



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2022 – 07:43 PM EST

PDB ID : 7LXR  
Title : Kinesin-like protein at 61F (Klp61f) bound to AMPPNP  
Authors : Worthylake, D.K.; Wojcik, E.J.  
Deposited on : 2021-03-04  
Resolution : 1.74 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](mailto: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>.

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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 : 2.31.2  
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) : 2.31.2

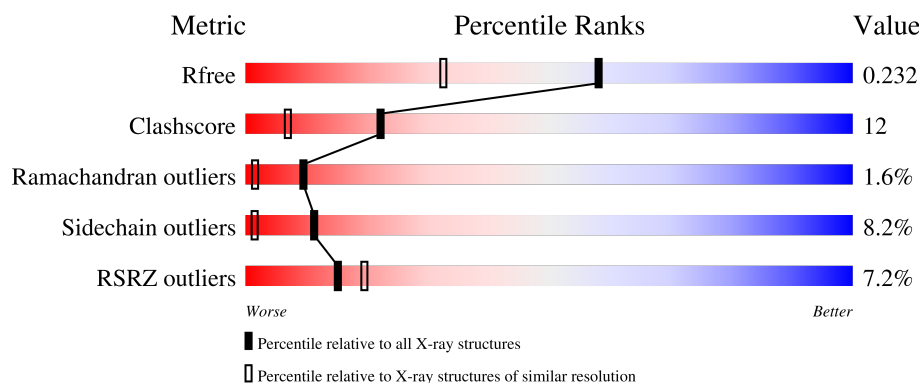
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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  $\geq 3$ , 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	369	<div> <div>4%</div> <div>70%</div> <div>19%</div> <div>• • 8%</div> </div>
1	B	369	<div> <div>9%</div> <div>70%</div> <div>18%</div> <div>• • 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	402	-	-	X	-
2	EDO	B	401	-	-	X	-
2	EDO	B	402	-	-	X	-
5	IOD	A	405	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11595 atoms, of which 5686 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.

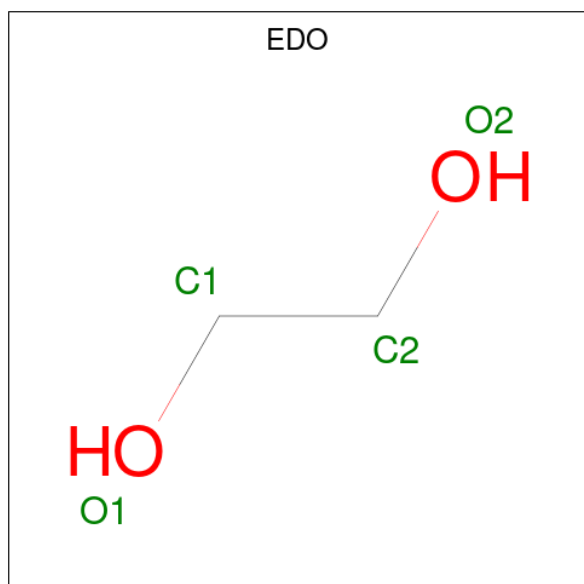
- Molecule 1 is a protein called Kinesin-like protein Klp61F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	H	N	O	S	97	14	0
			5612	1731	2847	482	540	12			
1	B	344	Total	C	H	N	O	S	89	2	0
			5522	1702	2789	486	535	10			

There are 4 discrepancies between the modelled and reference sequences:

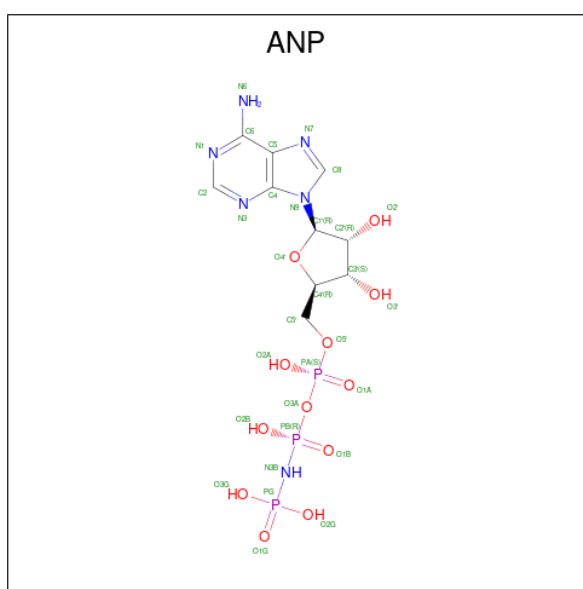
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P46863
A	0	ALA	-	expression tag	UNP P46863
B	-1	GLY	-	expression tag	UNP P46863
B	0	ALA	-	expression tag	UNP P46863

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	1	0
2	A	1	Total C H O 10 2 6 2	1	0
2	B	1	Total C H O 10 2 6 2	1	0
2	B	1	Total C H O 10 2 6 2	1	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O P 44 10 13 6 12 3	2	0
3	B	1	Total C H N O P 44 10 13 6 12 3	2	0

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

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

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total I 2 2	0	0

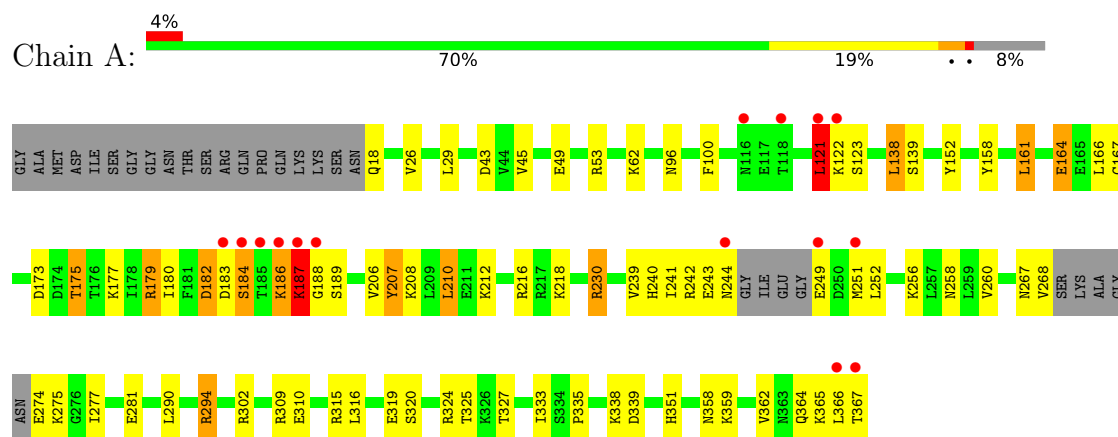
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	219	Total O 219 219	0	0
6	B	110	Total O 110 110	0	0

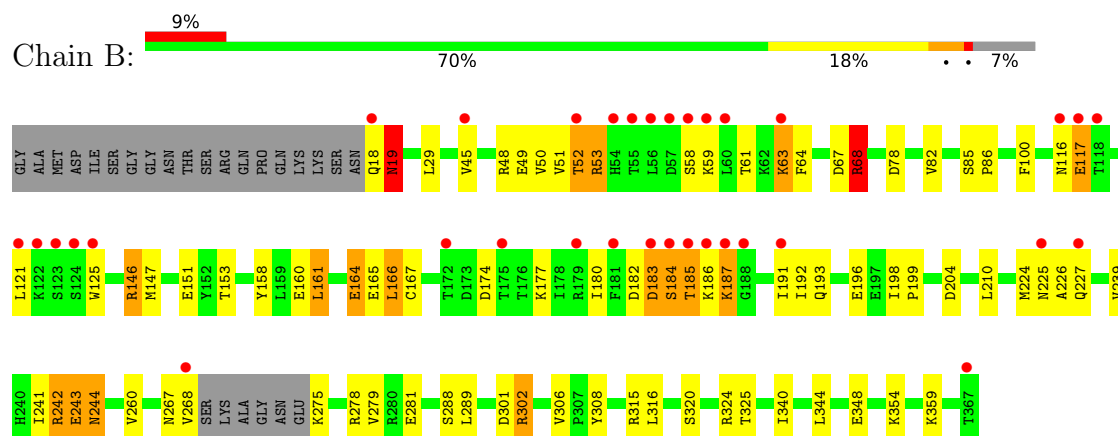
### 3 Residue-property plots [i](#)

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: Kinesin-like protein Klp61F



#### • Molecule 1: Kinesin-like protein Klp61F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.69Å 50.81Å 93.34Å 78.53° 77.87° 73.20°	Depositor
Resolution (Å)	48.11 – 1.74 48.11 – 1.74	Depositor EDS
% Data completeness (in resolution range)	90.6 (48.11-1.74) 90.6 (48.11-1.74)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.185 , 0.224 0.193 , 0.232	Depositor DCC
$R_{free}$ test set	2669 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: IOD, MG, EDO, 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	0.93	1/2836 (0.0%)	1.13	11/3829 (0.3%)
1	B	0.78	0/2775	1.00	7/3744 (0.2%)
All	All	0.86	1/5611 (0.0%)	1.07	18/7573 (0.2%)

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	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	ARG	CD-NE	-5.05	1.37	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ARG	NE-CZ-NH2	-13.83	113.38	120.30
1	A	230	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	A	294	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	146	ARG	NE-CZ-NH1	-8.61	115.99	120.30
1	A	315	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	B	242	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	146	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	B	68	ARG	NE-CZ-NH1	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	225	ASN	CB-CA-C	6.46	123.31	110.40
1	A	315	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	243	GLU	CB-CA-C	-5.89	98.61	110.40
1	A	294	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	207	TYR	CB-CG-CD1	5.21	124.13	121.00
1	A	242	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	309	ARG	CB-CG-CD	5.10	124.85	111.60
1	A	210	LEU	CB-CG-CD2	5.09	119.66	111.00
1	B	164	GLU	CB-CA-C	5.06	120.52	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	LEU	Peptide
1	A	182	ASP	Peptide
1	A	274	GLU	Peptide
1	B	53	ARG	Peptide

## 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	2765	2847	2844	76	0
1	B	2733	2789	2776	54	0
2	A	8	12	10	8	0
2	B	8	12	10	12	0
3	A	31	13	13	0	0
3	B	31	13	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	2	0
6	A	219	0	0	12	0
6	B	110	0	0	7	0
All	All	5909	5686	5666	132	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 12.

All (132) 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:164:GLU:OE1	2:B:402:EDO:O2	1.74	1.06
1:A:243:GLU:O	1:A:244:ASN:HB2	1.49	1.05
1:A:167[B]:CYS:SG	6:A:681:HOH:O	2.10	1.00
1:A:179:ARG:HH11	1:A:179:ARG:HG3	1.19	1.00
1:A:320:SER:HA	1:A:325[A]:THR:HG21	1.42	0.99
1:A:294:ARG:NH2	1:A:310:GLU:OE1	2.09	0.84
1:A:179:ARG:HD3	2:A:402:EDO:O2	1.78	0.83
1:B:161:LEU:HD13	2:B:402:EDO:H21	1.60	0.83
2:A:401:EDO:O2	5:A:405:IOD:I	2.69	0.80
1:A:138[B]:LEU:HD22	1:A:206[B]:VAL:HG11	1.63	0.79
1:A:365:LYS:HG2	1:A:365:LYS:O	1.81	0.79
1:A:18:GLN:NE2	6:A:502:HOH:O	2.14	0.77
1:A:244:ASN:HB3	6:A:700:HOH:O	1.84	0.77
1:A:179:ARG:HG3	1:A:179:ARG:NH1	1.98	0.76
1:B:116:ASN:O	1:B:117:GLU:O	2.04	0.74
1:A:358:ASN:O	1:A:359:LYS:HE2	1.87	0.74
1:A:230:ARG:HD3	1:A:281:GLU:OE1	1.88	0.73
1:A:179:ARG:NH1	1:B:301:ASP:OD2	2.20	0.71
1:B:153:THR:HB	2:B:401:EDO:H12	1.71	0.70
1:A:243:GLU:O	1:A:244:ASN:CB	2.36	0.70
1:B:68:ARG:HG3	1:B:68:ARG:HH11	1.58	0.69
1:A:179:ARG:CD	2:A:402:EDO:O2	2.40	0.69
1:B:49:GLU:HG3	6:B:565:HOH:O	1.92	0.69
1:A:320:SER:HA	1:A:325[A]:THR:CG2	2.20	0.68
1:A:173:ASP:OD1	1:A:175:THR:HB	1.94	0.67
1:A:183:ASP:HB3	1:A:189:SER:C	2.15	0.66
1:B:63:LYS:HE2	1:B:64:PHE:N	2.14	0.62
1:B:164:GLU:OE1	2:B:402:EDO:C2	2.47	0.62
1:A:45[A]:VAL:HG23	1:A:49:GLU:HB2	1.81	0.62
1:A:367:THR:O	1:A:367:THR:HG22	2.00	0.61
1:A:138[A]:LEU:HG	1:A:206[A]:VAL:HG21	1.82	0.61
1:A:290:LEU:HD12	6:A:554:HOH:O	2.01	0.60
1:B:227:GLN:HA	1:B:227:GLN:HE21	1.66	0.59
1:B:244:ASN:HA	6:B:531:HOH:O	2.02	0.59
1:A:62:LYS:HE2	6:A:506:HOH:O	2.03	0.59
1:B:192:ILE:N	1:B:192:ILE:HD12	2.17	0.58
1:B:161:LEU:HD13	2:B:402:EDO:C2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HD2	6:B:518:HOH:O	2.01	0.58
1:A:164:GLU:HG3	6:A:622:HOH:O	2.03	0.58
1:B:196:GLU:HB3	1:B:198:ILE:HD11	1.85	0.57
1:B:226:ALA:O	1:B:227:GLN:NE2	2.38	0.57
1:B:52:THR:HG21	1:B:344:LEU:HD21	1.87	0.56
1:B:183:ASP:O	1:B:185:THR:N	2.40	0.55
1:A:319:GLU:OE2	1:A:324:ARG:HG2	2.07	0.54
1:A:161:LEU:HD13	5:A:405:IOD:I	2.77	0.54
1:B:227:GLN:HA	1:B:227:GLN:NE2	2.21	0.54
1:A:183:ASP:CB	1:A:189:SER:HB3	2.38	0.54
1:B:18:GLN:HA	1:B:354:LYS:O	2.07	0.54
1:B:45:VAL:HG22	1:B:49:GLU:HB2	1.90	0.53
1:A:251:MET:HE1	1:A:364:GLN:CG	2.39	0.53
1:A:256:LYS:HE2	1:A:258:ASN:HD21	1.73	0.53
1:B:151:GLU:OE1	1:B:242:ARG:HD2	2.08	0.53
1:A:173:ASP:CG	1:A:175:THR:HB	2.29	0.52
1:A:365:LYS:O	1:A:365:LYS:CG	2.53	0.52
1:A:230:ARG:CD	1:A:281:GLU:OE1	2.56	0.52
1:A:251:MET:HE1	1:A:364:GLN:HG2	1.92	0.52
1:A:26:VAL:HG22	1:A:333:ILE:HD11	1.91	0.51
1:A:180:ILE:HG22	2:A:402:EDO:O1	2.11	0.51
1:B:51:VAL:HG22	1:B:63:LYS:HG2	1.91	0.51
1:A:362:VAL:CG1	1:A:364:GLN:HG3	2.41	0.51
1:A:367:THR:O	1:A:367:THR:CG2	2.58	0.51
1:A:249:GLU:CG	1:A:367:THR:OXT	2.60	0.50
1:A:121:LEU:O	1:A:121:LEU:HG	2.12	0.50
2:B:401:EDO:C1	6:B:556:HOH:O	2.60	0.49
1:A:218:LYS:HE3	6:A:711:HOH:O	2.12	0.49
1:A:123:SER:HB2	6:A:568:HOH:O	2.11	0.49
1:B:199:PRO:HB3	2:B:401:EDO:H22	1.94	0.49
1:A:43:ASP:OD2	1:A:53:ARG:NE	2.32	0.49
1:A:180:ILE:CG2	2:A:402:EDO:H12	2.43	0.49
1:A:249:GLU:OE2	1:A:366:LEU:HB3	2.13	0.48
1:B:288:SER:HB3	2:B:402:EDO:H11	1.95	0.48
1:B:121:LEU:HD11	1:B:204:ASP:HB2	1.94	0.48
1:A:180:ILE:HG22	2:A:402:EDO:C1	2.43	0.48
1:B:166:LEU:HD21	1:B:180:ILE:HG13	1.95	0.48
1:B:239:VAL:HG12	1:B:241:ILE:HG13	1.95	0.48
1:B:278[A]:ARG:NH1	1:B:281:GLU:OE1	2.46	0.48
1:B:100:PHE:HB3	1:B:260:VAL:HB	1.95	0.47
1:A:138[B]:LEU:CD2	1:A:206[B]:VAL:HG11	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLU:HB3	1:B:167:CYS:HB3	1.96	0.47
1:A:164:GLU:CG	6:A:622:HOH:O	2.62	0.47
1:A:183:ASP:OD2	1:A:189:SER:HB3	2.14	0.47
1:A:324:ARG:O	1:A:324:ARG:HG3	2.14	0.47
1:B:161:LEU:HD22	2:B:402:EDO:C2	2.44	0.47
1:B:161:LEU:CD1	2:B:402:EDO:H21	2.40	0.47
1:B:306:VAL:HG22	1:B:308:TYR:CE2	2.50	0.47
1:A:29:LEU:HD13	1:A:335:PRO:HG2	1.97	0.47
1:B:244:ASN:HD22	1:B:244:ASN:C	2.17	0.47
1:B:146:ARG:HG3	6:B:564:HOH:O	2.16	0.46
1:B:183:ASP:HB3	1:B:191:ILE:CG1	2.45	0.46
1:A:180:ILE:HG22	2:A:402:EDO:H12	1.98	0.46
1:A:275:LYS:HG3	6:A:501:HOH:O	2.15	0.46
1:A:251:MET:HE3	1:A:252:LEU:N	2.31	0.46
1:B:182:ASP:O	1:B:184:SER:N	2.42	0.46
1:B:18:GLN:O	1:B:19:ASN:CB	2.64	0.45
1:A:184:SER:O	1:A:187:LYS:HG2	2.17	0.45
2:B:401:EDO:H12	6:B:556:HOH:O	2.17	0.45
1:B:48:ARG:NH1	1:B:67:ASP:O	2.50	0.45
1:A:239[A]:VAL:HG12	1:A:241:ILE:HG13	1.97	0.45
1:B:63:LYS:HE2	1:B:63:LYS:C	2.36	0.45
1:B:85:SER:N	1:B:86:PRO:CD	2.80	0.45
1:A:179:ARG:HD3	2:A:402:EDO:C2	2.46	0.45
1:A:294:ARG:HH22	1:A:310:GLU:CD	2.12	0.44
1:A:362:VAL:HG12	1:A:364:GLN:HG3	1.99	0.44
1:B:301:ASP:C	1:B:302:ARG:HG2	2.38	0.44
1:A:183:ASP:CG	1:A:189:SER:HB3	2.38	0.43
1:B:183:ASP:HB3	1:B:191:ILE:HG13	2.01	0.43
1:A:249:GLU:HG2	1:A:367:THR:OXT	2.19	0.43
1:B:125:TRP:HD1	6:B:555:HOH:O	2.02	0.43
1:A:121:LEU:CD1	6:A:697:HOH:O	2.67	0.42
1:A:249:GLU:HG3	1:A:367:THR:OXT	2.19	0.42
1:A:186:LYS:HG3	1:A:324:ARG:CZ	2.50	0.42
1:B:196:GLU:HB3	1:B:198:ILE:CD1	2.48	0.42
1:B:340:ILE:HD12	1:B:340:ILE:HA	1.86	0.42
1:A:325[A]:THR:CG2	1:A:327:THR:OG1	2.67	0.42
1:B:226:ALA:O	1:B:227:GLN:CD	2.58	0.42
1:B:78:ASP:O	1:B:82:VAL:HG13	2.19	0.42
1:A:121:LEU:HD13	6:A:697:HOH:O	2.19	0.41
1:B:58:SER:OG	1:B:59:LYS:N	2.53	0.41
1:A:139:SER:HB2	1:A:207:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:MET:HE1	1:A:364:GLN:CB	2.51	0.41
1:A:325[A]:THR:HG23	1:A:327:THR:OG1	2.21	0.41
1:A:179:ARG:NH1	1:A:179:ARG:CG	2.72	0.41
1:A:338:LYS:HE3	1:A:339:ASP:OD2	2.21	0.41
1:B:306:VAL:CG2	1:B:308:TYR:CE2	3.04	0.41
1:B:100:PHE:CB	1:B:260:VAL:HB	2.50	0.41
1:A:325[B]:THR:HG22	1:A:327:THR:OG1	2.21	0.40
1:B:320:SER:HA	1:B:325:THR:OG1	2.22	0.40
1:B:164:GLU:HA	2:B:402:EDO:H22	2.03	0.40
1:A:100:PHE:HB3	1:A:260:VAL:HB	2.03	0.40
1:A:212:LYS:HE2	1:A:216:ARG:HH22	1.86	0.40
1:A:183:ASP:HB3	1:A:189:SER:O	2.21	0.40
1:A:152:TYR:HA	1:A:240:HIS:O	2.21	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	349/369 (95%)	339 (97%)	6 (2%)	4 (1%)	14	3
1	B	342/369 (93%)	324 (95%)	11 (3%)	7 (2%)	7	1
All	All	691/738 (94%)	663 (96%)	17 (2%)	11 (2%)	9	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	B	19	ASN
1	B	117	GLU
1	B	184	SER
1	B	187	LYS

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Mol	Chain	Res	Type
1	B	267	ASN
1	A	184	SER
1	A	187	LYS
1	A	188	GLY
1	B	183	ASP
1	B	185	THR

### 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	325/331 (98%)	303 (93%)	22 (7%)	16	2
1	B	313/331 (95%)	282 (90%)	31 (10%)	8	1
All	All	638/662 (96%)	585 (92%)	53 (8%)	11	1

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	121	LEU
1	A	138[A]	LEU
1	A	138[B]	LEU
1	A	158	TYR
1	A	161	LEU
1	A	164	GLU
1	A	166	LEU
1	A	175	THR
1	A	177	LYS
1	A	179	ARG
1	A	182	ASP
1	A	186	LYS
1	A	187	LYS
1	A	208	LYS
1	A	210	LEU
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	268	VAL
1	A	277[A]	ILE
1	A	277[B]	ILE
1	A	316	LEU
1	A	351	HIS
1	B	19	ASN
1	B	29	LEU
1	B	50	VAL
1	B	52	THR
1	B	53	ARG
1	B	61	THR
1	B	63	LYS
1	B	68	ARG
1	B	147	MET
1	B	158	TYR
1	B	161	LEU
1	B	165	GLU
1	B	166	LEU
1	B	174	ASP
1	B	177	LYS
1	B	186	LYS
1	B	187	LYS
1	B	193	GLN
1	B	210	LEU
1	B	224	MET
1	B	243	GLU
1	B	244	ASN
1	B	268	VAL
1	B	275	LYS
1	B	279	VAL
1	B	289	LEU
1	B	302	ARG
1	B	316	LEU
1	B	324	ARG
1	B	348	GLU
1	B	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	227	GLN

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Mol	Chain	Res	Type
1	A	258	ASN
1	A	318	GLN
1	B	193	GLN
1	B	227	GLN
1	B	244	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	EDO	A	401	-	3,3,3	0.65	0	2,2,2	0.91	0
2	EDO	B	402	-	3,3,3	1.71	1 (33%)	2,2,2	0.61	0
2	EDO	A	402	-	3,3,3	1.17	0	2,2,2	0.76	0
3	ANP	A	403	4	29,33,33	1.30	4 (13%)	31,52,52	1.28	5 (16%)
2	EDO	B	401	-	3,3,3	0.17	0	2,2,2	0.31	0
3	ANP	B	403	4	29,33,33	1.48	2 (6%)	31,52,52	1.23	4 (12%)

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	EDO	A	401	-	-	1/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
3	ANP	A	403	4	-	3/14/38/38	0/3/3/3
2	EDO	B	401	-	-	0/1/1/1	-
3	ANP	B	403	4	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	ANP	PG-O1G	5.21	1.54	1.46
3	B	403	ANP	PB-O1B	4.17	1.52	1.46
3	A	403	ANP	PG-O1G	3.20	1.51	1.46
3	A	403	ANP	PG-O2G	-3.10	1.48	1.56
3	A	403	ANP	PB-O1B	3.04	1.51	1.46
2	B	402	EDO	O2-C2	-2.75	1.27	1.42
3	A	403	ANP	PG-O3G	-2.08	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	ANP	O2B-PB-O1B	3.91	118.12	109.92
3	A	403	ANP	O2B-PB-O1B	3.40	117.05	109.92
3	B	403	ANP	O1B-PB-N3B	-2.86	107.56	111.77
3	B	403	ANP	O1G-PG-N3B	-2.78	107.67	111.77
3	A	403	ANP	O2G-PG-O1G	-2.53	107.10	113.45
3	A	403	ANP	C5-C6-N6	2.37	123.96	120.35
3	A	403	ANP	O1B-PB-N3B	-2.25	108.46	111.77
3	A	403	ANP	O3A-PB-N3B	-2.13	100.67	106.59
3	B	403	ANP	C5-C6-N6	2.08	123.52	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	ANP	PG-N3B-PB-O1B
3	A	403	ANP	PA-O3A-PB-O1B
3	A	403	ANP	PA-O3A-PB-O2B

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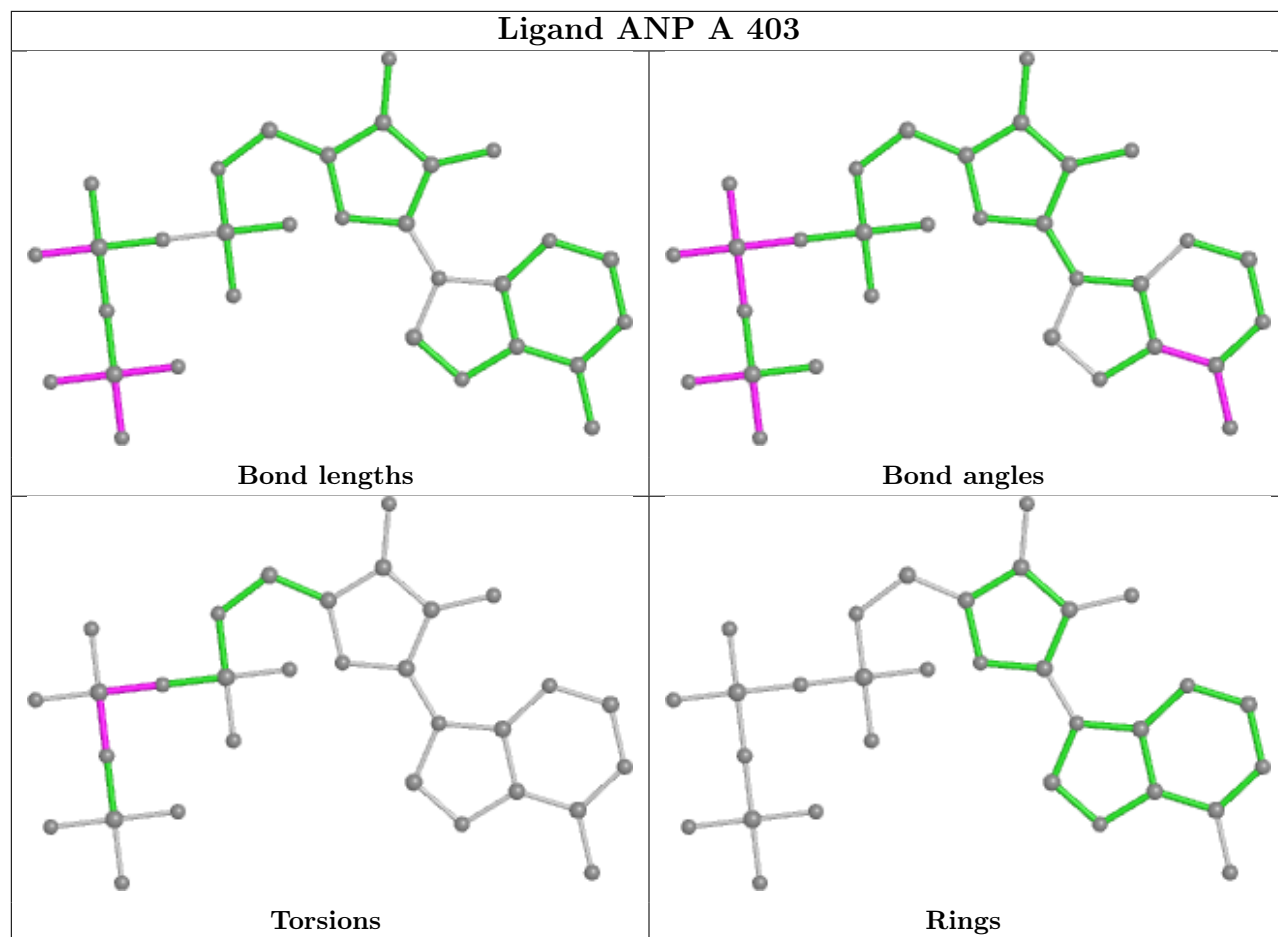
Mol	Chain	Res	Type	Atoms
3	B	403	ANP	PG-N3B-PB-O1B
3	B	403	ANP	PA-O3A-PB-O1B
3	B	403	ANP	PA-O3A-PB-O2B
2	A	401	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	B	402	EDO	O1-C1-C2-O2
3	B	403	ANP	PG-N3B-PB-O3A

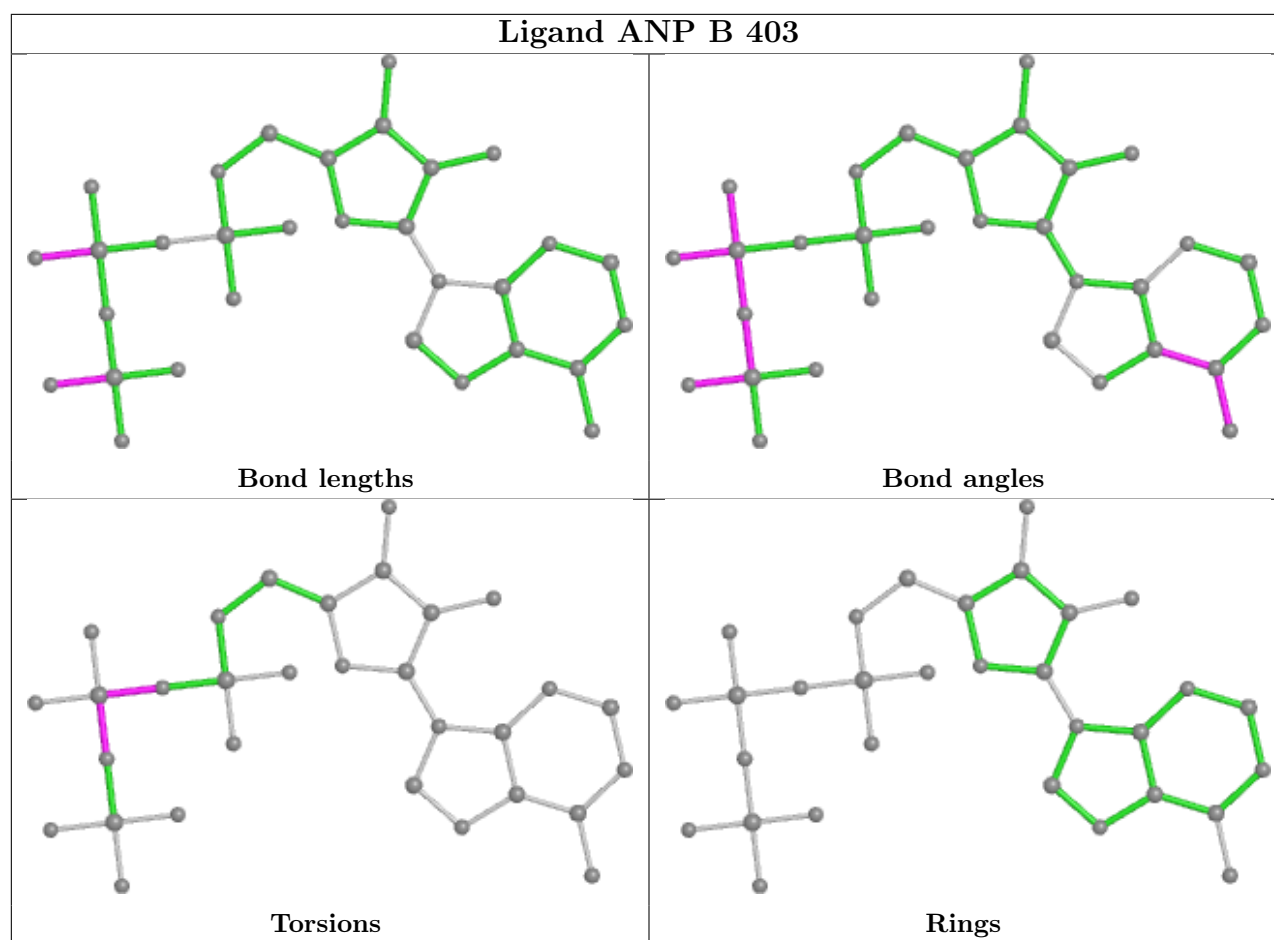
There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	EDO	1	0
2	B	402	EDO	8	0
2	A	402	EDO	7	0
2	B	401	EDO	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/369 (92%)	0.29	15 (4%) 34 39	10, 20, 51, 114	0
1	B	344/369 (93%)	0.55	34 (9%) 7 9	18, 33, 80, 106	0
All	All	685/738 (92%)	0.42	49 (7%) 15 19	10, 27, 68, 114	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	THR	12.9
1	A	188	GLY	11.0
1	B	18	GLN	8.0
1	A	184	SER	8.0
1	B	122	LYS	6.9
1	B	185	THR	6.7
1	B	56	LEU	6.5
1	B	58	SER	6.3
1	B	118	THR	6.2
1	A	121	LEU	6.0
1	B	186	LYS	5.9
1	B	187	LYS	5.8
1	B	59	LYS	5.8
1	B	121	LEU	5.6
1	B	55	THR	5.6
1	B	123	SER	5.2
1	A	186	LYS	5.0
1	B	60	LEU	4.9
1	A	366	LEU	4.4
1	B	117	GLU	4.2
1	B	54	HIS	4.0
1	B	116	ASN	4.0
1	B	181	PHE	3.7
1	B	57	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	367	THR	3.3
1	B	367	THR	3.3
1	B	125	TRP	3.3
1	B	45	VAL	3.2
1	A	249	GLU	3.1
1	B	225	ASN	2.8
1	A	187	LYS	2.8
1	B	63	LYS	2.7
1	B	268	VAL	2.7
1	A	122	LYS	2.6
1	B	52	THR	2.6
1	B	227	GLN	2.6
1	A	183	ASP	2.5
1	B	191	ILE	2.5
1	B	124	SER	2.5
1	B	184	SER	2.5
1	A	244	ASN	2.4
1	B	175	THR	2.2
1	A	116	ASN	2.2
1	B	179	ARG	2.2
1	A	118	THR	2.2
1	B	172	THR	2.1
1	A	251	MET	2.1
1	B	188	GLY	2.1
1	B	183	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

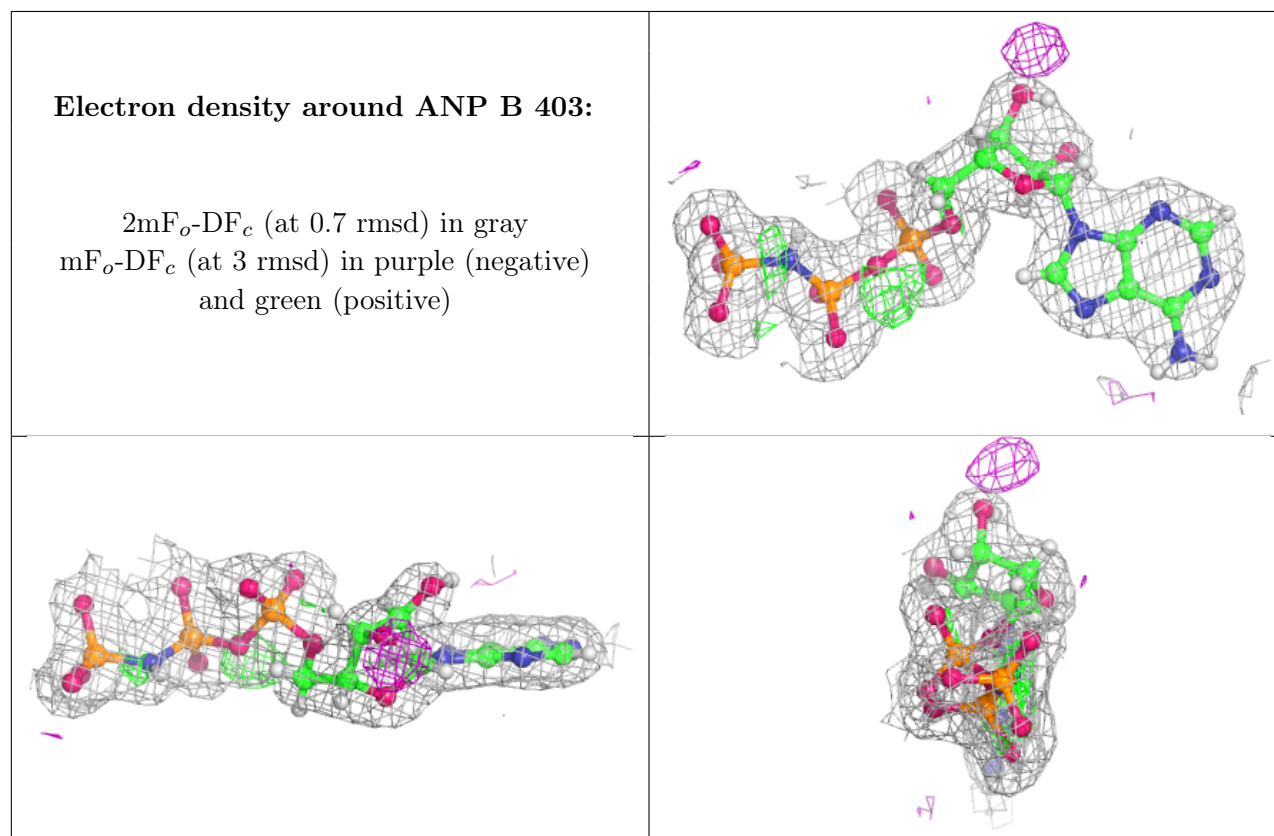
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

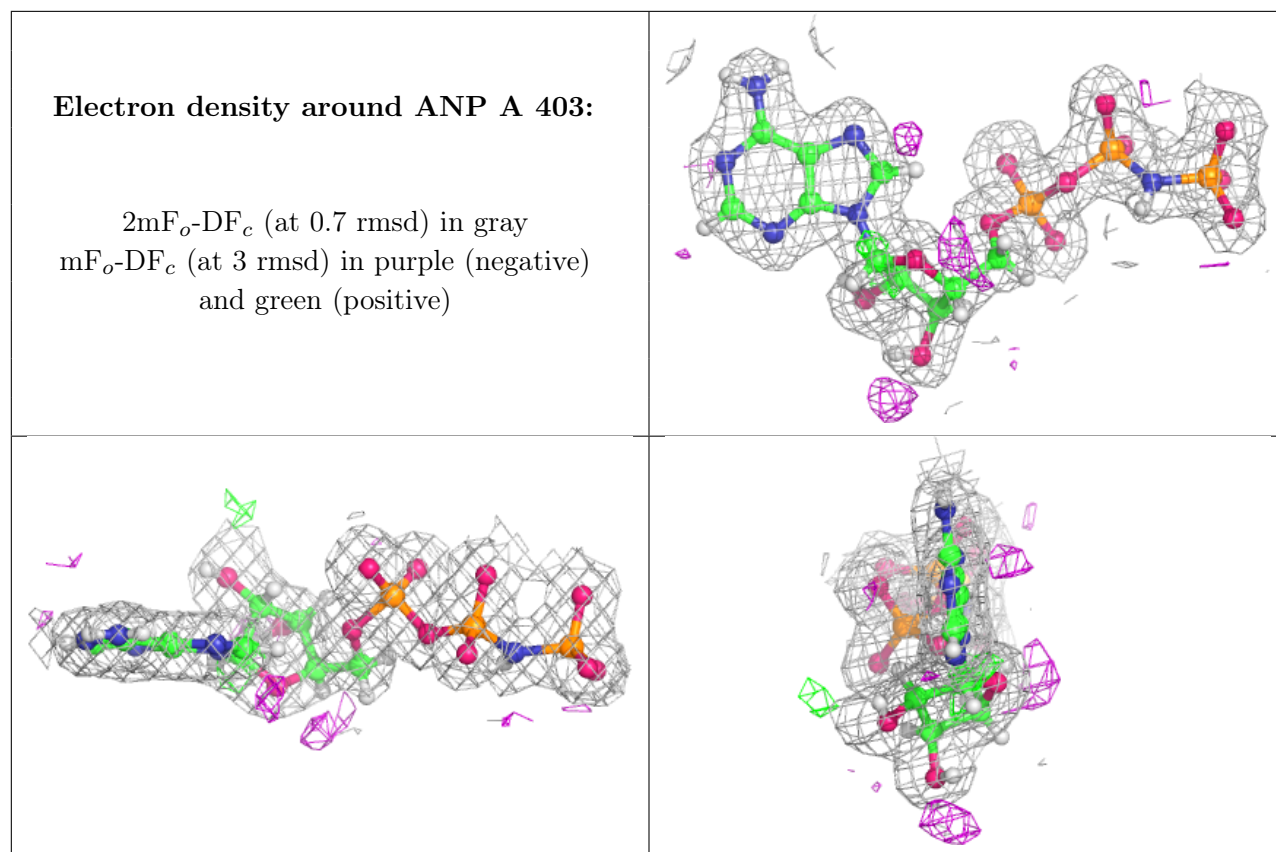
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	402	4/4	0.88	0.12	24,28,30,33	1
2	EDO	A	401	4/4	0.93	0.14	14,21,23,28	1
2	EDO	B	401	4/4	0.93	0.31	35,36,38,46	1
2	EDO	B	402	4/4	0.93	0.17	17,20,24,24	1
3	ANP	B	403	31/31	0.97	0.09	19,28,35,48	2
3	ANP	A	403	31/31	0.99	0.09	8,16,23,33	2
4	MG	B	404	1/1	0.99	0.04	22,22,22,22	0
5	IOD	A	405	1/1	0.99	0.04	38,38,38,38	0
5	IOD	A	406	1/1	0.99	0.05	50,50,50,50	0
4	MG	A	404	1/1	1.00	0.07	10,10,10,10	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.