLU:OE1	4:A:602:HOH:O	2.14	0.64
1:B:312:GLU:OE2	4:B:603:HOH:O	2.13	0.64
1:B:257:ASP:OD2	4:B:605:HOH:O	2.14	0.64
1:A:205:TYR:CE1	1:A:209[B]:LYS:HG3	2.36	0.61
1:A:245:VAL:O	4:A:604:HOH:O	2.17	0.60
1:A:192:LYS:NZ	4:A:611:HOH:O	2.30	0.59
1:B:344:LEU:O	1:B:347:GLU:HB2	2.03	0.58
1:A:225:GLN:NE2	4:A:603:HOH:O	2.15	0.58
1:B:19:ARG:HD3	1:B:111:GLY:O	2.03	0.58
1:B:52:THR:HB	1:B:74:LYS:HB3	1.85	0.58
1:B:51:GLU:HG2	1:B:58:VAL:HG21	1.89	0.54
1:B:28:THR:HG23	3:B:502:ANP:O3G	2.07	0.54
1:B:28:THR:HB	4:B:822:HOH:O	2.07	0.53
1:B:243[A]:ARG:NH2	4:B:612:HOH:O	2.39	0.53
1:B:45:ALA:CB	1:B:65:ARG:HE	2.22	0.52
1:A:156:GLY:O	4:A:606:HOH:O	2.19	0.51
1:A:211:THR:OG1	1:A:251:MLY:HH11	2.11	0.51
1:A:41:ILE:HD13	1:A:103:ALA:HB2	1.94	0.50
1:B:45:ALA:HB1	1:B:65:ARG:HE	1.77	0.49
1:A:220:GLU:HG3	1:A:223:MLY:HH23	1.94	0.49
1:A:200[B]:GLU:HG2	4:A:616:HOH:O	2.13	0.49
1:A:94:GLU:OE2	4:A:605:HOH:O	2.19	0.49
1:A:141:LEU:HD22	1:A:344:LEU:HB2	1.94	0.49
1:A:20:MLY:HH13	1:A:105:VAL:HG11	1.94	0.48
1:B:143:GLN:OE1	1:B:343:ARG:NH2	2.40	0.48
1:B:300:GLY:HA2	1:B:326:GLN:HG3	1.95	0.47
1:A:223:MLY:HH12	1:A:223:MLY:HD2	1.66	0.47
1:B:209:LYS:HB2	4:B:839:HOH:O	2.14	0.46
1:A:223:MLY:HE3	1:A:223:MLY:HB2	1.43	0.45
1:A:251:MLY:HD2	1:A:251:MLY:HH13	1.68	0.45
1:B:243[B]:ARG:NH1	1:B:248:GLY:HA2	2.32	0.45
1:B:56:LYS:HA	1:B:56:LYS:HD2	1.83	0.44
1:B:99[B]:ILE:HD12	1:B:99[B]:ILE:HA	1.83	0.44
1:A:312:GLU:OE1	4:A:607:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:O	1:A:200[B]:GLU:HG3	2.18	0.43
1:B:41:ILE:HD13	1:B:103:ALA:HB2	2.01	0.43
1:A:22:ILE:HG12	1:A:35:ILE:HG12	2.00	0.43
1:A:49:ALA:HB3	1:A:59:ALA:HB3	2.00	0.43
1:A:222:ILE:HA	1:A:238:MET:SD	2.59	0.43
1:B:52:THR:OG1	1:B:76:GLU:HG3	2.19	0.43
1:B:153:LEU:HD13	1:B:159:ILE:HG12	2.00	0.42
1:A:248:GLY:HA3	4:A:661:HOH:O	2.18	0.42
1:B:49:ALA:HB3	1:B:59:ALA:HB3	2.01	0.42
1:B:125:LEU:HD23	1:B:125:LEU:HA	1.89	0.42
1:B:143:GLN:NE2	1:B:145:GLU:OE2	2.37	0.42
1:B:155:ALA:O	1:B:320:MLY:HH22	2.20	0.41
1:B:154:GLY:HA3	1:B:328:ALA:O	2.20	0.41
1:A:20:MLY:HH12	1:A:20:MLY:HD3	1.78	0.41
1:A:308:MLY:HH12	1:A:312:GLU:OE1	2.20	0.41
1:B:338:MLY:HD3	1:B:338:MLY:HH23	1.78	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:NH2	1:B:323:MLY:CH2[2_454]	1.44	0.76
4:A:636:HOH:O	4:A:909:HOH:O[2_445]	2.03	0.17
4:A:604:HOH:O	4:A:852:HOH:O[2_455]	2.11	0.09
4:A:779:HOH:O	4:A:986:HOH:O[1_655]	2.11	0.09
4:A:778:HOH:O	4:A:907:HOH:O[1_655]	2.17	0.03
4:A:970:HOH:O	4:A:1020:HOH:O[2_445]	2.18	0.02
4:A:959:HOH:O	4:A:1035:HOH:O[2_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	313/355 (88%)	309 (99%)	4 (1%)	0	100	100
1	B	312/355 (88%)	303 (97%)	9 (3%)	0	100	100
All	All	625/710 (88%)	612 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/272 (93%)	254 (100%)	0	100	100
1	B	253/272 (93%)	249 (98%)	4 (2%)	62	45
All	All	507/544 (93%)	503 (99%)	4 (1%)	81	72

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

Mol	Chain	Res	Type
1	B	56	LYS
1	B	72	HIS
1	B	110	LYS
1	B	166	PHE

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

Mol	Chain	Res	Type
1	A	106	GLN
1	B	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	MLY	B	251	1	9,10,11	0.61	0	6,11,13	0.86	0
1	MLY	B	237	1	9,10,11	0.60	0	6,11,13	0.82	0
1	MLY	B	233	1	9,10,11	0.60	0	6,11,13	1.33	1 (16%)
1	MLY	A	320	1	9,10,11	0.71	0	6,11,13	0.96	0
1	MLY	B	308	1	9,10,11	0.58	0	6,11,13	0.80	0
1	MLY	B	223	1	9,10,11	0.55	0	6,11,13	1.28	2 (33%)
1	MLY	A	251	1	9,10,11	0.58	0	6,11,13	1.12	0
1	MLY	A	135	1	9,10,11	0.57	0	6,11,13	0.72	0
1	MLY	B	236	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	A	120	1	9,10,11	0.60	0	6,11,13	0.73	0
1	MLY	B	55	1	9,10,11	0.57	0	6,11,13	0.82	0
1	MLY	B	204	1	9,10,11	0.57	0	6,11,13	0.83	0
1	MLY	A	66	1	9,10,11	0.49	0	6,11,13	0.91	0
1	MLY	A	189	1	9,10,11	0.58	0	6,11,13	0.61	0
1	MLY	A	237	1	9,10,11	0.59	0	6,11,13	0.74	0
1	MLY	B	338	1	9,10,11	0.57	0	6,11,13	0.70	0
1	MLY	A	236	1	9,10,11	0.57	0	6,11,13	0.93	0
1	MLY	A	224	1	9,10,11	0.56	0	6,11,13	1.15	0
1	MLY	A	20	1	9,10,11	0.61	0	6,11,13	0.69	0
1	MLY	B	323	1	9,10,11	0.66	0	6,11,13	0.60	0
1	MLY	B	70	1	9,10,11	0.61	0	6,11,13	1.30	1 (16%)
1	MLY	B	174	1	9,10,11	0.52	0	6,11,13	0.87	0
1	MLY	A	223	1	9,10,11	0.66	0	6,11,13	0.77	0
1	MLY	B	120	1	9,10,11	0.46	0	6,11,13	0.92	0
1	MLY	B	231	1	9,10,11	0.65	0	6,11,13	0.70	0
1	MLY	A	233	1	9,10,11	0.61	0	6,11,13	0.77	0
1	MLY	A	174	1	9,10,11	0.57	0	6,11,13	0.97	0
1	MLY	B	163	1	9,10,11	0.56	0	6,11,13	0.92	0
1	MLY	A	55	1	9,10,11	0.52	0	6,11,13	1.05	0
1	MLY	A	204	1	9,10,11	0.70	0	6,11,13	0.77	0
1	MLY	B	20	1	9,10,11	0.52	0	6,11,13	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	338	1	9,10,11	0.61	0	6,11,13	0.83	0
1	MLY	B	320	1	9,10,11	0.75	0	6,11,13	0.67	0
1	MLY	B	66	1	9,10,11	0.56	0	6,11,13	0.84	0
1	MLY	A	323	1	9,10,11	0.54	0	6,11,13	0.89	0
1	MLY	A	70	1	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	B	189	1	9,10,11	0.62	0	6,11,13	0.73	0
1	MLY	A	231	1	9,10,11	0.47	0	6,11,13	1.13	0
1	MLY	B	224	1	9,10,11	0.53	0	6,11,13	1.05	0
1	MLY	A	163	1	9,10,11	0.60	0	6,11,13	0.96	0
1	MLY	B	135	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	A	308	1	9,10,11	0.57	0	6,11,13	0.78	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
1	MLY	B	251	1	-	0/8/9/11	-
1	MLY	B	237	1	-	1/8/9/11	-
1	MLY	B	233	1	-	0/8/9/11	-
1	MLY	A	320	1	-	0/8/9/11	-
1	MLY	B	308	1	-	1/8/9/11	-
1	MLY	B	223	1	-	2/8/9/11	-
1	MLY	A	251	1	-	2/8/9/11	-
1	MLY	A	135	1	-	0/8/9/11	-
1	MLY	B	236	1	-	0/8/9/11	-
1	MLY	A	120	1	-	1/8/9/11	-
1	MLY	B	55	1	-	2/8/9/11	-
1	MLY	B	204	1	-	0/8/9/11	-
1	MLY	A	66	1	-	2/8/9/11	-
1	MLY	A	189	1	-	0/8/9/11	-
1	MLY	A	237	1	-	1/8/9/11	-
1	MLY	B	338	1	-	3/8/9/11	-
1	MLY	A	236	1	-	0/8/9/11	-
1	MLY	A	224	1	-	0/8/9/11	-
1	MLY	A	20	1	-	2/8/9/11	-
1	MLY	B	323	1	-	2/8/9/11	-
1	MLY	B	70	1	-	1/8/9/11	-
1	MLY	B	174	1	-	2/8/9/11	-
1	MLY	A	223	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	120	1	-	0/8/9/11	-
1	MLY	B	231	1	-	1/8/9/11	-
1	MLY	A	233	1	-	3/8/9/11	-
1	MLY	A	174	1	-	2/8/9/11	-
1	MLY	B	163	1	-	3/8/9/11	-
1	MLY	A	55	1	-	0/8/9/11	-
1	MLY	A	204	1	-	0/8/9/11	-
1	MLY	B	20	1	-	5/8/9/11	-
1	MLY	A	338	1	-	0/8/9/11	-
1	MLY	B	320	1	-	1/8/9/11	-
1	MLY	B	66	1	-	2/8/9/11	-
1	MLY	A	323	1	-	1/8/9/11	-
1	MLY	A	70	1	-	1/8/9/11	-
1	MLY	B	189	1	-	0/8/9/11	-
1	MLY	A	231	1	-	1/8/9/11	-
1	MLY	B	224	1	-	0/8/9/11	-
1	MLY	A	163	1	-	1/8/9/11	-
1	MLY	B	135	1	-	0/8/9/11	-
1	MLY	A	308	1	-	1/8/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	MLY	CH2-NZ-CH1	-2.79	102.51	109.73
1	B	70	MLY	CH2-NZ-CH1	-2.44	103.42	109.73
1	B	223	MLY	CH1-NZ-CE	-2.32	101.54	110.74
1	B	223	MLY	CD-CE-NZ	-2.01	108.34	113.79

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	MLY	O-C-CA-CB
1	A	70	MLY	O-C-CA-CB
1	A	120	MLY	O-C-CA-CB
1	A	251	MLY	O-C-CA-CB
1	B	20	MLY	O-C-CA-CB
1	B	55	MLY	N-CA-CB-CG
1	B	55	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	66	MLY	C-CA-CB-CG
1	B	163	MLY	N-CA-CB-CG
1	B	163	MLY	C-CA-CB-CG
1	B	174	MLY	O-C-CA-CB
1	B	231	MLY	O-C-CA-CB
1	A	223	MLY	CE-CD-CG-CB
1	A	223	MLY	CD-CE-NZ-CH2
1	B	20	MLY	CD-CE-NZ-CH1
1	B	223	MLY	CG-CD-CE-NZ
1	B	323	MLY	CG-CD-CE-NZ
1	A	308	MLY	CG-CD-CE-NZ
1	B	66	MLY	CG-CD-CE-NZ
1	A	223	MLY	CG-CD-CE-NZ
1	B	20	MLY	CD-CE-NZ-CH2
1	B	338	MLY	CD-CE-NZ-CH2
1	A	20	MLY	CA-CB-CG-CD
1	A	223	MLY	CD-CE-NZ-CH1
1	A	231	MLY	CD-CE-NZ-CH2
1	B	163	MLY	CD-CE-NZ-CH2
1	B	20	MLY	CA-CB-CG-CD
1	B	70	MLY	CA-CB-CG-CD
1	A	223	MLY	CA-CB-CG-CD
1	B	323	MLY	CA-CB-CG-CD
1	B	338	MLY	CA-CB-CG-CD
1	A	174	MLY	CG-CD-CE-NZ
1	B	338	MLY	CG-CD-CE-NZ
1	B	237	MLY	CG-CD-CE-NZ
1	B	223	MLY	CD-CE-NZ-CH2
1	A	163	MLY	CD-CE-NZ-CH1
1	A	233	MLY	CE-CD-CG-CB
1	A	233	MLY	CG-CD-CE-NZ
1	A	233	MLY	CD-CE-NZ-CH1
1	A	251	MLY	CE-CD-CG-CB
1	A	174	MLY	CA-CB-CG-CD
1	B	320	MLY	CD-CE-NZ-CH1
1	A	237	MLY	CD-CE-NZ-CH2
1	B	174	MLY	CE-CD-CG-CB
1	B	20	MLY	CE-CD-CG-CB
1	A	323	MLY	CA-CB-CG-CD
1	A	20	MLY	CD-CE-NZ-CH1
1	B	308	MLY	CD-CE-NZ-CH2
1	A	66	MLY	CD-CE-NZ-CH2

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	223	MLY	1	0
1	A	251	MLY	2	0
1	B	338	MLY	1	0
1	A	20	MLY	2	0
1	B	323	MLY	0	1
1	A	223	MLY	3	0
1	B	320	MLY	1	0
1	A	308	MLY	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	502	2	29,33,33	1.09	3 (10%)	31,52,52	1.11	3 (9%)
3	ANP	B	502	2	29,33,33	1.02	2 (6%)	31,52,52	1.25	3 (9%)

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	A	502	2	-	1/14/38/38	0/3/3/3
3	ANP	B	502	2	-	1/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PG-O1G	3.30	1.51	1.46
3	A	502	ANP	PG-O1G	2.95	1.50	1.46
3	A	502	ANP	PG-N3B	2.62	1.70	1.63
3	A	502	ANP	PB-N3B	2.27	1.69	1.63
3	B	502	ANP	PG-N3B	2.10	1.68	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ANP	O1B-PB-N3B	-4.59	105.01	111.77
3	A	502	ANP	O1B-PB-N3B	-3.38	106.79	111.77
3	A	502	ANP	O2B-PB-O3A	2.43	112.76	104.64
3	B	502	ANP	C5-C6-N6	2.36	123.94	120.35
3	A	502	ANP	C5-C6-N6	2.21	123.70	120.35
3	B	502	ANP	O2B-PB-O3A	2.06	111.53	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

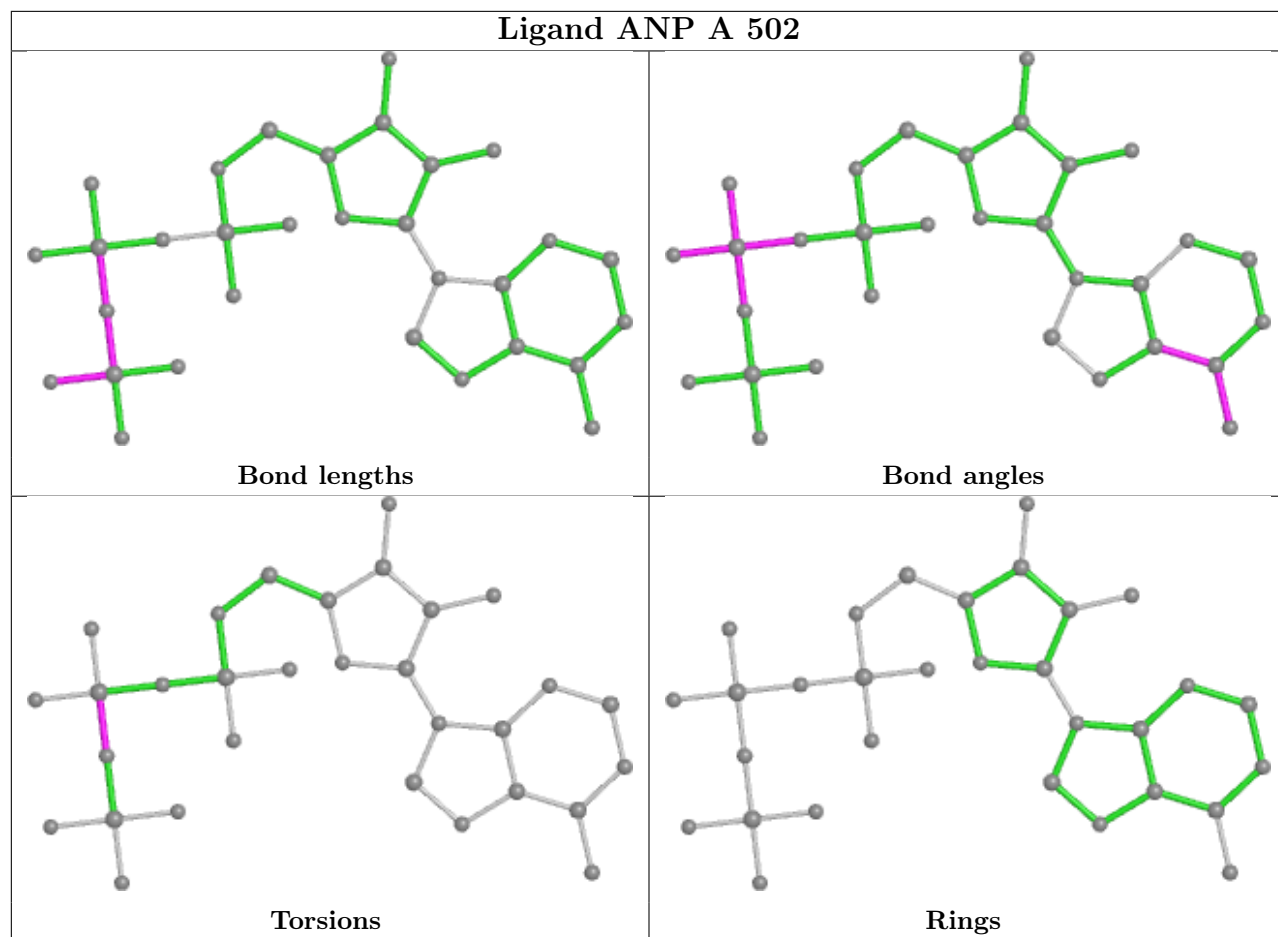
Mol	Chain	Res	Type	Atoms
3	A	502	ANP	PG-N3B-PB-O1B
3	B	502	ANP	PG-N3B-PB-O1B

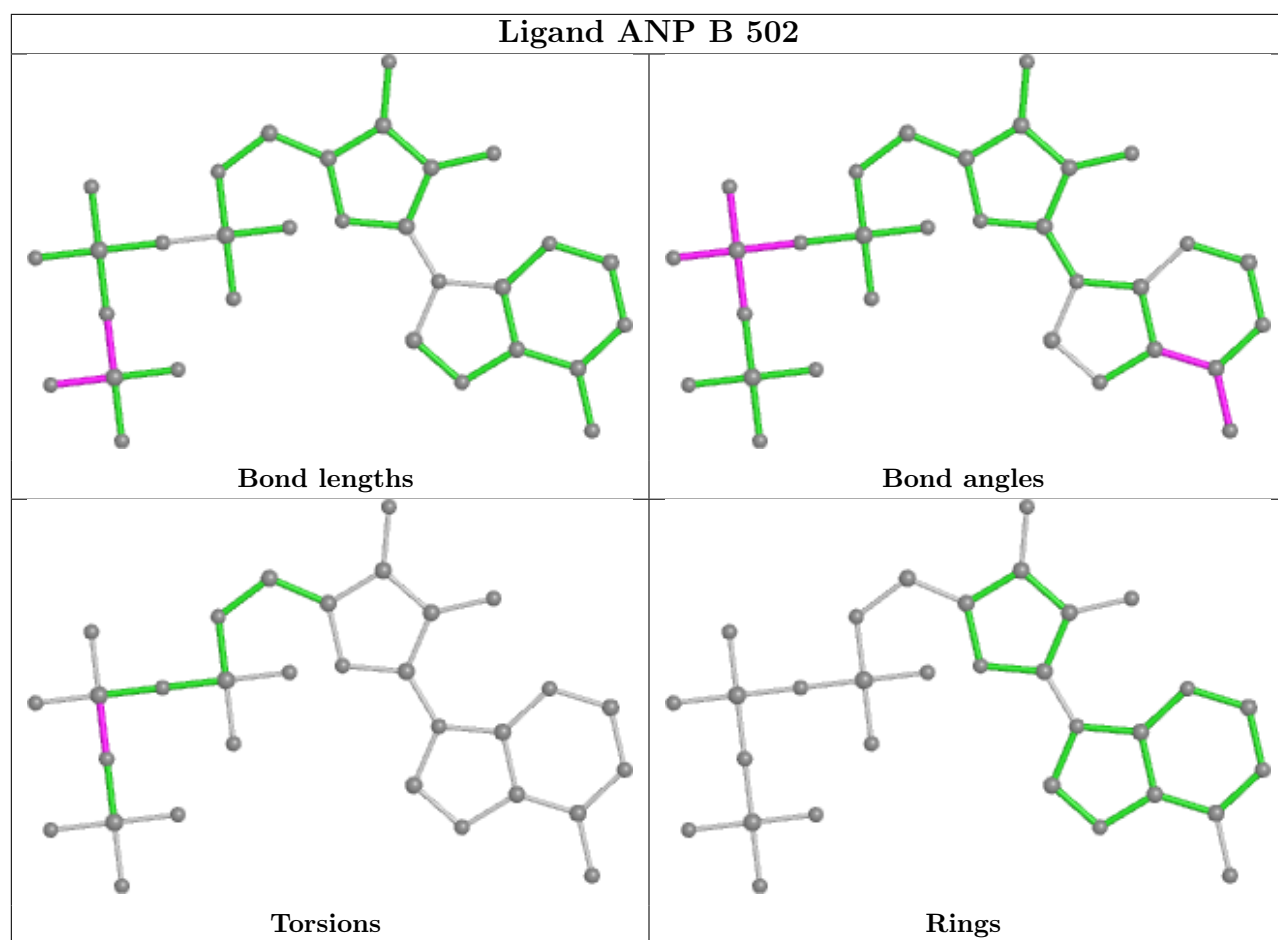
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ANP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	311/355 (87%)	0.04	10 (3%) 47 54	11, 17, 36, 69	0
1	B	309/355 (87%)	0.23	34 (11%) 5 7	14, 23, 60, 74	0
All	All	620/710 (87%)	0.13	44 (7%) 16 21	11, 20, 55, 74	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PRO	9.0
1	A	345	ILE	7.2
1	B	75	ILE	6.2
1	B	72	HIS	5.5
1	B	57	LEU	4.9
1	B	54	THR	4.7
1	B	56	LYS	4.7
1	B	53	GLY	4.4
1	A	346	GLU	4.0
1	B	77	ILE	4.0
1	B	347	GLU	4.0
1	B	58	VAL	4.0
1	B	68	ILE	4.0
1	B	50	TYR	3.9
1	B	69	GLY	3.8
1	B	107	ASP	3.8
1	B	99[A]	ILE	3.7
1	B	73	ASP	3.6
1	B	18	PRO	3.5
1	B	105	VAL	3.3
1	B	106	GLN	3.3
1	B	78	TYR	3.3
1	A	344	LEU	3.2
1	B	74	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	3.0
1	B	344	LEU	3.0
1	B	83	ASN	3.0
1	B	345	ILE	2.9
1	A	17	PRO	2.9
1	A	348	ASN	2.8
1	A	19	ARG	2.7
1	A	347	GLU	2.7
1	A	136[A]	HIS	2.7
1	B	59	ALA	2.7
1	B	104	LYS	2.7
1	B	87	THR	2.5
1	B	51	GLU	2.4
1	A	104	LYS	2.3
1	B	52	THR	2.3
1	B	101	ASN	2.3
1	B	346	GLU	2.2
1	B	65	ARG	2.0
1	B	60	LEU	2.0
1	B	79	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	B	55	11/12	0.67	0.24	57,62,67,70	0
1	MLY	B	66	11/12	0.71	0.38	55,60,67,70	0
1	MLY	B	70	11/12	0.83	0.29	49,55,60,65	0
1	MLY	B	20	11/12	0.87	0.18	27,37,49,52	0
1	MLY	B	163	11/12	0.89	0.26	26,32,51,56	0
1	MLY	B	323	11/12	0.89	0.20	23,33,66,70	0
1	MLY	B	231	11/12	0.90	0.14	18,22,34,42	0
1	MLY	A	233	11/12	0.91	0.12	29,35,38,42	0
1	MLY	B	223	11/12	0.91	0.12	14,19,30,32	0
1	MLY	A	251	11/12	0.91	0.14	18,23,40,45	0
1	MLY	B	233	11/12	0.91	0.20	22,31,72,74	0
1	MLY	A	20	11/12	0.91	0.16	25,33,44,51	0
1	MLY	A	135	11/12	0.92	0.15	24,31,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	A	223	11/12	0.92	0.14	14,17,22,30	0
1	MLY	A	338	11/12	0.92	0.13	25,33,45,46	0
1	MLY	B	320	11/12	0.92	0.11	16,19,37,41	0
1	MLY	A	231	11/12	0.92	0.13	19,26,39,42	0
1	MLY	B	237	11/12	0.93	0.13	18,27,51,53	0
1	MLY	B	189	11/12	0.94	0.11	17,22,30,31	0
1	MLY	A	70	11/12	0.94	0.10	12,14,17,19	0
1	MLY	A	323	11/12	0.94	0.13	14,24,42,46	0
1	MLY	A	120	11/12	0.94	0.12	17,21,42,43	0
1	MLY	B	236	11/12	0.94	0.12	20,25,45,52	0
1	MLY	B	120	11/12	0.94	0.12	21,28,37,43	0
1	MLY	B	135	11/12	0.94	0.09	20,25,27,28	0
1	MLY	A	237	11/12	0.94	0.10	20,24,36,38	0
1	MLY	B	338	11/12	0.94	0.17	24,31,44,46	0
1	MLY	B	204	11/12	0.95	0.10	18,22,38,44	0
1	MLY	A	174	11/12	0.95	0.10	12,20,32,33	0
1	MLY	B	251	11/12	0.95	0.08	16,18,24,28	0
1	MLY	A	236	11/12	0.96	0.09	20,25,37,37	0
1	MLY	B	224	11/12	0.96	0.08	15,21,29,36	0
1	MLY	A	204	11/12	0.96	0.11	11,14,27,34	0
1	MLY	A	55	11/12	0.96	0.11	17,21,40,40	0
1	MLY	A	308	11/12	0.96	0.11	10,12,37,38	0
1	MLY	A	320	11/12	0.96	0.10	11,15,28,29	0
1	MLY	A	224	11/12	0.96	0.10	15,18,27,34	0
1	MLY	B	308	11/12	0.96	0.09	15,19,34,39	0
1	MLY	B	174	11/12	0.96	0.10	16,26,38,45	0
1	MLY	A	163	11/12	0.96	0.11	14,16,41,42	0
1	MLY	A	66	11/12	0.96	0.11	11,16,37,38	0
1	MLY	A	189	11/12	0.98	0.10	11,13,29,29	0

6.3 Carbohydrates ⓘ

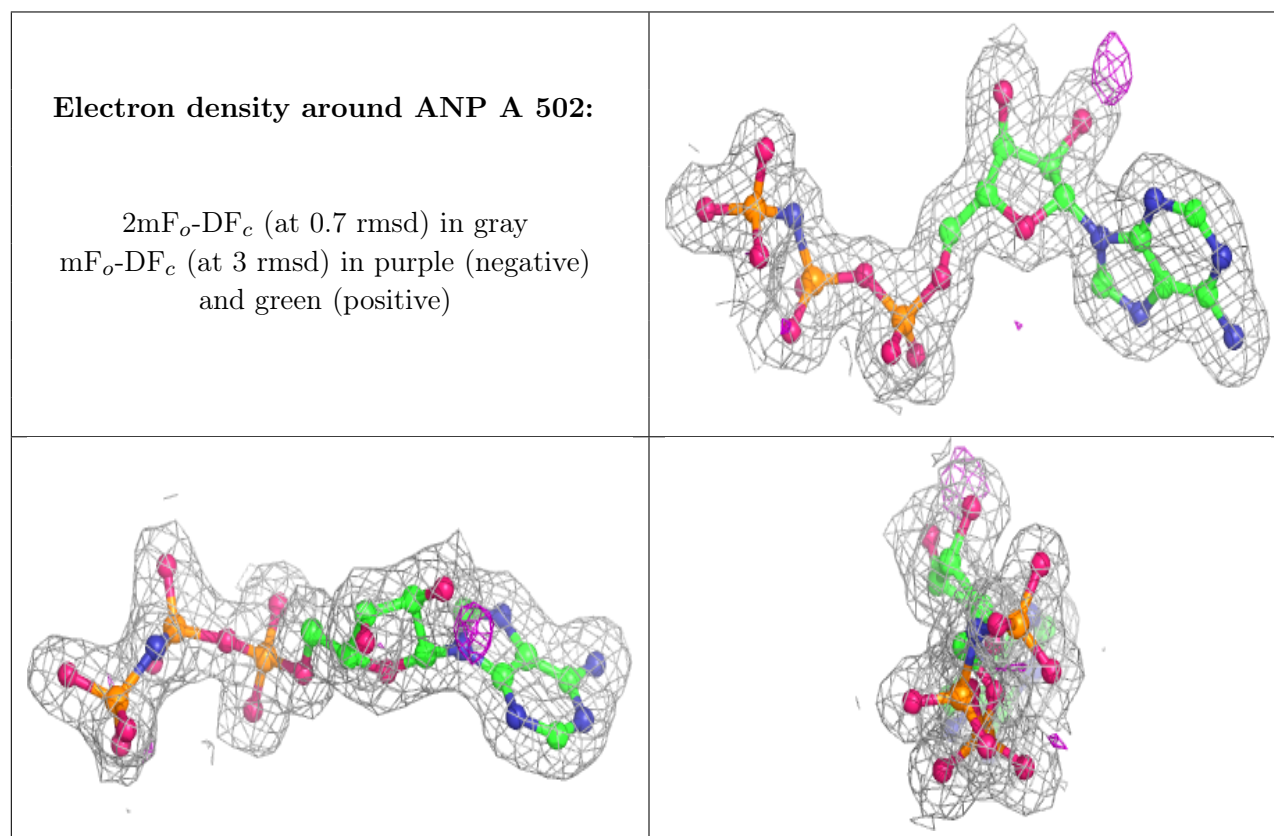
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

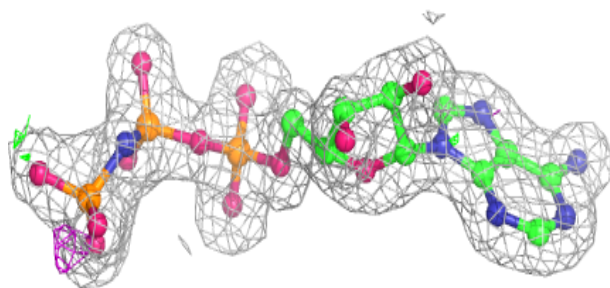
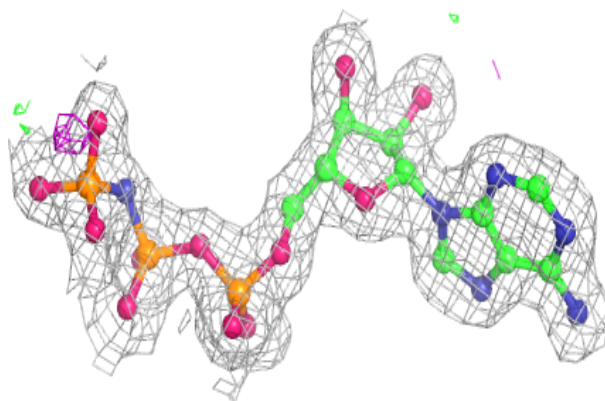
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ANP	A	502	31/31	0.97	0.09	10,15,20,22	0
3	ANP	B	502	31/31	0.97	0.07	13,18,25,28	0
2	MG	A	501	1/1	0.98	0.06	19,19,19,19	0
2	MG	B	501	1/1	0.99	0.07	23,23,23,23	0

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.



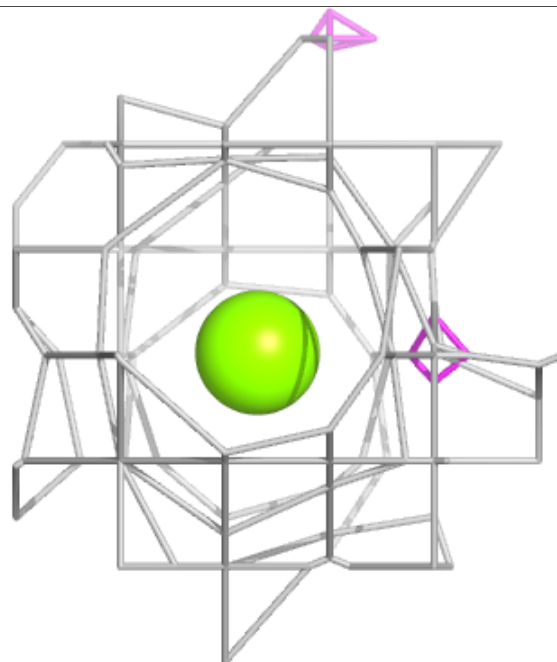
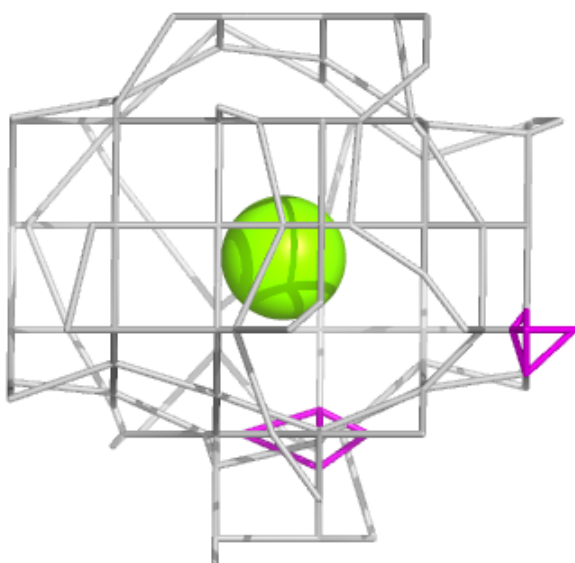
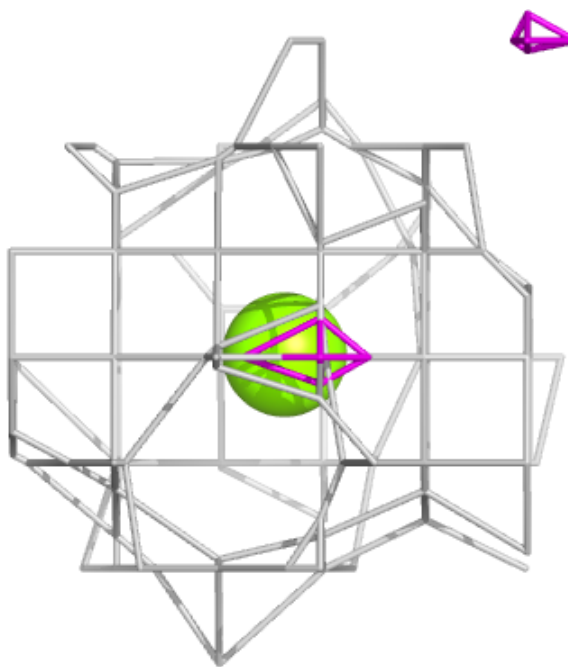
Electron density around ANP B 502:

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



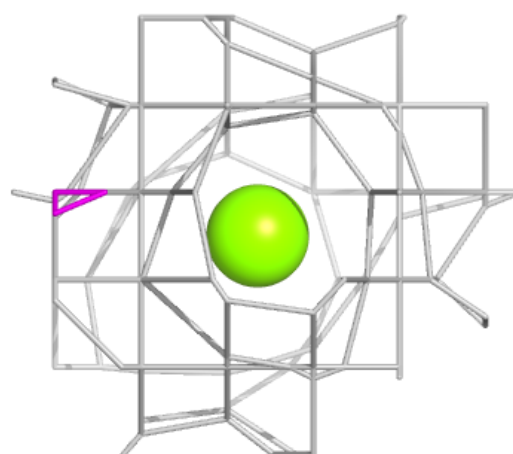
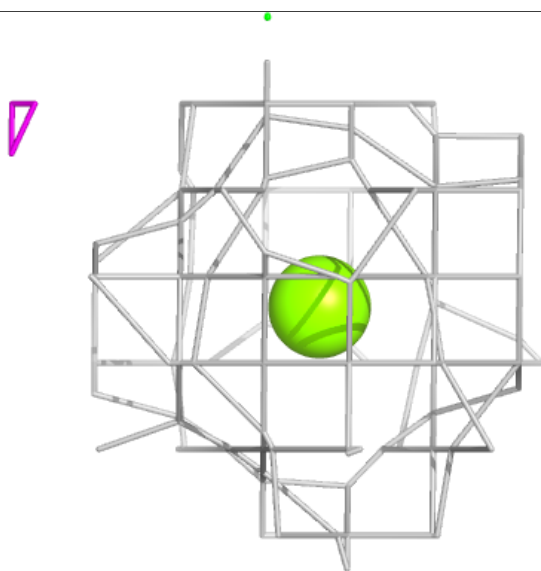
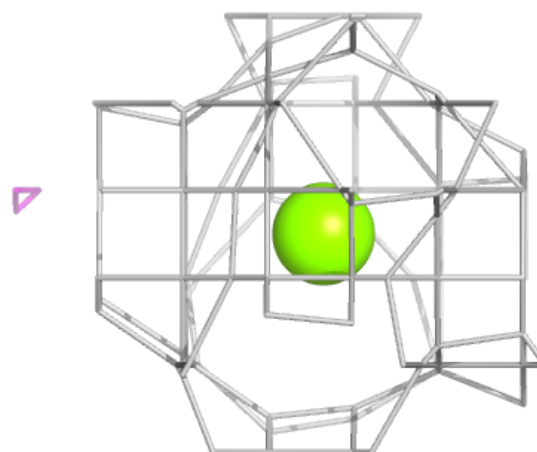
Electron density around MG A 501:

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



Electron density around MG B 501:

$2mF_o-DF_c$ (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.