



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2021 – 12:30 AM JST

PDB ID : 7EXP  
Title : Crystal structure of zebrafish TRAP1 with AMPPNP and MitoQ  
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Deposited on : 2021-05-28  
Resolution : 2.30 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.

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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 : 2.25  
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) : 2.25

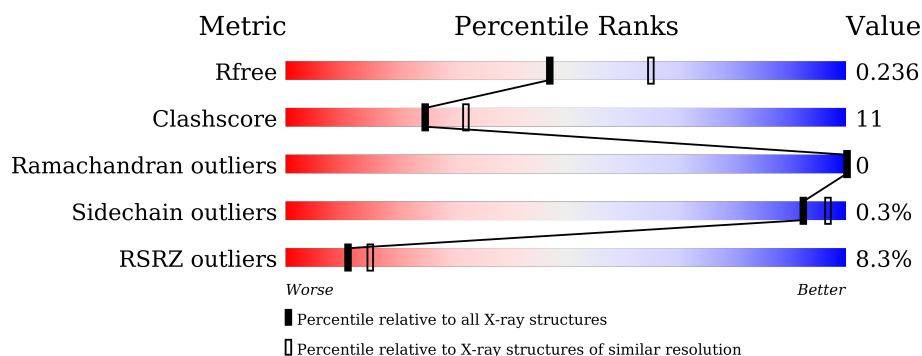
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	647	 7% 69% 19% • 11%
1	B	647	 8% 73% 19% • 7%

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
4	CO	A	804	-	-	-	X
4	CO	B	804	-	-	-	X

## 2 Entry composition [i](#)

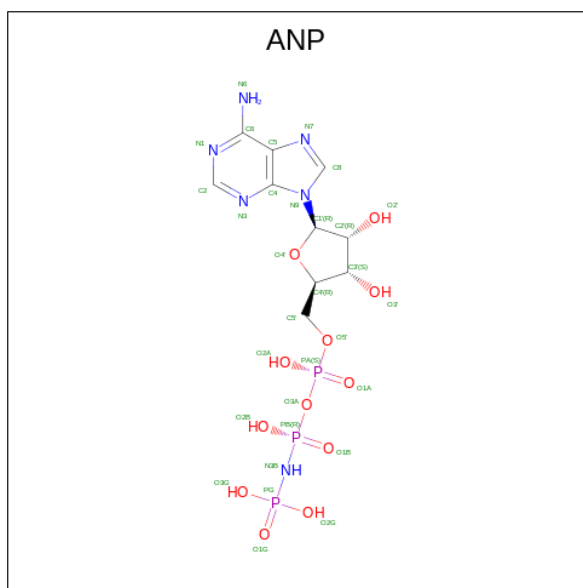
There are 6 unique types of molecules in this entry. The entry contains 9793 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	1	0
			4608	2924	796	868	20			
1	B	599	Total	C	N	O	S	0	3	0
			4855	3080	837	916	22			

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

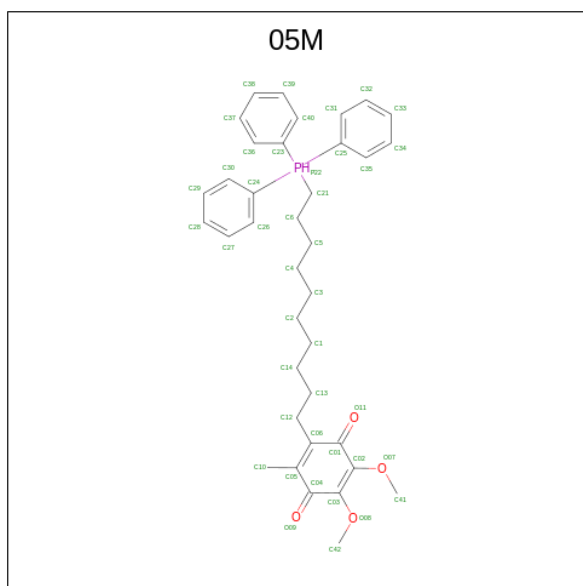


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Co 2 2	0	0
4	B	2	Total Co 2 2	0	0

- Molecule 5 is 2,3-dimethoxy-5-methyl-6-[10-(triphenyl- $\text{P}$ -phosphanyl)decyl]cyclohexa-2,5-diene-1,4-dione (three-letter code: 05M) (formula:  $\text{C}_{37}\text{H}_{45}\text{O}_4\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P 36 31 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	109	Total O 109 109	0	0

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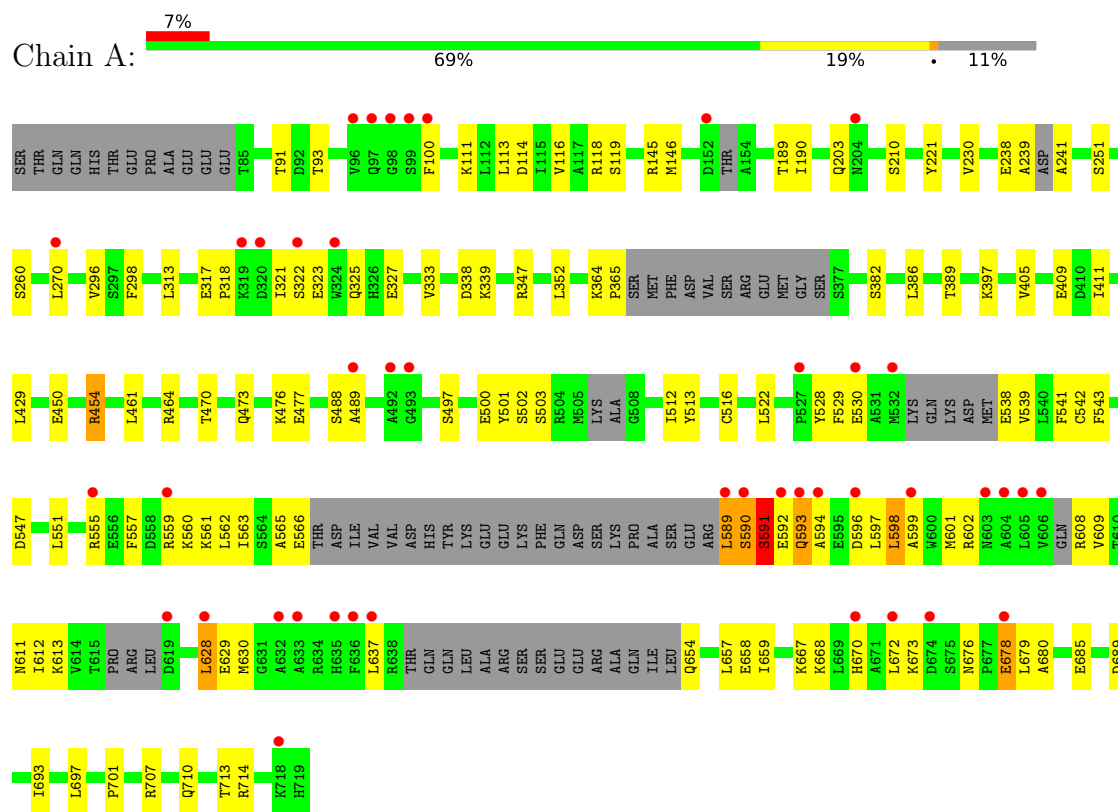
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	117	Total 117	O 117	0	0

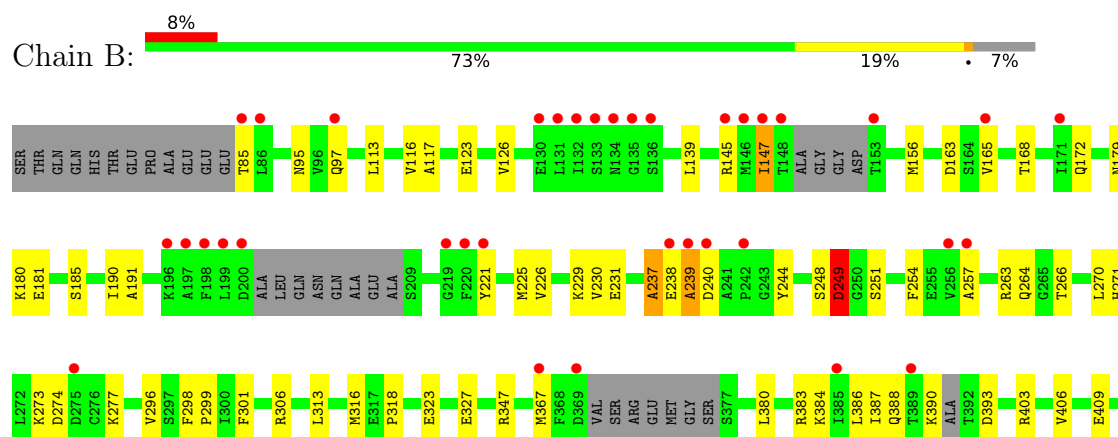
### 3 Residue-property plots [i](#)

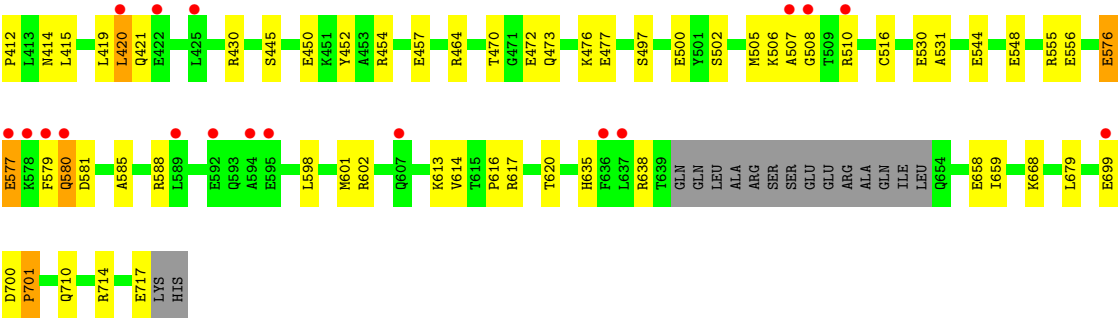
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TNF receptor-associated protein 1



#### • Molecule 1: TNF receptor-associated protein 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.34Å 96.52Å 125.61Å 90.00° 134.39° 90.00°	Depositor
Resolution (Å)	31.20 – 2.30 31.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (31.20-2.30) 98.7 (31.21-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.195 , 0.241 0.197 , 0.236	Depositor DCC
$R_{free}$ test set	2011 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h+2*l,k,-h-l 0.016 for h,-k,-h-l 0.024 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: MG, CO, 05M, 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	0.44	2/4691 (0.0%)	0.90	25/6317 (0.4%)
1	B	0.46	7/4953 (0.1%)	0.65	12/6672 (0.2%)
All	All	0.45	9/9644 (0.1%)	0.78	37/12989 (0.3%)

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	2
1	B	0	4
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	699	GLU	C-O	-7.53	1.09	1.23
1	B	668	LYS	CE-NZ	7.20	1.67	1.49
1	B	700	ASP	C-O	-6.37	1.11	1.23
1	B	701	PRO	CA-CB	-5.69	1.42	1.53
1	B	457	GLU	CB-CG	5.65	1.62	1.52
1	A	609	VAL	CB-CG1	5.56	1.64	1.52
1	B	457	GLU	CD-OE2	5.47	1.31	1.25
1	A	559	ARG	CZ-NH2	-5.21	1.26	1.33
1	B	700	ASP	CA-C	-5.00	1.40	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	628	LEU	CB-CG-CD2	-23.77	70.59	111.00
1	A	628	LEU	CB-CG-CD1	15.02	136.54	111.00
1	A	454	ARG	CB-CG-CD	-13.64	76.12	111.60
1	A	591	SER	N-CA-CB	12.97	129.96	110.50
1	A	590	SER	CB-CA-C	12.70	134.23	110.10
1	A	611	ASN	CB-CA-C	-11.22	87.96	110.40
1	A	454	ARG	CG-CD-NE	10.23	133.29	111.80
1	A	454	ARG	CA-CB-CG	10.01	135.43	113.40
1	A	710	GLN	CA-CB-CG	9.26	133.78	113.40
1	A	654	GLN	N-CA-C	-8.98	86.75	111.00
1	A	609	VAL	CG1-CB-CG2	8.63	124.70	110.90
1	A	598	LEU	CA-CB-CG	8.22	134.20	115.30
1	A	654	GLN	CA-CB-CG	8.16	131.35	113.40
1	B	576	GLU	CB-CA-C	8.16	126.72	110.40
1	B	576	GLU	N-CA-C	-8.16	88.97	111.00
1	B	700	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	628	LEU	CD1-CG-CD2	-8.10	86.19	110.50
1	A	559	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	397	LYS	CB-CG-CD	7.33	130.65	111.60
1	A	591	SER	N-CA-C	-7.29	91.31	111.00
1	A	710	GLN	CB-CA-C	6.90	124.21	110.40
1	B	457	GLU	CA-CB-CG	6.86	128.49	113.40
1	B	577	GLU	N-CA-C	-6.76	92.76	111.00
1	B	249	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	B	700	ASP	C-N-CD	6.06	141.13	128.40
1	A	654	GLN	N-CA-CB	6.02	121.43	110.60
1	A	710	GLN	N-CA-CB	-5.92	99.94	110.60
1	A	529	PHE	N-CA-C	-5.73	95.53	111.00
1	B	147	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	B	701	PRO	CA-N-CD	-5.72	103.49	111.50
1	A	678	GLU	CG-CD-OE2	-5.70	106.89	118.30
1	B	97	GLN	C-N-CA	-5.61	110.51	122.30
1	A	598	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	502	SER	CB-CA-C	-5.43	99.77	110.10
1	B	457	GLU	CB-CA-C	-5.34	99.72	110.40
1	B	239	ALA	N-CA-C	-5.25	96.82	111.00
1	A	454	ARG	N-CA-CB	-5.15	101.33	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	593	GLN	Peptide
1	B	237	ALA	Peptide
1	B	249	ASP	Peptide
1	B	420	LEU	Peptide
1	B	580	GLN	Peptide

## 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	4608	0	4596	100	1
1	B	4855	0	4860	111	3
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	36	0	0	6	0
6	A	109	0	0	4	0
6	B	117	0	0	14	0
All	All	9793	0	9482	206	3

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 11.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD11	5:A:805:05M:C10	1.72	1.18
1:B:237:ALA:HB3	1:B:238:GLU:HG3	1.15	1.13
1:A:461:LEU:CG	5:A:805:05M:C10	2.29	1.10
1:B:414:ASN:ND2	1:B:419:LEU:H	1.49	1.08
1:B:237:ALA:CB	1:B:264:GLN:NE2	2.16	1.08
1:B:237:ALA:HB2	1:B:264:GLN:NE2	1.69	1.07
1:A:461:LEU:CD1	5:A:805:05M:C10	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:CB	1:B:238:GLU:HG3	1.87	1.04
1:A:672:LEU:O	1:A:680:ALA:HB2	1.56	1.03
1:A:461:LEU:HD21	5:A:805:05M:C10	1.89	1.02
1:A:592:GLU:HG2	1:A:593:GLN:H	1.24	1.02
1:A:593:GLN:HG2	1:A:596:ASP:HB3	1.39	1.02
1:B:414:ASN:HD21	1:B:419:LEU:N	1.56	1.02
1:B:380:LEU:HD12	1:B:406:VAL:O	1.65	0.97
1:B:237:ALA:HB2	1:B:264:GLN:HE21	1.22	0.95
1:A:461:LEU:CD2	5:A:805:05M:C10	2.46	0.94
1:A:713:THR:O	6:A:901:HOH:O	1.85	0.94
1:B:383:ARG:NH1	6:B:901:HOH:O	2.02	0.92
1:B:380:LEU:HD23	1:B:420:LEU:HD11	1.53	0.91
1:B:414:ASN:ND2	1:B:419:LEU:N	2.17	0.90
1:A:461:LEU:HG	5:A:805:05M:C10	2.03	0.87
1:B:414:ASN:HD21	1:B:419:LEU:H	0.86	0.85
1:B:237:ALA:HB3	1:B:238:GLU:CG	2.03	0.84
1:B:163:ASP:HB3	1:B:168:THR:HG22	1.58	0.84
1:A:598:LEU:HD12	1:A:659:ILE:HD11	1.59	0.81
1:B:237:ALA:CB	1:B:264:GLN:HE22	1.95	0.80
1:A:352:LEU:HD11	1:A:429:LEU:HD13	1.67	0.77
1:B:454:ARG:NH1	6:B:903:HOH:O	2.19	0.76
1:A:593:GLN:CG	1:A:596:ASP:HB3	2.16	0.76
1:A:678:GLU:HG2	1:A:714:ARG:HH12	1.51	0.74
1:B:506:LYS:HD2	1:B:508:GLY:H	1.51	0.74
1:A:628:LEU:HD23	1:A:629:GLU:HG3	1.68	0.74
1:B:237:ALA:CA	1:B:264:GLN:NE2	2.51	0.74
1:A:676:ASN:ND2	1:A:679:LEU:HB2	2.04	0.73
1:B:249:ASP:HB2	1:B:251:SER:H	1.53	0.73
1:A:464:ARG:NH2	1:A:547:ASP:OD1	2.22	0.72
1:A:628:LEU:CD2	1:A:629:GLU:HG3	2.20	0.72
1:B:679:LEU:HD13	1:B:714:ARG:HG2	1.71	0.72
1:B:387:ILE:HG21	1:B:420:LEU:HD21	1.72	0.71
1:A:592:GLU:HG2	1:A:593:GLN:N	2.03	0.71
1:B:367:MET:SD	1:B:403[B]:ARG:NH2	2.65	0.69
1:A:382:SER:HB2	1:A:411:ILE:HD11	1.74	0.68
1:B:384:LYS:O	6:B:902:HOH:O	2.11	0.68
1:A:593:GLN:HB3	1:A:597:LEU:H	1.57	0.68
1:A:678:GLU:CG	1:A:714:ARG:HH12	2.07	0.67
1:A:238:GLU:HG2	1:A:239:ALA:H	1.58	0.67
1:A:592:GLU:CG	1:A:593:GLN:H	2.04	0.67
1:A:590:SER:OG	1:A:594:ALA:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:O	1:B:430:ARG:NH1	2.28	0.66
1:B:380:LEU:CD2	1:B:420:LEU:HD11	2.25	0.66
1:B:237:ALA:HA	1:B:264:GLN:NE2	2.11	0.66
1:B:414:ASN:ND2	1:B:419:LEU:CA	2.60	0.65
1:A:590:SER:OG	1:A:591:SER:HA	1.97	0.64
1:A:239:ALA:O	1:A:241:ALA:N	2.31	0.64
1:A:488:SER:OG	1:A:539:VAL:N	2.28	0.63
1:B:530:GLU:OE2	1:B:620:THR:HB	2.00	0.62
1:B:237:ALA:HB1	1:B:264:GLN:HE22	1.64	0.62
1:B:414:ASN:HD22	1:B:419:LEU:C	2.02	0.62
1:B:581:ASP:OD2	1:B:588:ARG:NH1	2.33	0.62
1:A:593:GLN:HB2	1:A:670:HIS:CE1	2.35	0.61
1:B:390:LYS:NZ	6:B:906:HOH:O	2.21	0.61
1:A:100:PHE:HA	1:B:257:ALA:HB2	1.83	0.61
1:A:386:LEU:HD21	1:A:389:THR:HG22	1.83	0.60
1:A:322:SER:HB2	1:A:325:GLN:HG2	1.83	0.60
1:B:367:MET:HA	6:B:942:HOH:O	2.02	0.59
1:B:635:HIS:ND1	6:B:904:HOH:O	2.32	0.59
1:B:414:ASN:ND2	1:B:419:LEU:HB2	2.18	0.59
1:B:638:ARG:NH2	6:B:904:HOH:O	2.19	0.59
1:A:528:TYR:HE2	1:A:629:GLU:HG2	1.69	0.57
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.86	0.57
1:B:116:VAL:HG11	1:B:221:TYR:HB2	1.87	0.57
1:A:516:CYS:SG	1:A:542[A]:CYS:HB2	2.44	0.57
1:B:472:GLU:O	1:B:476:LYS:HG3	2.04	0.56
1:B:470:THR:HG23	1:B:476:LYS:HG2	1.87	0.56
1:B:414:ASN:ND2	1:B:419:LEU:O	2.36	0.56
1:A:597:LEU:O	1:A:601:MET:HG3	2.06	0.56
1:A:672:LEU:O	1:A:680:ALA:CB	2.43	0.56
1:A:599:ALA:HA	1:A:602:ARG:HG3	1.87	0.55
1:A:260:SER:O	1:B:95:ASN:N	2.30	0.55
1:B:248:SER:OG	1:B:249:ASP:N	2.40	0.55
1:B:380:LEU:CD2	1:B:420:LEU:CD1	2.83	0.55
1:B:497:SER:OG	1:B:500:GLU:HG3	2.07	0.55
1:B:180:LYS:HB2	1:B:244:TYR:CZ	2.42	0.54
1:B:580:GLN:HG3	1:B:581:ASP:H	1.73	0.54
1:A:597:LEU:HD23	1:A:670:HIS:HA	1.89	0.54
1:B:581:ASP:OD2	1:B:588:ARG:CZ	2.56	0.53
1:A:637:LEU:HD21	1:A:697:LEU:HD23	1.90	0.53
1:B:117:ALA:O	1:B:225:MET:HG2	2.09	0.53
1:B:598:LEU:HD11	1:B:614:VAL:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ARG:NH1	6:A:906:HOH:O	2.35	0.53
1:A:339:LYS:N	1:A:339:LYS:HD3	2.24	0.53
1:A:497:SER:OG	1:A:500:GLU:HG3	2.09	0.53
1:A:318:PRO:HD3	1:A:347:ARG:HD2	1.90	0.53
1:B:387:ILE:HG22	1:B:388:GLN:H	1.74	0.52
1:A:473:GLN:OE1	1:A:477:GLU:OE1	2.27	0.52
1:B:414:ASN:ND2	1:B:419:LEU:CB	2.73	0.52
1:B:147:ILE:O	1:B:147:ILE:HG22	2.10	0.52
1:B:531:ALA:O	1:B:617:ARG:NH2	2.41	0.51
1:A:513:TYR:CD1	1:A:563:ILE:HB	2.45	0.51
1:A:313:LEU:HD21	1:A:325:GLN:HB3	1.93	0.51
1:B:555:ARG:NH2	1:B:556:GLU:OE2	2.43	0.51
1:B:598:LEU:O	1:B:602:ARG:HG3	2.11	0.50
1:A:522:LEU:HB3	1:A:630:MET:HE2	1.92	0.50
1:A:561:LYS:HB3	1:A:563:ILE:HD11	1.93	0.50
1:B:168:THR:HG23	6:B:917:HOH:O	2.10	0.50
1:B:502:SER:HA	1:B:505:MET:HG3	1.93	0.50
1:B:577:GLU:HG2	1:B:579:PHE:HD2	1.77	0.49
1:A:210:SER:HB2	1:A:409:GLU:CD	2.32	0.49
1:A:557:PHE:O	1:A:560:LYS:HG2	2.12	0.49
1:A:323:GLU:O	1:A:327:GLU:HG3	2.13	0.49
1:A:501:TYR:CE2	1:A:538:GLU:HG2	2.47	0.49
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.34	0.49
1:A:592:GLU:CG	1:A:593:GLN:N	2.72	0.49
1:B:85:THR:N	6:B:921:HOH:O	2.46	0.49
1:B:516:CYS:SG	1:B:548:GLU:HB2	2.53	0.49
1:B:367:MET:HG3	1:B:367:MET:O	2.12	0.48
1:A:470:THR:HG23	1:A:476:LYS:HG3	1.95	0.48
1:A:333:VAL:HG21	1:A:405:VAL:HG23	1.95	0.48
1:A:317:GLU:CD	1:A:347:ARG:HH12	2.16	0.48
1:B:506:LYS:HD2	1:B:507:ALA:N	2.29	0.48
1:B:313:LEU:HA	1:B:316:MET:HE2	1.94	0.48
1:A:296:VAL:HG12	1:A:298:PHE:H	1.78	0.48
1:A:668:LYS:O	1:A:672:LEU:HD12	2.13	0.48
1:A:313:LEU:HG	1:A:321:ILE:HD12	1.96	0.47
1:A:676:ASN:HD22	1:A:679:LEU:HB2	1.79	0.47
1:B:616:PRO:O	6:B:905:HOH:O	2.20	0.47
1:A:450:GLU:HG2	1:A:454:ARG:NH1	2.29	0.47
1:B:390:LYS:NZ	6:B:924:HOH:O	2.47	0.47
1:B:601:MET:HE1	1:B:659:ILE:HD13	1.97	0.47
1:A:500:GLU:HA	1:A:503:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ILE:HG13	1:A:560:LYS:HG3	1.97	0.47
1:B:409:GLU:HG2	6:B:901:HOH:O	2.14	0.47
1:A:364:LYS:HG2	1:A:365:PRO:HD2	1.95	0.47
1:B:445:SER:HB2	1:B:452:TYR:CD2	2.51	0.46
1:B:613:LYS:HG3	1:B:658:GLU:HG2	1.97	0.46
1:B:248:SER:HB2	1:B:254:PHE:HB3	1.97	0.46
1:B:412:PRO:HB2	1:B:421:GLN:HB2	1.97	0.46
1:A:338:ASP:C	1:A:339:LYS:HD3	2.36	0.46
1:A:114:ASP:OD2	1:A:118:ARG:NH1	2.49	0.46
1:B:263:ARG:NH1	6:B:925:HOH:O	2.48	0.46
1:B:414:ASN:HD22	1:B:419:LEU:CA	2.25	0.46
1:A:114:ASP:OD1	1:A:118:ARG:HD3	2.14	0.46
1:A:116:VAL:HG11	1:A:221:TYR:HB2	1.96	0.46
1:B:274:ASP:HA	1:B:277:LYS:NZ	2.31	0.46
1:B:323:GLU:O	1:B:327:GLU:HG3	2.16	0.46
1:A:551:LEU:HD22	1:A:562:LEU:HD22	1.99	0.45
1:A:322:SER:H	1:A:325:GLN:HG3	1.80	0.45
1:A:113:LEU:HG	1:A:190:ILE:HD11	1.98	0.45
1:A:594:ALA:O	1:A:598:LEU:HB2	2.16	0.45
1:A:589:LEU:HD22	1:A:667:LYS:NZ	2.31	0.45
1:B:172:GLN:NE2	1:B:263:ARG:HD2	2.31	0.45
1:B:473:GLN:O	1:B:477:GLU:HG3	2.17	0.45
1:B:181:GLU:O	1:B:185:SER:HB3	2.17	0.45
1:B:145:ARG:HD3	1:B:145:ARG:HA	1.62	0.45
1:B:226:VAL:O	1:B:273:LYS:HG2	2.17	0.44
1:B:710:GLN:NE2	1:B:714:ARG:HH21	2.14	0.44
1:B:139:LEU:HD22	1:B:156:MET:HB3	1.98	0.44
1:B:230:VAL:HG22	1:B:270:LEU:HD22	1.98	0.44
1:B:450:GLU:HG3	6:B:955:HOH:O	2.17	0.44
1:B:464:ARG:CZ	1:B:544:GLU:HG2	2.47	0.44
1:A:608:ARG:NH1	1:A:685:GLU:OE1	2.47	0.44
1:B:296:VAL:HG12	1:B:298:PHE:H	1.83	0.44
1:A:668:LYS:HE3	1:B:717:GLU:C	2.38	0.43
1:B:163:ASP:OD1	1:B:165:VAL:HG22	2.17	0.43
1:A:612:ILE:HA	1:A:657:LEU:O	2.18	0.43
1:A:513:TYR:HD1	1:A:563:ILE:HB	1.82	0.43
1:B:237:ALA:C	1:B:238:GLU:HG3	2.38	0.43
1:B:470:THR:CG2	1:B:476:LYS:HG2	2.49	0.43
1:A:673:LYS:HB3	1:A:673:LYS:HE3	1.76	0.43
1:B:386:LEU:HG	1:B:387:ILE:O	2.18	0.43
1:A:528:TYR:HB3	1:A:565:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:HB3	1:A:630:MET:CE	2.49	0.43
1:A:111:LYS:HG2	1:B:191:ALA:O	2.19	0.43
1:A:145:ARG:HB2	6:A:994:HOH:O	2.19	0.43
1:B:179:ASN:OD1	1:B:181:GLU:HG3	2.19	0.43
1:A:541:PHE:HB3	1:A:543:PHE:CE1	2.54	0.42
1:B:113:LEU:CD2	1:B:190:ILE:HD11	2.49	0.42
1:B:249:ASP:OD2	1:B:251:SER:OG	2.37	0.42
1:B:613:LYS:HB2	1:B:613:LYS:HE2	1.63	0.42
1:A:91:THR:O	1:A:93:THR:HG22	2.20	0.42
1:A:470:THR:O	1:A:476:LYS:HE3	2.20	0.42
1:B:239:ALA:O	1:B:240:ASP:HB2	2.20	0.41
1:B:318:PRO:HD3	1:B:347:ARG:HD2	2.01	0.41
1:A:119:SER:O	1:B:415:LEU:N	2.36	0.41
1:A:693:ILE:HD11	1:A:701:PRO:HB3	2.02	0.41
1:B:229:LYS:HD2	1:B:248:SER:O	2.20	0.41
1:A:489:ALA:HB3	1:A:538:GLU:OE1	2.20	0.41
1:A:528:TYR:CD2	1:A:566:GLU:HG2	2.55	0.41
1:B:576:GLU:N	1:B:576:GLU:OE1	2.53	0.41
1:B:614:VAL:HG12	1:B:659:ILE:HD11	2.02	0.41
1:A:555:ARG:O	1:A:561:LYS:HD3	2.20	0.41
1:A:613:LYS:HG2	1:A:658:GLU:HG2	2.03	0.41
1:A:689:ASP:OD2	1:A:707:ARG:NH2	2.38	0.41
1:B:299:PRO:HB3	1:B:306:ARG:CZ	2.51	0.41
1:B:585:ALA:HA	1:B:588:ARG:CZ	2.51	0.41
1:B:172:GLN:HA	1:B:266:THR:O	2.21	0.41
1:B:248:SER:HB2	1:B:254:PHE:CB	2.51	0.41
1:B:301:PHE:CE2	1:B:306:ARG:HB2	2.55	0.40
1:A:628:LEU:HD23	1:A:629:GLU:N	2.37	0.40
1:A:251:SER:O	1:A:251:SER:OG	2.36	0.40
1:A:593:GLN:O	1:A:597:LEU:HB3	2.21	0.40
1:B:123:GLU:O	1:B:126:VAL:HG22	2.21	0.40
1:B:237:ALA:CA	1:B:238:GLU:HG3	2.50	0.40
1:A:189:THR:O	6:A:902:HOH:O	2.22	0.40
1:A:146:MET:HE2	1:A:146:MET:HB2	1.99	0.40
1:A:318:PRO:HD3	1:A:347:ARG:CD	2.51	0.40

All (3) 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:510:ARG:NH1	1:B:576:GLU:OE2[2_557]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:NE2	1:B:472:GLU:OE2[4_558]	2.05	0.15
1:B:510:ARG:NH1	1:B:576:GLU:CD[2_557]	2.17	0.03

## 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	555/647 (86%)	535 (96%)	20 (4%)	0	100	100
1	B	590/647 (91%)	568 (96%)	22 (4%)	0	100	100
All	All	1145/1294 (88%)	1103 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	502/569 (88%)	500 (100%)	2 (0%)	91	96
1	B	535/569 (94%)	534 (100%)	1 (0%)	93	97
All	All	1037/1138 (91%)	1034 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	530	GLU

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Mol	Chain	Res	Type
1	A	591	SER
1	B	701	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	473	GLN
1	A	521	HIS
1	A	670	HIS
1	A	676	ASN
1	B	97	GLN
1	B	264	GLN
1	B	580	GLN
1	B	710	GLN

### 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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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
5	05M	A	805	-	38,38,45	1.67	9 (23%)	49,52,60	2.17	7 (14%)
2	ANP	A	801	3,1	29,33,33	1.38	7 (24%)	31,52,52	1.38	7 (22%)
2	ANP	B	801	3	29,33,33	1.03	2 (6%)	31,52,52	1.01	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
5	05M	A	805	-	-	3/25/49/60	0/4/4/4
2	ANP	A	801	3,1	-	2/14/38/38	0/3/3/3
2	ANP	B	801	3	-	1/14/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	805	05M	P22-C23	4.05	1.86	1.79
5	A	805	05M	P22-C24	3.52	1.85	1.79
2	A	801	ANP	C4-N3	3.26	1.40	1.35
5	A	805	05M	P22-C25	2.96	1.84	1.79
5	A	805	05M	C06-C05	2.93	1.40	1.35
5	A	805	05M	C03-C04	-2.91	1.40	1.48
2	A	801	ANP	C8-N7	-2.89	1.29	1.34
5	A	805	05M	C02-C01	-2.83	1.40	1.48
5	A	805	05M	P22-C21	2.80	1.86	1.79
2	A	801	ANP	PG-N3B	2.65	1.70	1.63
2	B	801	ANP	PG-N3B	2.62	1.70	1.63
5	A	805	05M	O08-C03	2.58	1.43	1.36
2	A	801	ANP	PG-O1G	2.54	1.50	1.46
2	A	801	ANP	C5-C4	-2.33	1.34	1.40
2	B	801	ANP	PG-O1G	2.27	1.49	1.46
5	A	805	05M	C06-C01	-2.16	1.40	1.46
2	A	801	ANP	PB-N3B	2.09	1.68	1.63
2	A	801	ANP	PB-O1B	2.03	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	05M	C23-P22-C24	8.77	124.67	109.44
5	A	805	05M	C25-P22-C24	-6.88	97.49	109.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	05M	C10-C05-C06	-5.05	116.17	124.40
5	A	805	05M	C12-C06-C01	4.42	124.23	117.00
5	A	805	05M	C25-P22-C23	-3.90	102.66	109.44
2	A	801	ANP	C5-C6-N6	3.59	125.81	120.35
5	A	805	05M	C06-C05-C04	3.46	121.92	119.18
2	A	801	ANP	O1B-PB-N3B	-3.15	107.14	111.77
5	A	805	05M	C13-C12-C06	2.59	118.52	113.08
2	B	801	ANP	O2B-PB-O3A	2.53	113.07	104.64
2	B	801	ANP	C5-C6-N6	2.48	124.12	120.35
2	A	801	ANP	C1'-N9-C4	2.37	130.80	126.64
2	B	801	ANP	O1B-PB-N3B	-2.33	108.33	111.77
2	A	801	ANP	PB-O3A-PA	-2.30	124.52	132.62
2	A	801	ANP	C4-C5-N7	-2.27	107.04	109.40
2	A	801	ANP	C5-C6-N1	-2.02	115.77	120.35
2	A	801	ANP	O2G-PG-O1G	-2.01	108.41	113.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	A	801	ANP	PA-O3A-PB-O2B
2	B	801	ANP	PB-N3B-PG-O1G
5	A	805	05M	C01-C06-C12-C13
5	A	805	05M	C05-C06-C12-C13
5	A	805	05M	C06-C12-C13-C14

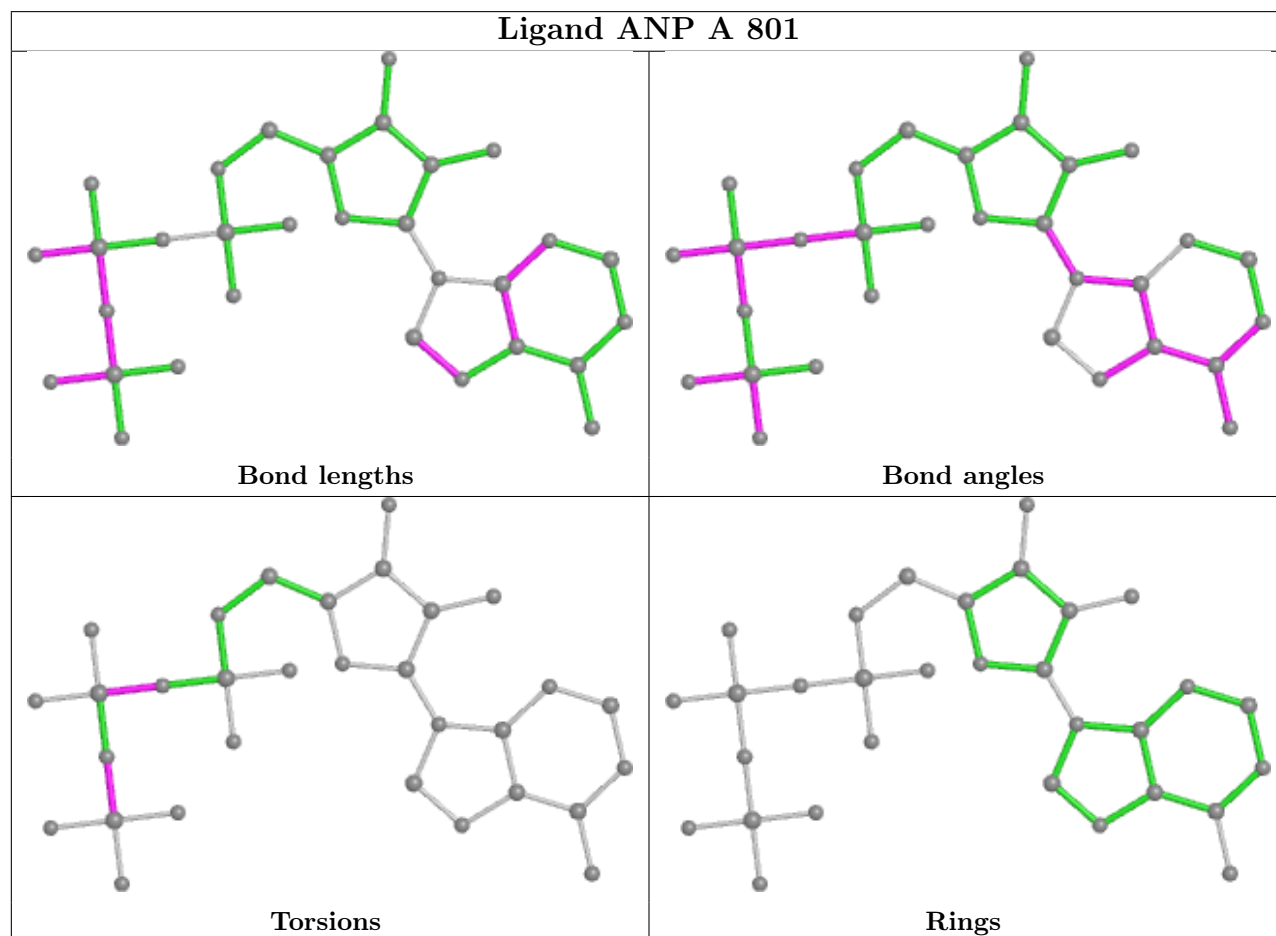
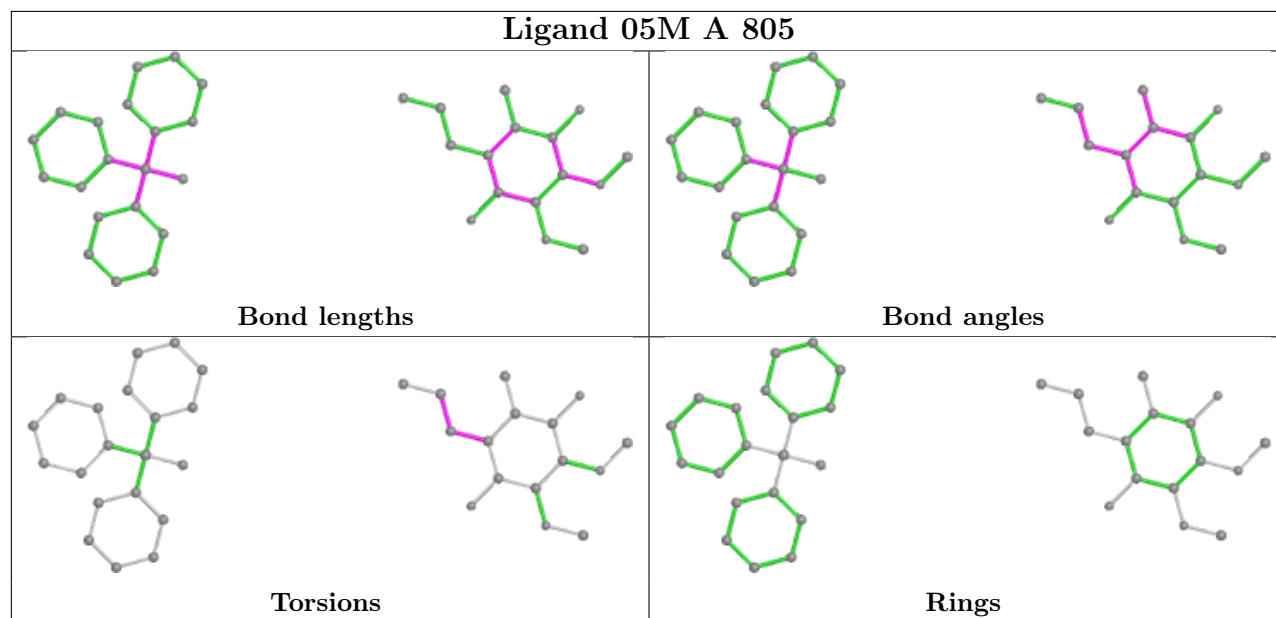
There are no ring outliers.

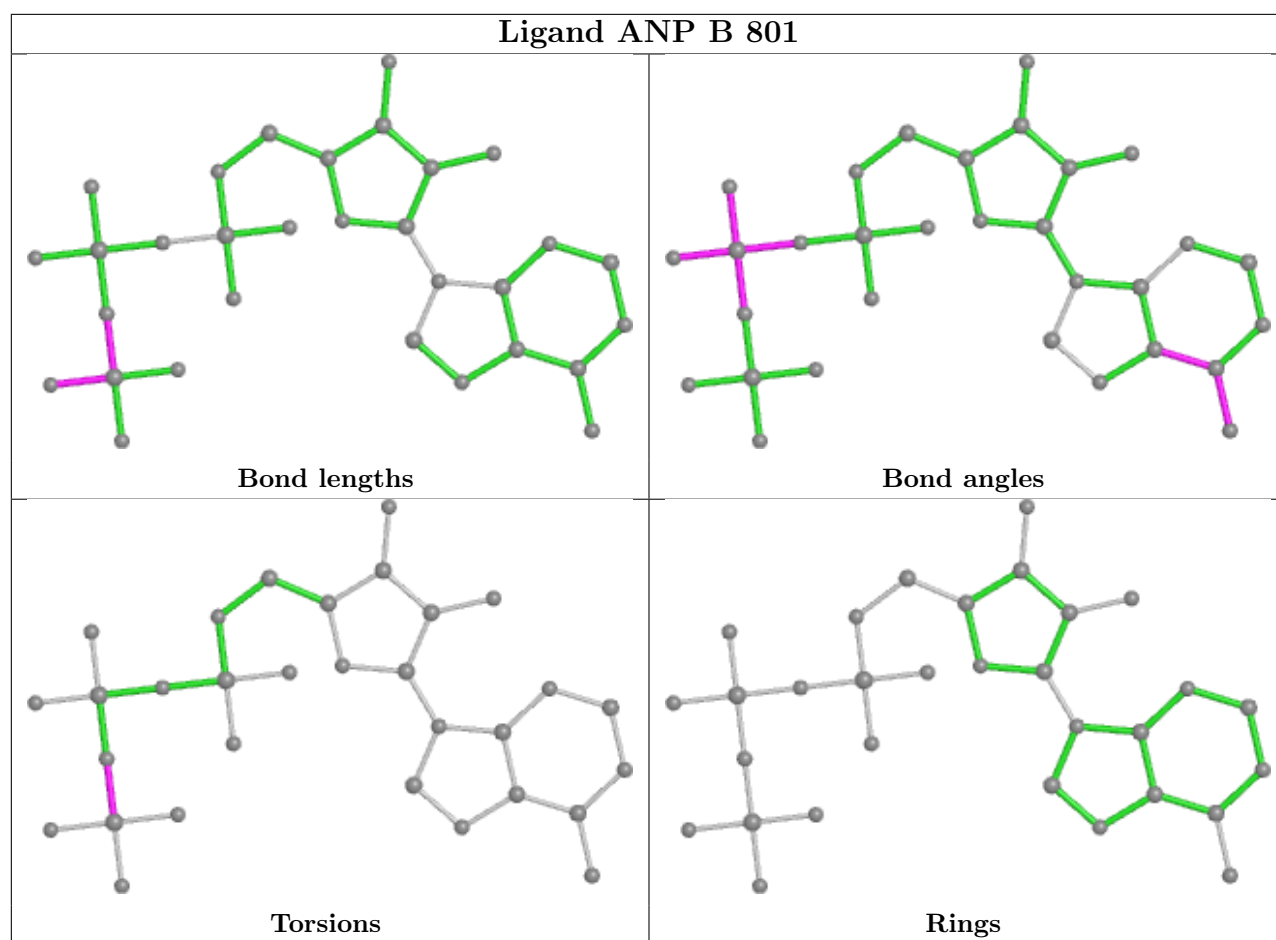
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	05M	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	574/647 (88%)	0.32	43 (7%)	14 19	27, 62, 118, 160	0
1	B	599/647 (92%)	0.35	54 (9%)	9 12	33, 59, 101, 138	0
All	All	1173/1294 (90%)	0.33	97 (8%)	11 15	27, 60, 114, 160	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	MET	5.7
1	A	152	ASP	5.1
1	B	199	LEU	5.1
1	B	147	ILE	4.9
1	B	165	VAL	4.9
1	B	200	ASP	4.7
1	B	238	GLU	4.5
1	A	100	PHE	4.5
1	A	606	VAL	4.4
1	B	510	ARG	4.2
1	A	98	GLY	4.2
1	B	198	PHE	4.2
1	A	605	LEU	4.1
1	B	257	ALA	4.0
1	B	131	LEU	4.0
1	B	153	THR	4.0
1	A	99	SER	4.0
1	B	580	GLN	3.7
1	B	607	GLN	3.7
1	B	239	ALA	3.5
1	B	507	ALA	3.5
1	A	527	PRO	3.5
1	A	632	ALA	3.5
1	B	220	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	240	ASP	3.5
1	A	492	ALA	3.5
1	A	590	SER	3.5
1	A	592	GLU	3.4
1	B	578	LYS	3.4
1	A	324	TRP	3.4
1	B	508	GLY	3.3
1	B	196	LYS	3.3
1	B	134	ASN	3.3
1	B	148	THR	3.3
1	A	674	ASP	3.3
1	A	593	GLN	3.3
1	B	85	THR	3.3
1	B	420	LEU	3.2
1	A	636	PHE	3.2
1	A	96	VAL	3.2
1	A	594	ALA	3.2
1	A	555	ARG	3.1
1	A	633	ALA	3.1
1	B	275	ASP	3.0
1	A	603	ASN	3.0
1	B	699	GLU	2.9
1	B	133	SER	2.9
1	A	604	ALA	2.9
1	B	132	ILE	2.8
1	B	145	ARG	2.8
1	A	319	LYS	2.8
1	B	389	THR	2.8
1	A	532	MET	2.7
1	B	219	GLY	2.7
1	A	678	GLU	2.7
1	A	672	LEU	2.7
1	B	577	GLU	2.7
1	A	589	LEU	2.7
1	A	559	ARG	2.6
1	A	322	SER	2.6
1	A	619	ASP	2.6
1	B	171	ILE	2.6
1	B	579	PHE	2.5
1	B	221	TYR	2.5
1	A	596	ASP	2.5
1	B	422	GLU	2.5

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	718	LYS	2.4
1	A	489	ALA	2.4
1	A	599	ALA	2.4
1	B	135	GLY	2.4
1	A	628	LEU	2.4
1	B	425	LEU	2.4
1	A	493	GLY	2.4
1	B	595	GLU	2.4
1	A	637	LEU	2.4
1	A	670	HIS	2.3
1	B	385	ILE	2.3
1	B	369	ASP	2.3
1	A	270	LEU	2.3
1	B	197	ALA	2.3
1	B	136	SER	2.3
1	A	320	ASP	2.2
1	B	636	PHE	2.2
1	A	635	HIS	2.2
1	B	86	LEU	2.2
1	A	530	GLU	2.1
1	B	637	LEU	2.1
1	A	204	ASN	2.1
1	B	592	GLU	2.1
1	B	242	PRO	2.1
1	B	589	LEU	2.1
1	B	367	MET	2.1
1	B	130	GLU	2.0
1	B	256	VAL	2.0
1	B	594	ALA	2.0
1	A	97	GLN	2.0
1	B	97	GLN	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 ⓘ

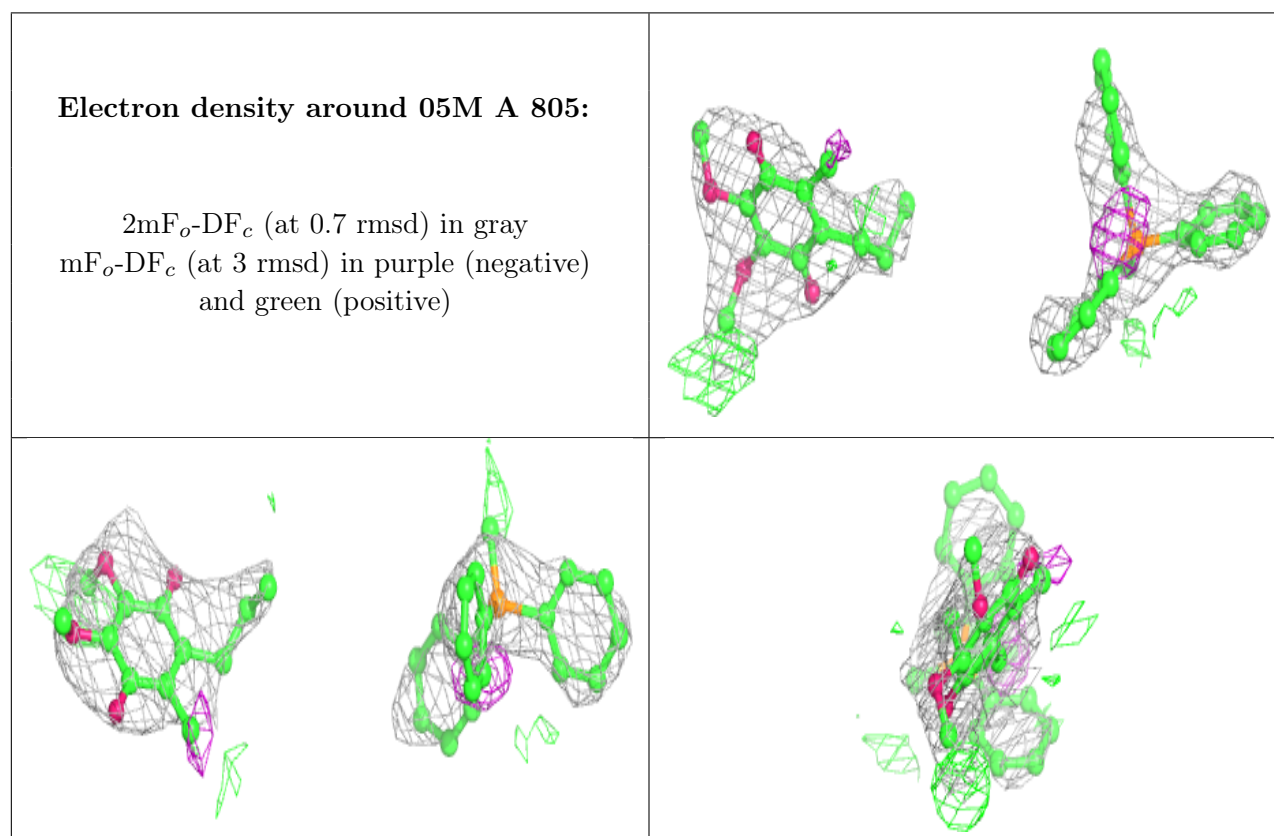
There are no monosaccharides in this entry.

## 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.

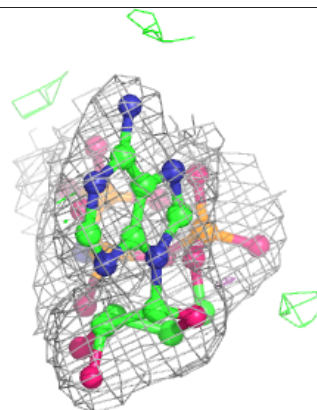
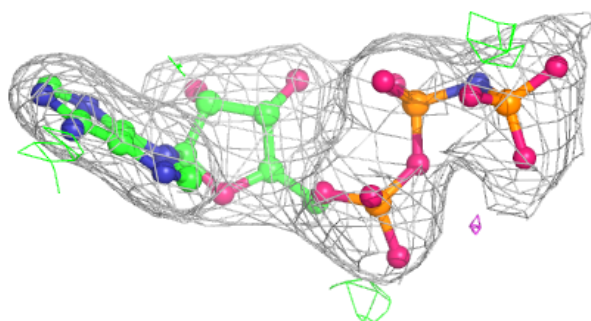
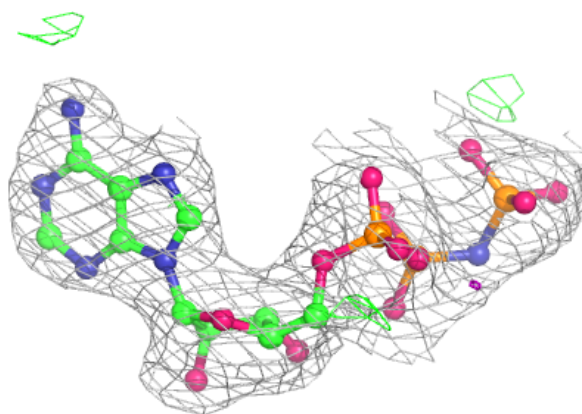
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CO	A	804	1/1	-0.03	0.49	292,292,292,292	0
4	CO	B	804	1/1	0.16	1.14	239,239,239,239	0
4	CO	A	803	1/1	0.81	0.39	200,200,200,200	0
5	05M	A	805	36/42	0.81	0.34	80,96,112,114	0
3	MG	B	802	1/1	0.93	0.23	60,60,60,60	0
4	CO	B	803	1/1	0.96	0.04	99,99,99,99	0
2	ANP	B	801	31/31	0.98	0.20	40,50,67,80	0
3	MG	A	802	1/1	0.98	0.18	25,25,25,25	0
2	ANP	A	801	31/31	0.99	0.18	22,34,40,44	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.

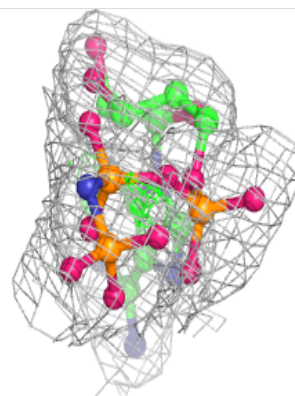
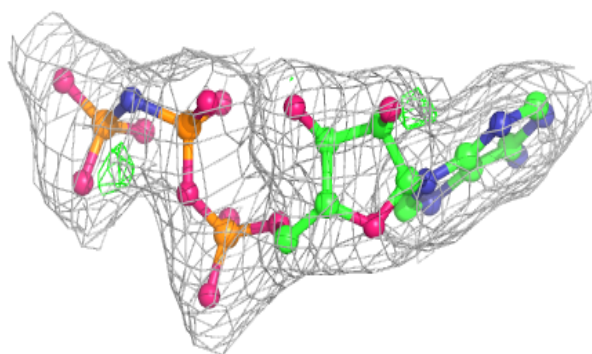
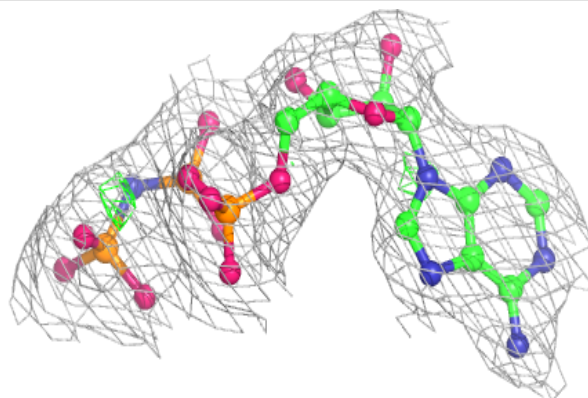


**Electron density around ANP B 801:**

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

**Electron density around ANP A 801:**

$2mF_o-DF_c$  (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.