



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 04:11 PM JST

PDB ID : 7XZR  
Title : Crystal structure of TNIK-AMPPNP-thiopeptide TP15 complex  
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Deposited on : 2022-06-03  
Resolution : 2.26 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

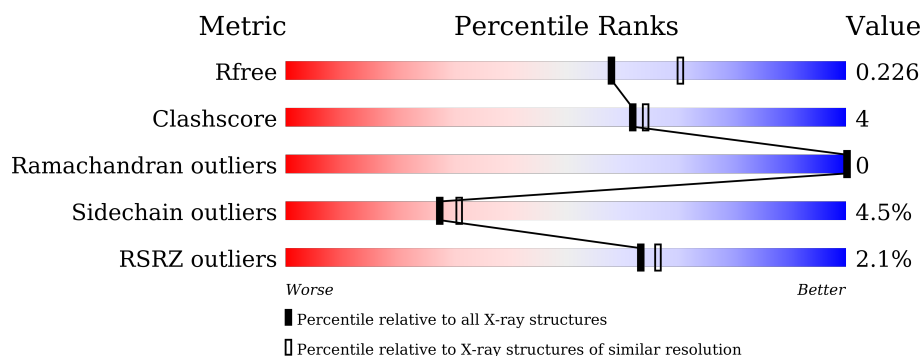
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 29%, green 75%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>82%</span> <span>14%</span> <span>..</span> </div> </div>
1	B	306	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 17%, yellow 31%, green 89%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>88%</span> <span>10%</span> <span>.</span> </div> </div>
2	C	18	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61%, yellow 39%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>61%</span> <span>39%</span> </div> </div>
2	D	18	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61%, yellow 39%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>61%</span> <span>39%</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DHA	C	16	-	X	-	-
2	DHA	D	16	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5337 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 TRAF2 and NCK-interacting protein kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	P	S	0	2	0
			2403	1521	423	442	2	15			
1	B	301	Total	C	N	O	P	S	0	2	0
			2409	1521	428	443	2	15			

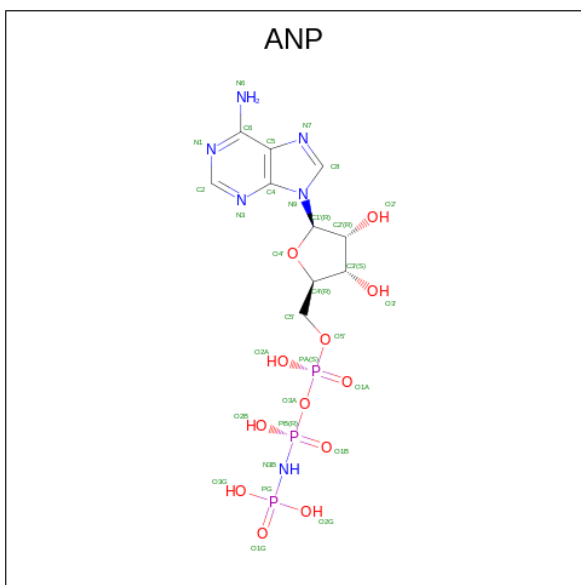
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP Q9UKE5
A	10	PRO	-	expression tag	UNP Q9UKE5
B	9	GLY	-	expression tag	UNP Q9UKE5
B	10	PRO	-	expression tag	UNP Q9UKE5

- Molecule 2 is a protein called thiopeptide TP15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	S	0	1	1
			127	80	26	18	3			
2	D	18	Total	C	N	O	S	0	0	1
			123	77	26	17	3			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

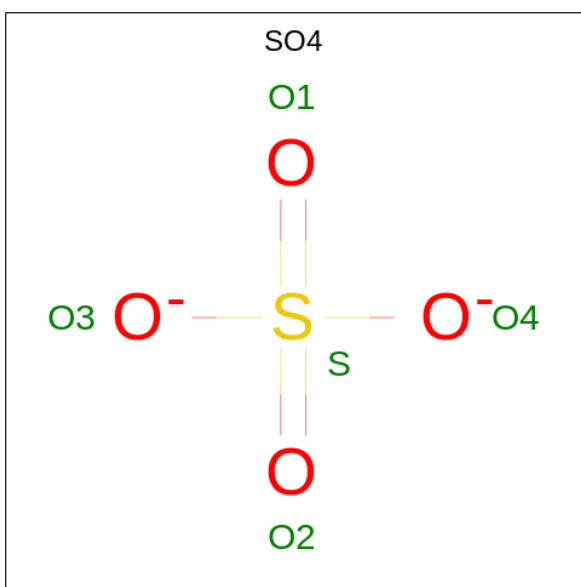


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
3	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

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

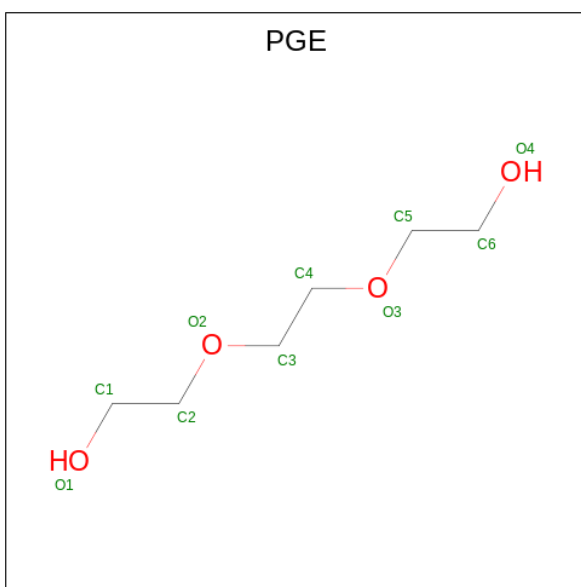
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

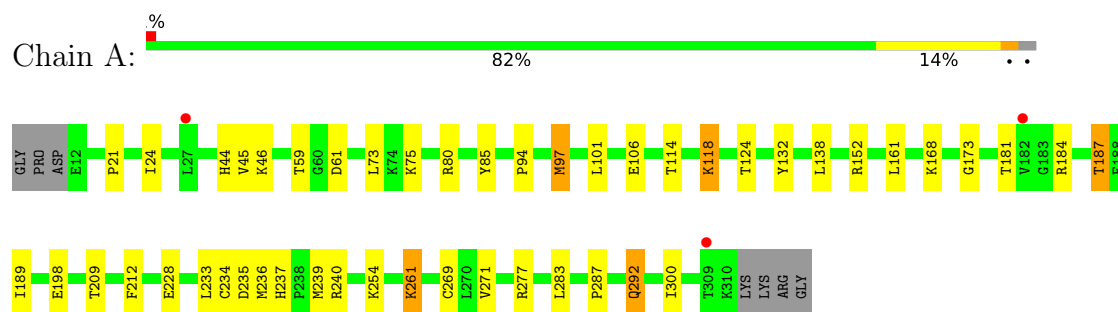
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total 90	O 90	0	0
7	B	87	Total 87	O 87	0	0
7	C	7	Total 7	O 7	0	0
7	D	2	Total 2	O 2	0	0

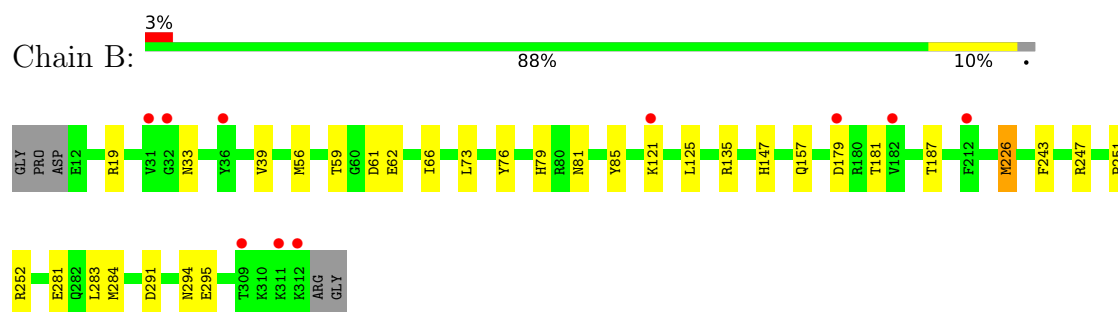
### 3 Residue-property plots [i](#)

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: TRAF2 and NCK-interacting protein kinase



- Molecule 1: TRAF2 and NCK-interacting protein kinase



- Molecule 2: thiopeptide TP15



- Molecule 2: thiopeptide TP15





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.11Å 167.65Å 53.71Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	43.34 – 2.26 43.34 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.34-2.26) 99.9 (43.34-2.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.182 , 0.226 0.181 , 0.226	Depositor DCC
$R_{free}$ test set	1957 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ANP, MOH, DHA, PGE, MG, BB9, TPO

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	0.41	0/2438	0.60	0/3291
1	B	0.42	0/2443	0.63	1/3297 (0.0%)
2	C	0.51	0/98	0.88	0/131
2	D	0.49	0/93	0.83	0/125
All	All	0.42	0/5072	0.63	1/6844 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	MET	CG-SD-CE	5.32	108.71	100.20

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	2403	0	2398	24	0
1	B	2409	0	2397	14	0
2	C	127	0	117	0	0
2	D	123	0	110	0	0
3	A	31	0	11	3	0
3	B	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	10	0	14	0	0
7	A	90	0	0	3	0
7	B	87	0	0	1	0
7	C	7	0	0	0	0
7	D	2	0	0	0	0
All	All	5337	0	5059	45	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 (45) 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)
3:B:1401:ANP:H8	3:B:1401:ANP:O2A	1.62	0.99
1:B:59:THR:HG22	1:B:61:ASP:H	1.37	0.87
3:A:1401:ANP:O3G	7:A:1501:HOH:O	1.93	0.87
1:B:56:MET:HE1	1:B:66:ILE:HD11	1.64	0.80
1:A:59:THR:HG22	1:A:61:ASP:H	1.50	0.75
3:A:1401:ANP:O3G	7:A:1502:HOH:O	2.07	0.73
1:A:187:TPO:HG23	1:A:189[A]:ILE:HG12	1.75	0.66
1:B:73:LEU:HB3	1:B:85:TYR:HB2	1.78	0.66
3:B:1401:ANP:O2'	7:B:1501:HOH:O	2.14	0.65
1:A:106:GLU:OE2	1:A:168:LYS:NZ	2.30	0.64
1:B:79:HIS:CD2	1:B:81:ASN:H	2.16	0.64
1:A:228:GLU:OE2	1:A:254:LYS:HG2	1.99	0.62
1:A:114:THR:O	1:A:118:LYS:HE2	2.00	0.61
1:B:59:THR:HG22	1:B:61:ASP:N	2.15	0.60
1:A:138:LEU:HD21	1:A:283:LEU:HD23	1.85	0.59
1:A:261:LYS:HE3	1:A:287:PRO:HB2	1.85	0.57
1:A:132:TYR:HA	1:A:292:GLN:HE22	1.69	0.57
1:A:80:ARG:O	1:A:168:LYS:HE2	2.05	0.56
1:A:269:CYS:O	1:A:277:ARG:HD2	2.06	0.55
1:B:121:LYS:C	1:B:121:LYS:HD3	2.27	0.55
1:B:243:PHE:O	1:B:247:ARG:HD2	2.09	0.53
1:A:24:ILE:N	1:A:24:ILE:HD13	2.24	0.52
1:A:152:ARG:CZ	1:A:189[A]:ILE:HD11	2.39	0.52
1:B:79:HIS:HD2	1:B:81:ASN:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:HG21	3:B:1401:ANP:O2A	2.11	0.51
1:A:184:ARG:HD3	1:A:209:THR:OG1	2.10	0.51
3:B:1401:ANP:O2A	3:B:1401:ANP:C8	2.48	0.51
1:A:198:GLU:OE2	1:A:277:ARG:NH2	2.43	0.49
1:B:251:PRO:O	1:B:252:ARG:NH1	2.46	0.49
3:A:1401:ANP:H8	3:A:1401:ANP:O5'	2.14	0.48
1:B:125:LEU:HD12	1:B:226:MET:HG2	1.97	0.46
1:A:59:THR:HG22	1:A:61:ASP:N	2.26	0.46
1:B:62:GLU:O	1:B:66:ILE:HG12	2.16	0.46
1:A:237:HIS:CD2	1:A:239:MET:HB2	2.52	0.45
1:A:271:VAL:O	1:A:277:ARG:HD3	2.16	0.45
1:A:94:PRO:HD2	1:A:97:MET:HE3	2.00	0.43
1:B:135:ARG:NH2	1:B:295:GLU:HG3	2.33	0.43
1:A:233:LEU:O	1:A:236:MET:HG2	2.19	0.42
1:B:76:TYR:HE1	1:B:147:HIS:CD2	2.38	0.42
1:A:173:GLY:HA3	7:A:1501:HOH:O	2.19	0.42
3:B:1401:ANP:O2A	3:B:1401:ANP:O4'	2.38	0.42
1:A:73:LEU:HB3	1:A:85:TYR:HB2	2.03	0.41
1:A:44:HIS:CE1	1:A:46:LYS:HB2	2.56	0.41
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.96	0.40
1:A:21:PRO:O	1:A:24:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/306 (97%)	285 (96%)	12 (4%)	0	100	100
1	B	299/306 (98%)	292 (98%)	7 (2%)	0	100	100
2	C	12/18 (67%)	12 (100%)	0	0	100	100
2	D	11/18 (61%)	10 (91%)	1 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	619/648 (96%)	599 (97%)	20 (3%)	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	258/264 (98%)	244 (95%)	14 (5%)	22	22
1	B	257/264 (97%)	248 (96%)	9 (4%)	36	43
2	C	10/9 (111%)	8 (80%)	2 (20%)	1	0
2	D	9/9 (100%)	8 (89%)	1 (11%)	6	4
All	All	534/546 (98%)	508 (95%)	26 (5%)	27	27

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	75	LYS
1	A	97	MET
1	A	101	LEU
1	A	118	LYS
1	A	124	THR
1	A	161	LEU
1	A	212	PHE
1	A	234[A]	CYS
1	A	234[B]	CYS
1	A	235	ASP
1	A	240	ARG
1	A	261	LYS
1	A	292	GLN
1	B	19	ARG
1	B	33	ASN
1	B	157	GLN

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Mol	Chain	Res	Type
1	B	179	ASP
1	B	281	GLU
1	B	283	LEU
1	B	284	MET
1	B	291	ASP
1	B	294	ASN
2	C	12[A]	THR
2	C	12[B]	THR
2	D	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	HIS
1	A	292	GLN
1	A	301	GLN
1	B	79	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	TPO	A	187	1	8,10,11	1.02	0	10,14,16	1.29	1 (10%)
2	BB9	D	15	2	2,4,6	2.06	1 (50%)	3,4,7	5.89	2 (66%)
2	BB9	C	13	2	3,5,6	2.44	2 (66%)	1,5,7	5.20	1 (100%)
1	TPO	A	181	1	8,10,11	1.63	1 (12%)	10,14,16	1.52	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DHA	D	14	2	3,3,5	2.77	1 (33%)	2,3,6	1.38	0
2	DHA	C	14	2	3,3,5	2.45	1 (33%)	2,3,6	3.33	1 (50%)
2	DHA	D	1	2	3,3,5	2.30	1 (33%)	2,2,6	1.92	1 (50%)
2	BB9	D	17	2	3,5,6	1.64	1 (33%)	1,5,7	6.85	1 (100%)
2	DHA	D	16	2	3,3,5	2.60	1 (33%)	2,3,6	2.81	2 (100%)
1	TPO	B	187	1	8,10,11	1.63	1 (12%)	10,14,16	1.48	2 (20%)
2	DHA	C	1	2	3,3,5	2.12	1 (33%)	2,2,6	1.76	1 (50%)
1	TPO	B	181	1	8,10,11	1.37	0	10,14,16	1.42	1 (10%)
2	BB9	D	13	2	3,5,6	0.97	0	1,5,7	5.93	1 (100%)
2	DHA	C	16	2	3,3,5	2.56	1 (33%)	2,3,6	2.33	2 (100%)
2	BB9	C	17	2	3,5,6	1.45	0	1,5,7	5.61	1 (100%)
2	BB9	C	15	2	2,4,6	1.92	1 (50%)	3,4,7	5.87	2 (66%)

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	TPO	A	187	1	-	0/9/11/13	-
2	BB9	D	15	2	-	0/0/2/6	-
2	BB9	C	13	2	-	0/0/4/6	-
1	TPO	A	181	1	-	3/9/11/13	-
2	DHA	D	1	2	-	0/0/1/4	-
2	BB9	D	17	2	-	0/0/4/6	-
1	TPO	B	187	1	-	0/9/11/13	-
2	DHA	C	1	2	-	0/0/1/4	-
1	TPO	B	181	1	-	2/9/11/13	-
2	BB9	D	13	2	-	0/0/4/6	-
2	BB9	C	17	2	-	0/0/4/6	-
2	BB9	C	15	2	-	0/0/2/6	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	14	DHA	CA-N	4.52	1.44	1.33
2	C	16	DHA	CB-CA	4.23	1.41	1.33
2	D	16	DHA	CB-CA	4.07	1.41	1.33
2	C	14	DHA	CA-N	4.04	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DHA	CB-CA	3.61	1.41	1.32
1	A	181	TPO	P-O1P	3.37	1.61	1.50
1	B	187	TPO	P-O1P	3.27	1.61	1.50
2	C	13	BB9	CA-N	3.21	1.43	1.35
2	C	1	DHA	CB-CA	3.16	1.40	1.32
2	D	15	BB9	CA-N	2.89	1.40	1.33
2	C	13	BB9	C-CA	2.71	1.49	1.45
2	C	15	BB9	CA-N	2.57	1.39	1.33
2	D	17	BB9	CA-N	2.52	1.41	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	BB9	C-CA-N	9.58	127.23	116.53
2	D	15	BB9	C-CA-N	9.43	127.06	116.53
2	D	17	BB9	O-C-CA	-6.85	116.69	125.39
2	D	13	BB9	O-C-CA	-5.93	117.85	125.39
2	C	17	BB9	O-C-CA	-5.61	118.26	125.39
2	C	13	BB9	O-C-CA	-5.20	118.78	125.39
2	C	14	DHA	C-CA-N	-4.59	110.50	115.40
1	A	181	TPO	P-OG1-CB	-4.20	110.52	123.21
1	B	181	TPO	P-OG1-CB	-4.08	110.89	123.21
2	D	15	BB9	CB-CA-N	-3.82	110.27	122.50
2	C	15	BB9	CB-CA-N	-3.42	111.56	122.50
2	D	16	DHA	C-CA-N	3.15	118.76	115.40
1	A	187	TPO	P-OG1-CB	-3.07	113.94	123.21
1	B	187	TPO	P-OG1-CB	-3.01	114.11	123.21
2	D	1	DHA	CB-CA-C	-2.61	117.22	122.32
1	B	187	TPO	CG2-CB-CA	-2.48	108.28	113.16
2	C	1	DHA	CB-CA-C	-2.48	117.47	122.32
2	D	16	DHA	CB-CA-N	-2.41	120.31	123.16
2	C	16	DHA	CB-CA-N	-2.36	120.38	123.16
2	C	16	DHA	C-CA-N	2.31	117.86	115.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	181	TPO	N-CA-CB-OG1
1	A	181	TPO	C-CA-CB-CG2
1	B	181	TPO	CB-OG1-P-O3P
1	A	181	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	B	181	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	187	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 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
3	ANP	A	1401	4	29,33,33	3.90	9 (31%)	31,52,52	2.56	11 (35%)
3	ANP	B	1401	4	29,33,33	3.68	10 (34%)	31,52,52	2.85	13 (41%)
5	SO4	A	1403	-	4,4,4	0.15	0	6,6,6	0.25	0
5	SO4	B	1403	-	4,4,4	0.16	0	6,6,6	0.32	0
6	PGE	A	1405	-	9,9,9	0.48	0	8,8,8	0.32	0
5	SO4	A	1404	-	4,4,4	0.17	0	6,6,6	0.12	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
6	PGE	A	1405	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1401	4	-	2/14/38/38	0/3/3/3
3	ANP	B	1401	4	-	7/14/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	ANP	PB-O3A	16.32	1.79	1.59
3	B	1401	ANP	PB-O3A	14.92	1.77	1.59
3	B	1401	ANP	PA-O5'	7.83	1.91	1.59
3	A	1401	ANP	PG-N3B	6.50	1.80	1.63
3	A	1401	ANP	PG-O1G	5.74	1.55	1.46
3	A	1401	ANP	PA-O5'	4.97	1.79	1.59
3	A	1401	ANP	PB-O1B	4.42	1.53	1.46
3	B	1401	ANP	PG-O1G	4.22	1.52	1.46
3	B	1401	ANP	PG-N3B	4.20	1.74	1.63
3	B	1401	ANP	PB-O1B	4.14	1.52	1.46
3	A	1401	ANP	O5'-C5'	-2.91	1.33	1.44
3	B	1401	ANP	O3'-C3'	-2.87	1.36	1.43
3	A	1401	ANP	O2'-C2'	-2.87	1.36	1.43
3	A	1401	ANP	C2-N3	2.82	1.36	1.32
3	A	1401	ANP	O3'-C3'	-2.66	1.36	1.43
3	B	1401	ANP	C2-N3	2.61	1.36	1.32
3	B	1401	ANP	O5'-C5'	-2.30	1.35	1.44
3	B	1401	ANP	C2'-C1'	2.25	1.57	1.53
3	B	1401	ANP	O4'-C1'	-2.04	1.38	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	ANP	O1G-PG-N3B	-8.10	99.84	111.77
3	A	1401	ANP	O1B-PB-N3B	6.69	121.62	111.77
3	A	1401	ANP	O1G-PG-N3B	-5.38	103.84	111.77
3	B	1401	ANP	O1B-PB-N3B	5.35	119.65	111.77
3	B	1401	ANP	O2B-PB-O1B	5.10	120.61	109.92
3	A	1401	ANP	O3A-PB-N3B	-5.00	92.71	106.59
3	B	1401	ANP	O3A-PB-N3B	-4.99	92.74	106.59
3	B	1401	ANP	C1'-N9-C4	-4.60	118.55	126.64
3	A	1401	ANP	O2B-PB-O3A	-4.31	90.25	104.64
3	A	1401	ANP	O2B-PB-O1B	4.25	118.84	109.92
3	B	1401	ANP	O2B-PB-O3A	-3.84	91.84	104.64
3	B	1401	ANP	C3'-C2'-C1'	3.26	105.88	100.98
3	A	1401	ANP	C1'-N9-C4	-3.12	121.16	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	ANP	O2A-PA-O5'	-3.01	93.77	107.75
3	A	1401	ANP	PB-O3A-PA	-2.93	122.28	132.62
3	B	1401	ANP	C4-C5-N7	2.75	112.27	109.40
3	A	1401	ANP	C2'-C3'-C4'	-2.70	97.39	102.64
3	B	1401	ANP	O5'-PA-O1A	-2.59	98.95	109.07
3	A	1401	ANP	O2A-PA-O5'	-2.57	95.82	107.75
3	B	1401	ANP	PB-O3A-PA	-2.40	124.17	132.62
3	A	1401	ANP	C4-C5-N7	2.37	111.87	109.40
3	B	1401	ANP	C2'-C3'-C4'	-2.22	98.33	102.64
3	B	1401	ANP	O2G-PG-O3G	2.15	113.36	107.64
3	A	1401	ANP	O5'-PA-O1A	-2.10	100.86	109.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	ANP	PB-N3B-PG-O1G
3	A	1401	ANP	PG-N3B-PB-O1B
3	B	1401	ANP	PG-N3B-PB-O1B
3	B	1401	ANP	C5'-O5'-PA-O3A
3	B	1401	ANP	C4'-C5'-O5'-PA
3	B	1401	ANP	C3'-C4'-C5'-O5'
6	A	1405	PGE	O1-C1-C2-O2
3	B	1401	ANP	PB-O3A-PA-O5'
3	B	1401	ANP	O4'-C4'-C5'-O5'
6	A	1405	PGE	C1-C2-O2-C3
3	B	1401	ANP	C5'-O5'-PA-O1A
6	A	1405	PGE	C4-C3-O2-C2
6	A	1405	PGE	C6-C5-O3-C4
6	A	1405	PGE	O2-C3-C4-O3

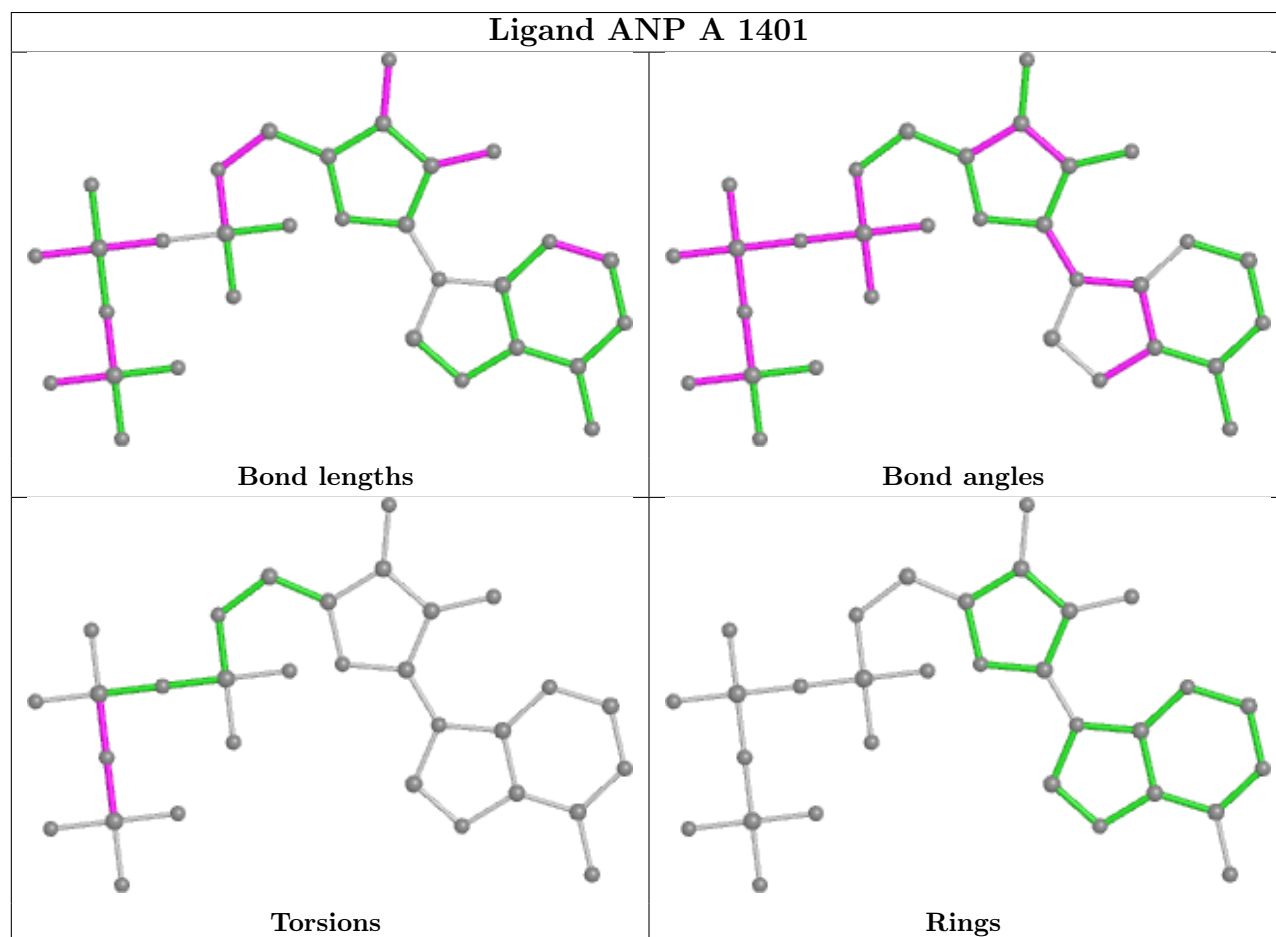
There are no ring outliers.

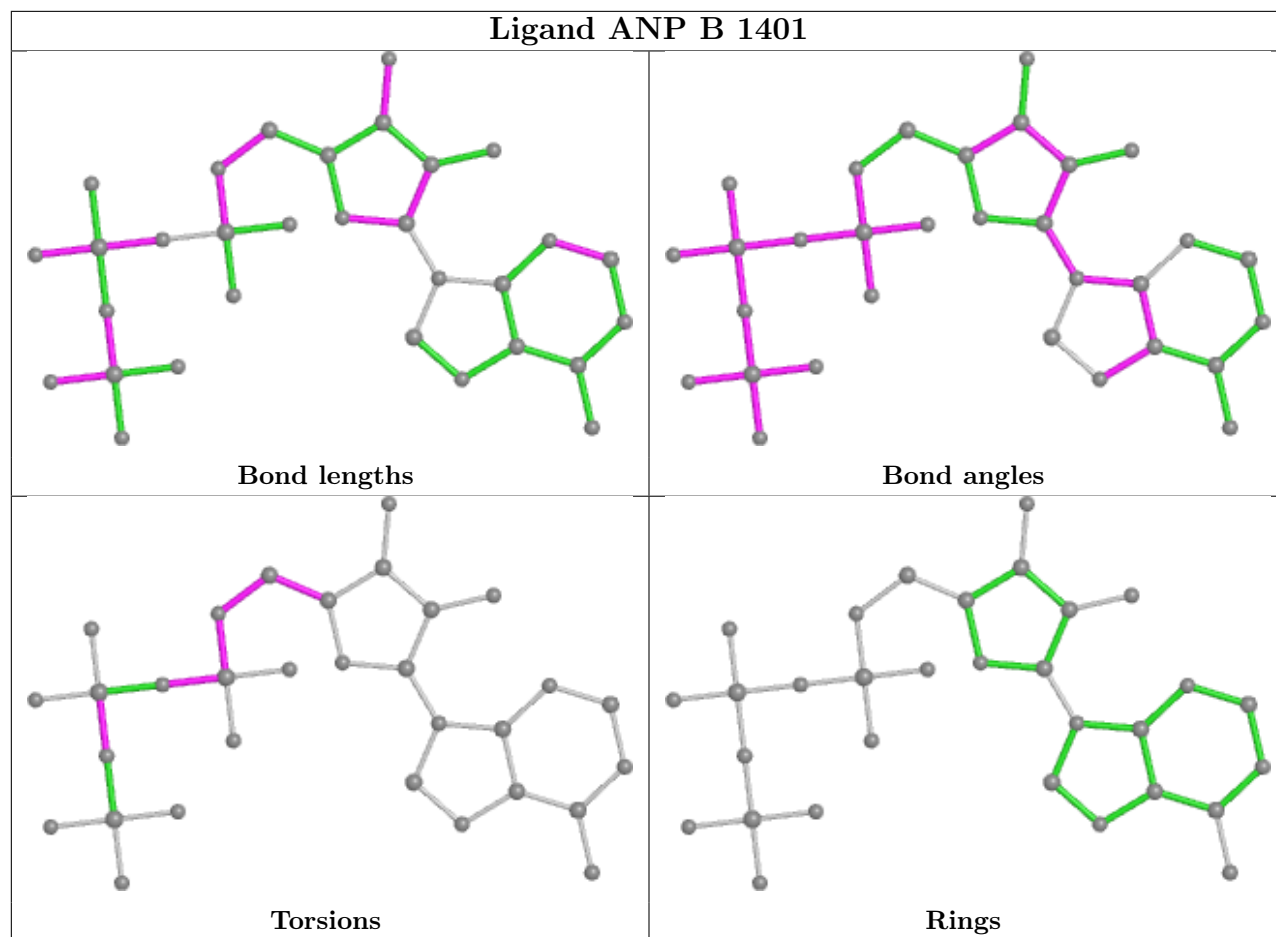
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401	ANP	3	0
3	B	1401	ANP	5	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	297/306 (97%)	0.17	3 (1%) 82 84	34, 49, 78, 110	0
1	B	299/306 (97%)	0.07	10 (3%) 46 48	34, 51, 80, 106	0
2	C	11/18 (61%)	-0.33	0 100 100	40, 44, 54, 58	0
2	D	11/18 (61%)	0.24	0 100 100	41, 49, 58, 58	0
All	All	618/648 (95%)	0.12	13 (2%) 63 66	34, 50, 78, 110	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	GLY	6.3
1	B	309	THR	4.4
1	B	182	VAL	3.9
1	A	182	VAL	3.8
1	B	31	VAL	3.3
1	B	312	LYS	2.7
1	A	27	LEU	2.5
1	B	36	TYR	2.5
1	B	311	LYS	2.2
1	B	179	ASP	2.2
1	B	212	PHE	2.2
1	B	121	LYS	2.1
1	A	309	THR	2.1

### 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, 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
1	TPO	B	181	11/12	0.81	0.22	92,98,110,114	0
1	TPO	A	181	11/12	0.91	0.30	80,93,104,105	0
2	DHA	D	1	4/6	0.95	0.13	41,42,43,49	0
2	BB9	C	13	6/7	0.95	0.11	45,49,52,54	0
2	DHA	D	14	4/6	0.95	0.17	45,45,45,48	0
1	TPO	B	187	11/12	0.96	0.11	49,52,58,59	0
1	TPO	A	187	11/12	0.97	0.12	34,42,49,50	0
2	DHA	D	16	4/6	0.97	0.12	40,42,43,48	0
2	DHA	C	14	4/6	0.98	0.13	42,45,47,51	0
2	DHA	C	1	4/6	0.98	0.08	42,43,43,44	0
2	BB9	D	13	6/7	0.98	0.11	46,47,51,54	0
2	BB9	C	17	6/7	0.98	0.10	45,47,48,48	0
2	BB9	D	17	6/7	0.98	0.09	46,48,50,52	0
2	BB9	C	15	5/7	0.99	0.07	45,46,48,48	0
2	BB9	D	15	5/7	0.99	0.11	42,43,45,49	0
2	DHA	C	16	4/6	0.99	0.09	44,45,45,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

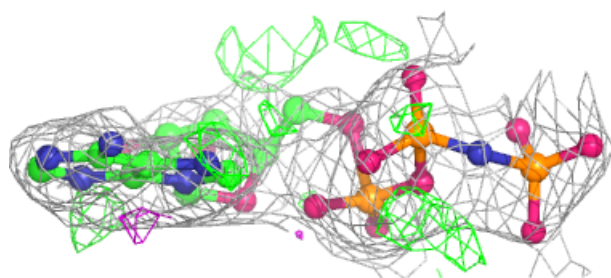
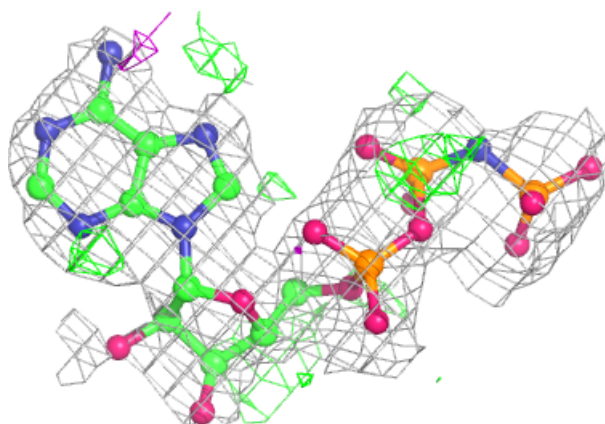
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1403	5/5	0.77	0.24	64,66,76,77	5
6	PGE	A	1405	10/10	0.78	0.23	62,67,70,74	0
3	ANP	B	1401	31/31	0.86	0.18	38,63,73,79	31
5	SO4	A	1404	5/5	0.93	0.17	62,63,65,75	5
4	MG	B	1402	1/1	0.94	0.17	63,63,63,63	0
5	SO4	A	1403	5/5	0.95	0.14	49,55,59,63	5
3	ANP	A	1401	31/31	0.97	0.13	35,41,60,77	0
4	MG	A	1402	1/1	0.98	0.12	41,41,41,41	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.

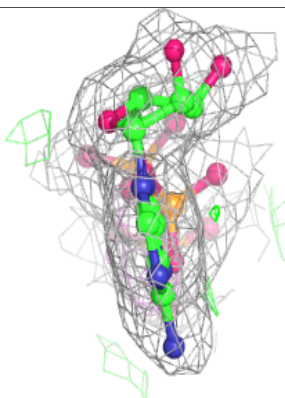
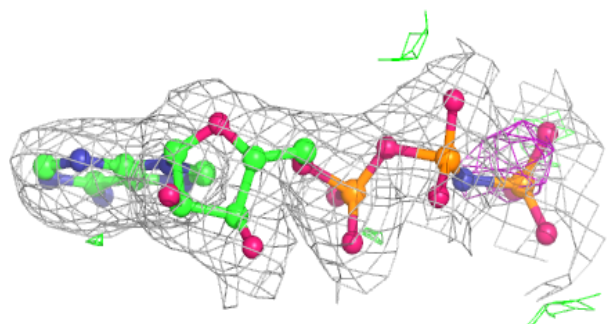
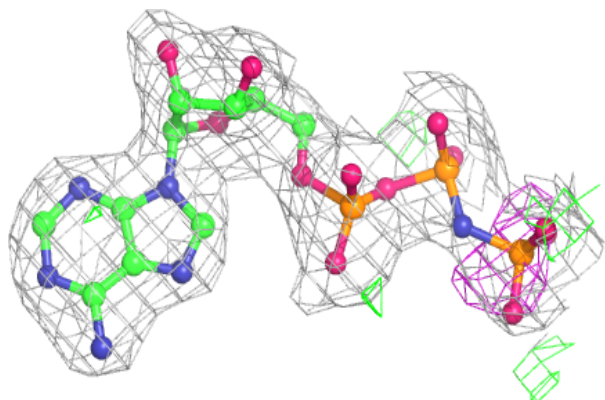


**Electron density around ANP B 1401:**

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

**Electron density around ANP A 1401:**

$2mF_o-DF_c$  (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.