



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:27 PM EDT

PDB ID : 6EQO  
Title : Tri-functional propionyl-CoA synthase of Erythrobacter sp. NAP1 with bound NADP<sup>+</sup> and phosphomethylphosphonic acid adenylate ester  
Authors : Zarzycki, J.; Bernhardsgruetter, I.; Voegeli, B.; Wagner, T.; Engilberge, S.; Girard, E.; Shima, S.; Erb, T.J.  
Deposited on : 2017-10-13  
Resolution : 2.70 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

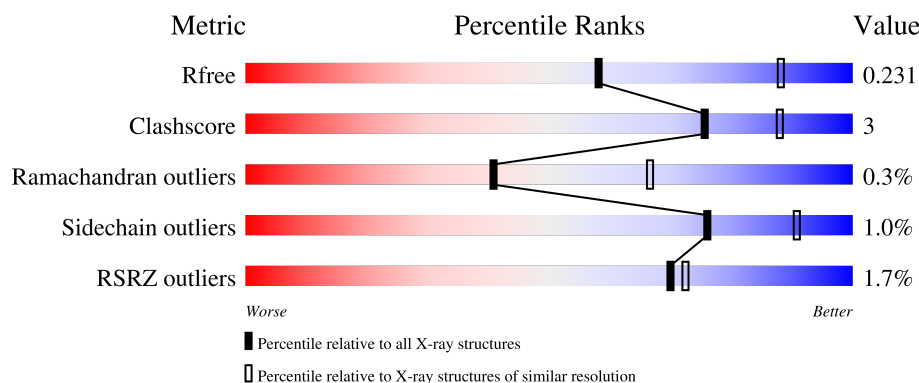
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	1850	<div> <div> <div>0%</div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	1850	<div> <div> <div>2%</div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

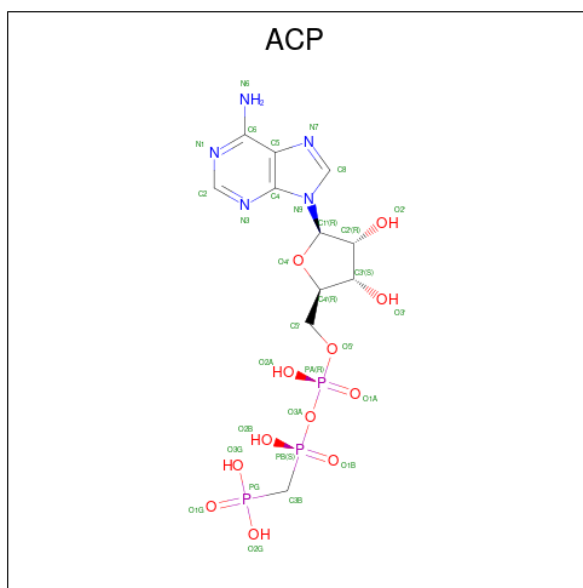
There are 4 unique types of molecules in this entry. The entry contains 28218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1804	Total	C	N	O	S	0	0	0
			13820	8700	2421	2651	48			
1	B	1803	Total	C	N	O	S	0	0	0
			13816	8698	2420	2650	48			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

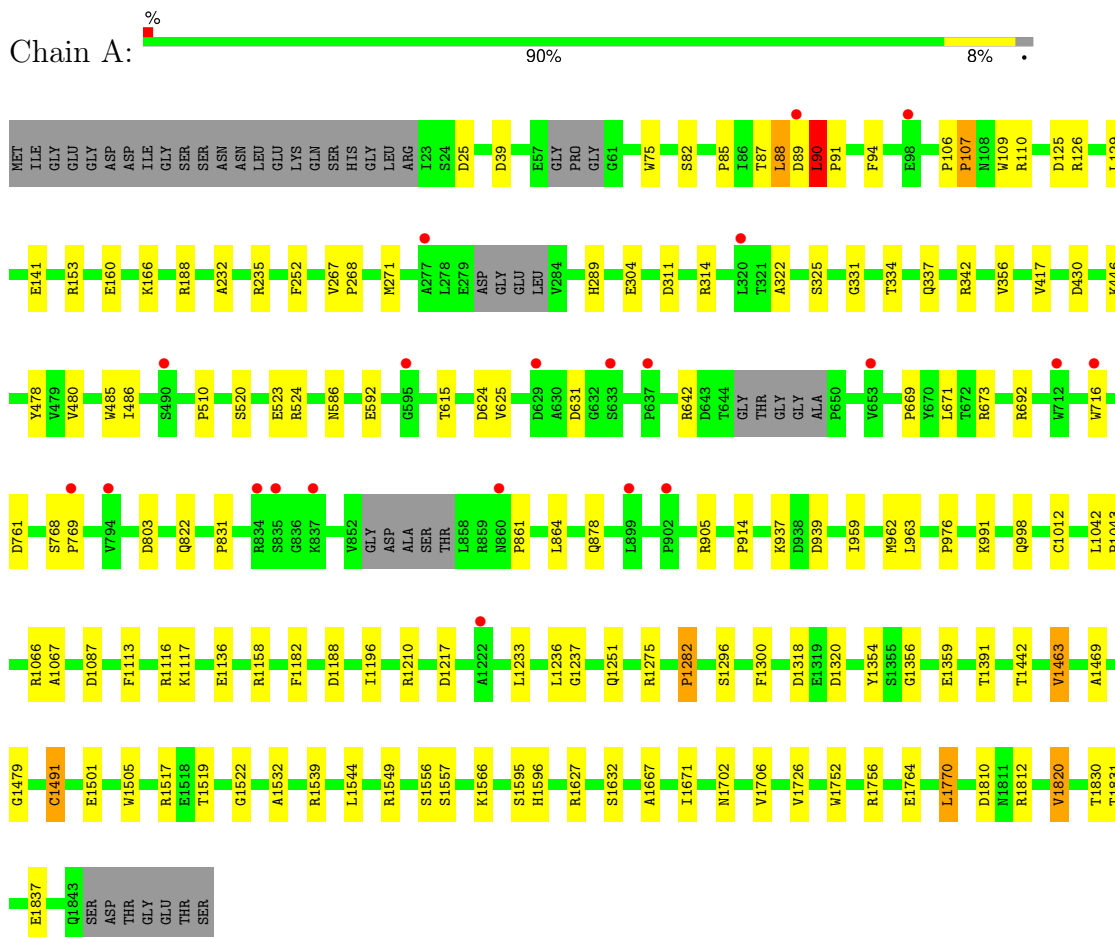
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	201	Total O 201 201	0	0
4	B	231	Total O 231 231	0	0

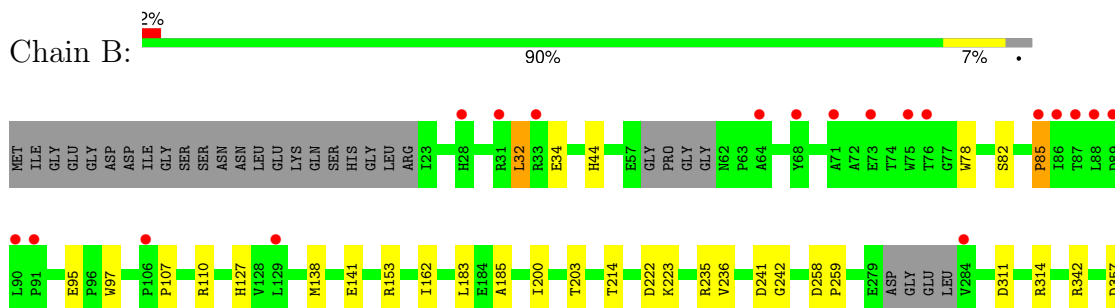
### 3 Residue-property plots [i](#)

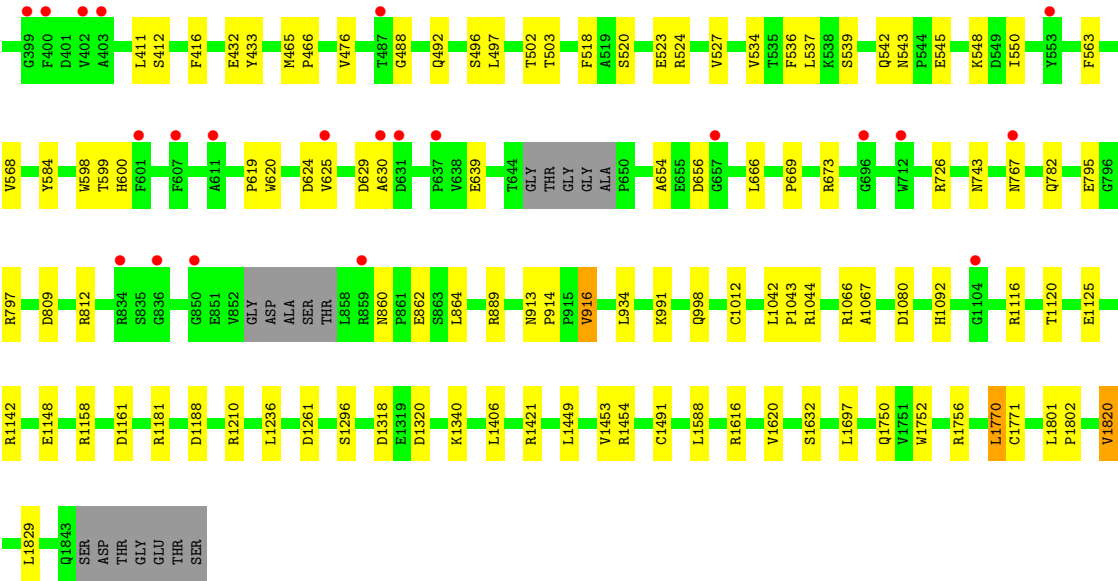
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Acetyl-coenzyme A synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	383.41Å 86.74Å 133.96Å 90.00° 108.89° 90.00°	Depositor
Resolution (Å)	46.18 – 2.70 46.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.18-2.70) 97.6 (46.18-2.70)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , 0.229 0.192 , 0.231	Depositor DCC
$R_{free}$ test set	2007 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28218	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 2.80% 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: ACP, NAP

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	0.35	0/14138	0.50	5/19223 (0.0%)
1	B	0.34	0/14134	0.49	3/19218 (0.0%)
All	All	0.35	0/28272	0.49	8/38441 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	PRO	N-CA-C	6.58	129.19	112.10
1	B	862	GLU	N-CA-C	6.51	128.59	111.00
1	A	914	PRO	CA-C-O	-5.70	106.52	120.20
1	B	914	PRO	N-CA-C	5.29	125.86	112.10
1	B	913	ASN	N-CA-C	-5.29	96.72	111.00
1	A	90	LEU	C-N-CD	5.16	139.24	128.40
1	A	1770	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	91	PRO	N-CA-C	5.03	125.18	112.10

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	13820	0	13424	86	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13816	0	13421	86	0
2	A	31	0	14	3	0
2	B	23	0	12	0	0
3	A	48	0	23	1	0
3	B	48	0	24	1	0
4	A	201	0	0	6	0
4	B	231	0	0	4	0
All	All	28218	0	26918	171	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 3.

All (171) 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:654:ALA:O	1:B:726:ARG:NH2	2.12	0.83
1:A:1066:ARG:NH1	1:A:1318:ASP:OD1	2.12	0.82
1:A:342:ARG:NH1	1:A:1632:SER:O	2.14	0.79
1:A:905:ARG:NE	1:A:939:ASP:OD2	2.17	0.78
1:B:32:LEU:O	1:B:32:LEU:HD13	1.82	0.78
1:B:520:SER:OG	1:B:524:ARG:NH1	2.17	0.77
1:A:822:GLN:NE2	1:A:878:GLN:OE1	2.19	0.75
1:A:937:LYS:O	1:A:991:LYS:NZ	2.19	0.74
1:B:1067:ALA:O	1:B:1210:ARG:NH1	2.20	0.74
1:A:1066:ARG:NH2	1:A:1320:ASP:OD1	2.21	0.74
1:B:1158:ARG:NH2	1:B:1188:ASP:OD2	2.21	0.73
1:B:809:ASP:OD2	1:B:812:ARG:NH2	2.22	0.72
1:B:141:GLU:OE1	1:B:524:ARG:NH2	2.23	0.72
1:A:624:ASP:OD1	1:A:625:VAL:N	2.23	0.71
1:B:1142:ARG:NH2	1:B:1261:ASP:OD1	2.25	0.70
1:B:624:ASP:OD1	1:B:726:ARG:NH1	2.23	0.70
1:A:141:GLU:OE2	1:A:524:ARG:NH2	2.25	0.70
1:A:430:ASP:OD1	1:A:692:ARG:NH1	2.25	0.69
1:A:1491:CYS:O	1:A:1539:ARG:NH1	2.26	0.69
1:B:1066:ARG:NH1	1:B:1320:ASP:OD1	2.27	0.67
1:B:110:ARG:NH2	1:B:432:GLU:OE2	2.27	0.67
1:B:1012:CYS:O	1:B:1116:ARG:NH1	2.28	0.67
1:A:322:ALA:O	1:A:325:SER:OG	2.11	0.66
1:A:1136:GLU:OE1	4:A:2001:HOH:O	2.13	0.66
1:A:88:LEU:HD12	1:A:88:LEU:O	1.99	0.63
1:B:153:ARG:NH1	1:B:523:GLU:OE2	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1549:ARG:NH1	1:A:1764:GLU:OE1	2.33	0.62
1:B:342:ARG:NH1	1:B:1632:SER:O	2.32	0.62
1:A:1210:ARG:NH2	1:A:1318:ASP:O	2.31	0.62
1:A:1830:THR:HG23	1:A:1831:THR:HG23	1.81	0.61
1:B:1044:ARG:NH2	1:B:1125:GLU:O	2.34	0.61
1:B:916:VAL:HG13	1:B:916:VAL:O	2.01	0.61
1:B:1616:ARG:NH1	1:B:1697:LEU:O	2.33	0.61
1:B:743:ASN:O	1:B:743:ASN:ND2	2.34	0.60
1:A:1087:ASP:O	1:B:1340:LYS:NZ	2.34	0.60
1:B:32:LEU:HD13	1:B:32:LEU:C	2.21	0.60
1:B:1161:ASP:OD2	1:B:1181:ARG:NH1	2.34	0.60
1:A:1296:SER:HB3	1:A:1820:VAL:HG13	1.84	0.59
1:A:1359:GLU:OE2	4:A:2002:HOH:O	2.16	0.59
1:B:534:VAL:HG22	1:B:563:PHE:CD1	2.36	0.59
1:B:545:GLU:HA	1:B:548:LYS:CE	2.33	0.58
1:A:486:ILE:HG22	2:A:1901:ACP:H3B1	1.85	0.58
1:A:1505:TRP:O	1:A:1539:ARG:NH2	2.36	0.58
1:A:160:GLU:OE2	1:A:166:LYS:NZ	2.37	0.57
1:A:671:LEU:O	1:A:673:ARG:NH1	2.37	0.57
1:B:534:VAL:HG21	1:B:568:VAL:HG12	1.86	0.56
1:B:311:ASP:OD1	1:B:314:ARG:NH2	2.40	0.55
1:A:109:TRP:O	1:A:110:ARG:NE	2.40	0.55
1:B:539:SER:HB3	1:B:782:GLN:NE2	2.22	0.55
1:A:485:TRP:HB3	2:A:1901:ACP:O1G	2.08	0.54
1:B:545:GLU:HA	1:B:548:LYS:HE3	1.89	0.54
1:B:934:LEU:O	1:B:991:LYS:NZ	2.37	0.53
1:B:539:SER:HB3	1:B:782:GLN:HE22	1.73	0.53
1:B:629:ASP:OD1	1:B:630:ALA:N	2.42	0.53
1:A:90:LEU:HB2	1:A:94:PHE:HB2	1.90	0.53
1:B:95:GLU:OE1	1:B:97:TRP:NE1	2.40	0.52
1:A:267:VAL:HG22	1:A:268:PRO:HD3	1.92	0.52
1:B:518:PHE:CE1	1:B:550:ILE:HD11	2.45	0.52
1:A:1282:PRO:HB2	1:A:1391:THR:HG23	1.93	0.51
1:B:624:ASP:OD1	1:B:625:VAL:N	2.40	0.51
1:B:1296:SER:OG	1:B:1820:VAL:HG13	2.11	0.51
1:A:1012:CYS:O	1:A:1116:ARG:NH1	2.45	0.50
1:B:411:LEU:HD11	1:B:416:PHE:HA	1.93	0.50
1:A:486:ILE:HG22	2:A:1901:ACP:C3B	2.42	0.50
1:B:860:ASN:N	1:B:860:ASN:OD1	2.44	0.50
1:A:1217:ASP:OD2	1:A:1275:ARG:NE	2.44	0.50
1:A:1595:SER:OG	1:A:1596:HIS:N	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:LEU:HB3	1:B:1043:PRO:HD3	1.94	0.50
1:A:1517:ARG:HG2	1:A:1522:GLY:HA2	1.93	0.49
1:B:542:GLN:NE2	1:B:782:GLN:OE1	2.46	0.49
1:A:1442:THR:OG1	3:A:1902:NAP:O3B	2.30	0.49
1:A:1463:VAL:HG11	1:A:1469:ALA:HB2	1.94	0.49
1:A:334:THR:O	1:A:337:GLN:N	2.45	0.49
1:A:188:ARG:NE	1:A:232:ALA:O	2.45	0.49
1:A:1236:LEU:HG	1:A:1237:GLY:N	2.27	0.49
1:B:534:VAL:CG2	1:B:568:VAL:HG12	2.42	0.49
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.94	0.48
1:B:1210:ARG:NH2	1:B:1318:ASP:O	2.43	0.48
1:A:1501:GLU:OE1	4:A:2004:HOH:O	2.20	0.48
1:A:1837:GLU:OE1	1:B:889:ARG:NH2	2.47	0.48
1:B:864:LEU:N	1:B:864:LEU:HD23	2.29	0.48
1:B:795:GLU:OE2	4:B:2001:HOH:O	2.20	0.48
1:B:258:ASP:HB2	1:B:259:PRO:HD3	1.96	0.48
1:A:1810:ASP:OD2	1:A:1812:ARG:NH2	2.46	0.47
1:A:1627:ARG:NH2	4:A:2031:HOH:O	2.47	0.47
1:A:592:GLU:OE1	1:A:592:GLU:N	2.43	0.47
1:A:311:ASP:OD1	1:A:314:ARG:NH2	2.47	0.47
1:A:39:ASP:OD1	4:A:2003:HOH:O	2.20	0.47
1:B:222:ASP:OD1	1:B:223:LYS:N	2.48	0.47
1:B:545:GLU:HA	1:B:548:LYS:HE2	1.96	0.47
1:A:520:SER:OG	1:A:524:ARG:NH1	2.47	0.47
1:B:185:ALA:O	1:B:433:TYR:OH	2.32	0.47
1:A:89:ASP:N	1:A:89:ASP:OD1	2.45	0.46
1:B:411:LEU:HD12	1:B:412:SER:O	2.15	0.46
1:B:539:SER:HA	1:B:542:GLN:HG2	1.97	0.46
1:A:153:ARG:NH1	1:A:523:GLU:OE2	2.48	0.46
1:B:543:ASN:N	1:B:543:ASN:OD1	2.47	0.46
1:A:126:ARG:NH1	4:A:2033:HOH:O	2.47	0.46
1:A:267:VAL:N	1:A:268:PRO:CD	2.78	0.46
1:B:496:SER:CB	1:B:503:THR:HG22	2.46	0.46
1:A:1726:VAL:O	1:A:1756:ARG:NH2	2.48	0.46
1:B:183:LEU:HD11	1:B:236:VAL:HG21	1.98	0.46
1:A:1702:ASN:ND2	1:A:1706:VAL:O	2.46	0.46
1:B:411:LEU:HD11	1:B:416:PHE:CA	2.46	0.46
1:A:669:PRO:O	1:A:673:ARG:NH1	2.47	0.45
1:A:289:HIS:NE2	1:A:331:GLY:HA3	2.32	0.45
1:A:1532:ALA:O	1:A:1556:SER:N	2.50	0.45
1:B:599:THR:OG1	1:B:600:HIS:N	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:ILE:HG22	1:A:1196:ILE:HG23	1.98	0.45
1:A:1158:ARG:NH2	1:A:1188:ASP:OD2	2.50	0.45
1:A:1354:TYR:CZ	1:A:1356:GLY:HA3	2.51	0.45
1:A:25:ASP:OD1	1:A:25:ASP:N	2.37	0.45
1:A:769:PRO:HG3	1:A:803:ASP:OD2	2.17	0.45
1:A:586:ASN:O	1:A:615:THR:HG22	2.17	0.44
1:A:90:LEU:HD13	1:A:90:LEU:N	2.31	0.44
1:A:87:THR:O	1:A:87:THR:OG1	2.35	0.44
1:B:767:ASN:O	1:B:797:ARG:NH2	2.51	0.44
1:B:1454:ARG:NE	4:B:2005:HOH:O	2.29	0.44
1:B:200:ILE:HA	1:B:203:THR:HG22	1.98	0.44
1:B:1148:GLU:OE1	4:B:2002:HOH:O	2.21	0.44
1:A:1042:LEU:HB3	1:A:1043:PRO:HD3	1.99	0.44
1:A:1113:PHE:O	1:A:1117:LYS:HG2	2.18	0.44
1:B:1750:GLN:O	1:B:1756:ARG:HD2	2.17	0.44
1:B:32:LEU:C	1:B:32:LEU:CD1	2.85	0.44
1:A:106:PRO:CB	1:A:107:PRO:HD3	2.48	0.43
1:A:761:ASP:OD2	1:A:768:SER:OG	2.31	0.43
1:B:669:PRO:O	1:B:673:ARG:NH2	2.37	0.43
1:B:465:MET:HB2	1:B:466:PRO:HD3	1.99	0.43
1:A:304:GLU:OE2	1:A:446:LYS:NZ	2.44	0.43
1:B:1421:ARG:HD2	1:B:1771:CYS:HA	1.99	0.43
1:B:1066:ARG:NH2	1:B:1318:ASP:OD1	2.43	0.43
1:B:241:ASP:OD1	1:B:242:GLY:N	2.51	0.43
1:B:639:GLU:HB2	1:B:666:LEU:HD11	2.01	0.43
1:B:1588:LEU:HD11	1:B:1620:VAL:HG23	2.00	0.43
1:A:1544:LEU:HB2	1:A:1566:LYS:HE3	2.01	0.42
1:B:34:GLU:HB2	1:B:619:PRO:HB3	2.00	0.42
1:A:1667:ALA:O	1:A:1671:ILE:HG13	2.19	0.42
1:B:1449:LEU:O	1:B:1453:VAL:HG23	2.20	0.42
1:A:1479:GLY:HA3	1:A:1519:THR:HG21	2.02	0.42
1:B:44:HIS:NE2	1:B:620:TRP:HB2	2.35	0.42
1:B:476:VAL:HG23	1:B:527:VAL:HA	2.02	0.42
1:B:235:ARG:O	1:B:357:ASP:N	2.43	0.42
1:A:75:TRP:HB2	1:A:87:THR:O	2.20	0.42
1:A:267:VAL:O	1:A:271:MET:HG2	2.20	0.42
1:B:1406:LEU:HD12	1:B:1829:LEU:HB2	2.02	0.42
1:A:480:VAL:HG11	1:A:510:PRO:HG3	2.02	0.41
1:B:476:VAL:HG12	1:B:502:THR:HB	2.01	0.41
1:A:1544:LEU:CB	1:A:1566:LYS:HE3	2.50	0.41
1:A:642:ARG:HD2	1:A:716:TRP:CE2	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:PRO:HG3	1:A:1182:PHE:HD2	1.85	0.41
1:A:106:PRO:HB2	1:A:716:TRP:CZ2	2.56	0.41
1:A:129:LEU:HD13	1:A:417:VAL:HG11	2.02	0.41
1:B:539:SER:CA	1:B:782:GLN:HE22	2.34	0.41
1:B:1116:ARG:HE	1:B:1120:THR:CG2	2.33	0.41
1:B:536:PHE:CZ	1:B:537:LEU:CD2	3.04	0.41
1:A:485:TRP:CD1	1:A:485:TRP:N	2.89	0.41
1:A:1233:LEU:CD1	1:A:1251:GLN:HA	2.50	0.41
1:B:1801:LEU:HB3	1:B:1802:PRO:HD3	2.02	0.41
1:A:235:ARG:O	1:A:356:VAL:HG22	2.21	0.41
1:A:959:ILE:HA	1:A:962:MET:HE2	2.02	0.41
1:B:127:HIS:NE2	1:B:497:LEU:O	2.54	0.41
1:B:214:THR:O	1:B:214:THR:HG23	2.20	0.41
1:A:963:LEU:HB2	1:A:1196:ILE:HG21	2.04	0.40
1:B:78:TRP:HA	1:B:85:PRO:CD	2.51	0.40
1:B:656:ASP:OD1	1:B:726:ARG:HD2	2.20	0.40
1:B:138:MET:CE	1:B:162:ILE:HG21	2.52	0.40
1:B:518:PHE:CZ	1:B:550:ILE:HD11	2.57	0.40
3:B:1902:NAP:H8A	4:B:2217:HOH:O	2.21	0.40
1:A:1067:ALA:O	1:A:1210:ARG:NH1	2.54	0.40
1:B:432:GLU:OE1	1:B:673:ARG:NH1	2.53	0.40
1:B:488:GLY:HA2	1:B:492:GLN:HB3	2.03	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	1794/1850 (97%)	1702 (95%)	87 (5%)	5 (0%)	41	66
1	B	1793/1850 (97%)	1703 (95%)	86 (5%)	4 (0%)	47	73
All	All	3587/3700 (97%)	3405 (95%)	173 (5%)	9 (0%)	41	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	PRO
1	A	82	SER
1	B	85	PRO
1	B	107	PRO
1	B	1770	LEU
1	A	107	PRO
1	B	82	SER
1	A	861	PRO
1	A	831	PRO

### 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	1416/1448 (98%)	1400 (99%)	16 (1%)	73	90
1	B	1416/1448 (98%)	1404 (99%)	12 (1%)	81	93
All	All	2832/2896 (98%)	2804 (99%)	28 (1%)	76	91

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	90	LEU
1	A	125	ASP
1	A	252	PHE
1	A	478	TYR
1	A	631	ASP
1	A	864	LEU
1	A	998	GLN
1	A	1282	PRO
1	A	1300	PHE
1	A	1463	VAL
1	A	1491	CYS
1	A	1557	SER
1	A	1752	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1770	LEU
1	A	1820	VAL
1	B	32	LEU
1	B	584	TYR
1	B	598	TRP
1	B	916	VAL
1	B	998	GLN
1	B	1080	ASP
1	B	1092	HIS
1	B	1236	LEU
1	B	1491	CYS
1	B	1752	TRP
1	B	1770	LEU
1	B	1820	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 ligands 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
2	ACP	A	1901	-	27,33,33	4.20	14 (51%)	33,52,52	2.08	8 (24%)
3	NAP	B	1902	-	46,52,52	4.03	18 (39%)	61,80,80	1.78	9 (14%)
3	NAP	A	1902	-	46,52,52	4.12	15 (32%)	61,80,80	1.71	10 (16%)
2	ACP	B	1901	-	21,25,33	4.48	7 (33%)	23,38,52	1.85	4 (17%)

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	ACP	A	1901	-	-	9/15/38/38	0/3/3/3
3	NAP	B	1902	-	-	4/31/67/67	0/5/5/5
3	NAP	A	1902	-	-	4/31/67/67	0/5/5/5
2	ACP	B	1901	-	-	3/6/26/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1902	NAP	O4B-C1B	16.37	1.62	1.40
3	A	1902	NAP	O4D-C1D	16.14	1.62	1.40
3	B	1902	NAP	O4B-C1B	15.72	1.61	1.40
3	B	1902	NAP	O4D-C1D	15.16	1.60	1.40
2	B	1901	ACP	O4'-C1'	12.25	1.57	1.40
2	A	1901	ACP	O4'-C1'	12.19	1.56	1.40
2	B	1901	ACP	C2'-C3'	-9.35	1.28	1.53
2	A	1901	ACP	C2'-C3'	-9.25	1.28	1.53
2	B	1901	ACP	O4'-C4'	-8.68	1.25	1.45
2	A	1901	ACP	O4'-C4'	-8.40	1.26	1.45
3	B	1902	NAP	C7N-N7N	7.30	1.46	1.33
3	A	1902	NAP	C7N-N7N	7.10	1.46	1.33
3	B	1902	NAP	O4B-C4B	-7.00	1.29	1.45
2	A	1901	ACP	C1'-N9	-6.88	1.32	1.49
3	A	1902	NAP	O4B-C4B	-6.60	1.30	1.45
2	B	1901	ACP	C1'-N9	-6.60	1.33	1.49
3	A	1902	NAP	O4D-C4D	-5.97	1.31	1.45
3	B	1902	NAP	O4D-C4D	-5.94	1.31	1.45
2	A	1901	ACP	PB-O2B	-4.76	1.44	1.56
2	A	1901	ACP	PG-O3G	-4.48	1.44	1.55
2	B	1901	ACP	C3'-C4'	4.40	1.64	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1901	ACP	C3'-C4'	4.23	1.63	1.53
3	B	1902	NAP	PN-O3	3.98	1.63	1.59
3	B	1902	NAP	P2B-O2B	3.80	1.66	1.59
2	A	1901	ACP	PG-O2G	-3.69	1.46	1.55
2	B	1901	ACP	C6-N6	3.62	1.47	1.34
3	A	1902	NAP	PN-O3	3.60	1.63	1.59
3	B	1902	NAP	PA-O3	3.31	1.63	1.59
3	A	1902	NAP	C6A-N6A	3.27	1.45	1.34
3	A	1902	NAP	P2B-O2B	3.24	1.65	1.59
3	A	1902	NAP	PA-O3	3.17	1.62	1.59
2	A	1901	ACP	C6-N6	3.15	1.45	1.34
3	B	1902	NAP	C6A-N6A	3.09	1.45	1.34
2	A	1901	ACP	PG-O1G	-3.07	1.44	1.50
3	A	1902	NAP	O7N-C7N	-3.06	1.18	1.24
3	B	1902	NAP	O3B-C3B	-2.88	1.35	1.43
3	A	1902	NAP	O3D-C3D	-2.85	1.35	1.43
3	A	1902	NAP	C4N-C3N	-2.79	1.35	1.39
3	B	1902	NAP	O7N-C7N	-2.75	1.19	1.24
3	A	1902	NAP	O2D-C2D	2.69	1.49	1.43
3	A	1902	NAP	O3B-C3B	-2.63	1.36	1.43
3	B	1902	NAP	C2A-N3A	2.60	1.36	1.32
3	A	1902	NAP	C2A-N3A	2.52	1.36	1.32
3	B	1902	NAP	O2D-C2D	2.49	1.49	1.43
3	B	1902	NAP	C3N-C7N	2.45	1.54	1.50
3	B	1902	NAP	C1B-N9A	-2.34	1.44	1.49
2	B	1901	ACP	C4-N3	-2.30	1.32	1.35
3	B	1902	NAP	O2B-C2B	2.17	1.51	1.44
2	A	1901	ACP	C4-N3	-2.12	1.32	1.35
3	B	1902	NAP	O3D-C3D	-2.10	1.37	1.43
2	A	1901	ACP	C8-N7	-2.09	1.30	1.34
2	A	1901	ACP	O2'-C2'	2.08	1.48	1.43
3	B	1902	NAP	C4N-C3N	-2.07	1.36	1.39
2	A	1901	ACP	C6-N1	-2.05	1.28	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1902	NAP	N3A-C2A-N1A	-6.85	119.38	128.67
3	B	1902	NAP	N3A-C2A-N1A	-6.11	120.37	128.67
3	B	1902	NAP	C4B-O4B-C1B	-5.95	104.47	109.92
2	B	1901	ACP	N3-C2-N1	-5.82	120.77	128.67
2	A	1901	ACP	C4'-O4'-C1'	-4.97	105.38	109.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	ACP	N3-C2-N1	-4.78	122.18	128.67
2	A	1901	ACP	C4-C5-N7	-4.54	104.54	109.34
3	B	1902	NAP	C1B-N9A-C4A	-4.43	118.86	126.64
3	A	1902	NAP	C1B-N9A-C4A	-4.35	119.00	126.64
3	A	1902	NAP	C5A-C6A-N6A	4.18	126.67	120.31
3	B	1902	NAP	O4B-C1B-N9A	-4.07	103.34	108.75
3	B	1902	NAP	C5A-C6A-N6A	4.07	126.51	120.31
2	B	1901	ACP	C4-C5-N7	-3.87	105.25	109.34
3	A	1902	NAP	C4B-O4B-C1B	-3.86	106.39	109.92
3	B	1902	NAP	C6N-N1N-C2N	-3.69	118.74	121.88
2	A	1901	ACP	PB-O3A-PA	-3.67	120.39	132.37
2	A	1901	ACP	O1G-PG-C3B	-3.56	103.60	111.37
3	A	1902	NAP	C6N-N1N-C2N	-3.53	118.87	121.88
2	A	1901	ACP	O2G-PG-C3B	3.23	114.23	106.40
2	A	1901	ACP	C5'-C4'-C3'	-3.21	103.64	115.21
3	A	1902	NAP	C4D-O4D-C1D	-2.86	107.30	109.92
3	B	1902	NAP	N6A-C6A-N1A	-2.66	112.66	118.33
3	A	1902	NAP	C2N-C3N-C4N	2.49	121.15	118.26
3	A	1902	NAP	P2B-O2B-C2B	-2.38	117.08	123.43
3	A	1902	NAP	N6A-C6A-N1A	-2.32	113.37	118.33
2	B	1901	ACP	O4'-C1'-N9	2.31	111.81	108.75
2	B	1901	ACP	C5-C6-N6	2.18	123.63	120.31
3	B	1902	NAP	C4D-O4D-C1D	-2.13	107.97	109.92
3	A	1902	NAP	O2N-PN-O5D	2.10	117.09	107.57
2	A	1901	ACP	O2A-PA-O3A	2.09	112.92	107.27
3	B	1902	NAP	O3B-C3B-C4B	-2.04	105.21	111.08

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1901	ACP	PG-C3B-PB-O1B
2	A	1901	ACP	PG-C3B-PB-O3A
2	B	1901	ACP	C5'-O5'-PA-O2A
2	B	1901	ACP	C5'-O5'-PA-O3A
3	A	1902	NAP	O4D-C1D-N1N-C6N
3	B	1902	NAP	O4D-C1D-N1N-C6N
2	A	1901	ACP	C3'-C4'-C5'-O5'
2	A	1901	ACP	O4'-C4'-C5'-O5'
3	A	1902	NAP	C2B-O2B-P2B-O1X
2	B	1901	ACP	C5'-O5'-PA-O1A
2	A	1901	ACP	PB-O3A-PA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	1901	ACP	C5'-O5'-PA-O1A
2	A	1901	ACP	C5'-O5'-PA-O2A
2	A	1901	ACP	C5'-O5'-PA-O3A
3	A	1902	NAP	O4D-C1D-N1N-C2N
3	B	1902	NAP	O4D-C1D-N1N-C2N
3	B	1902	NAP	C2B-O2B-P2B-O1X
2	A	1901	ACP	PB-O3A-PA-O2A
3	A	1902	NAP	O4B-C4B-C5B-O5B
3	B	1902	NAP	O4B-C4B-C5B-O5B

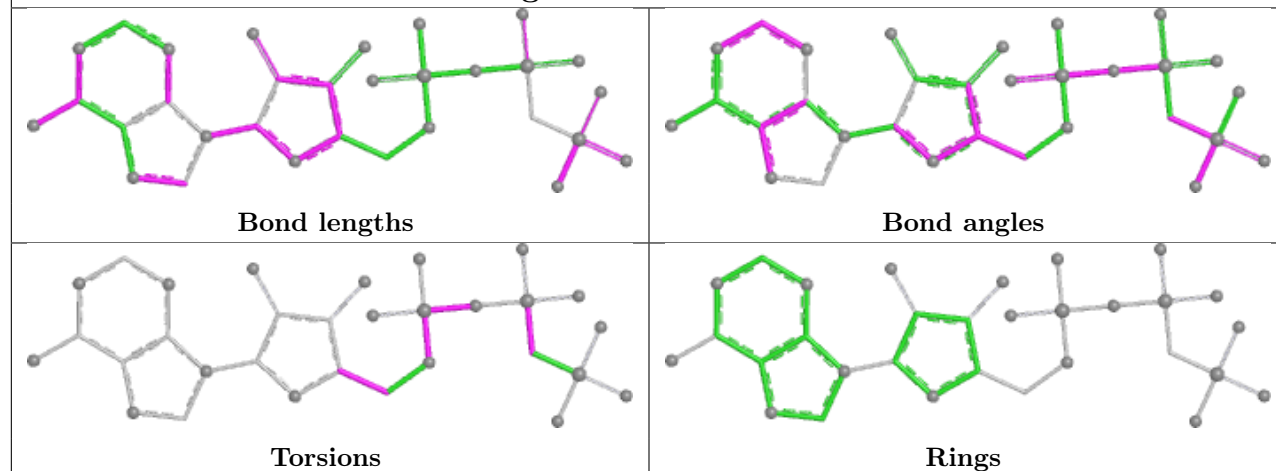
There are no ring outliers.

3 monomers are involved in 5 short contacts:

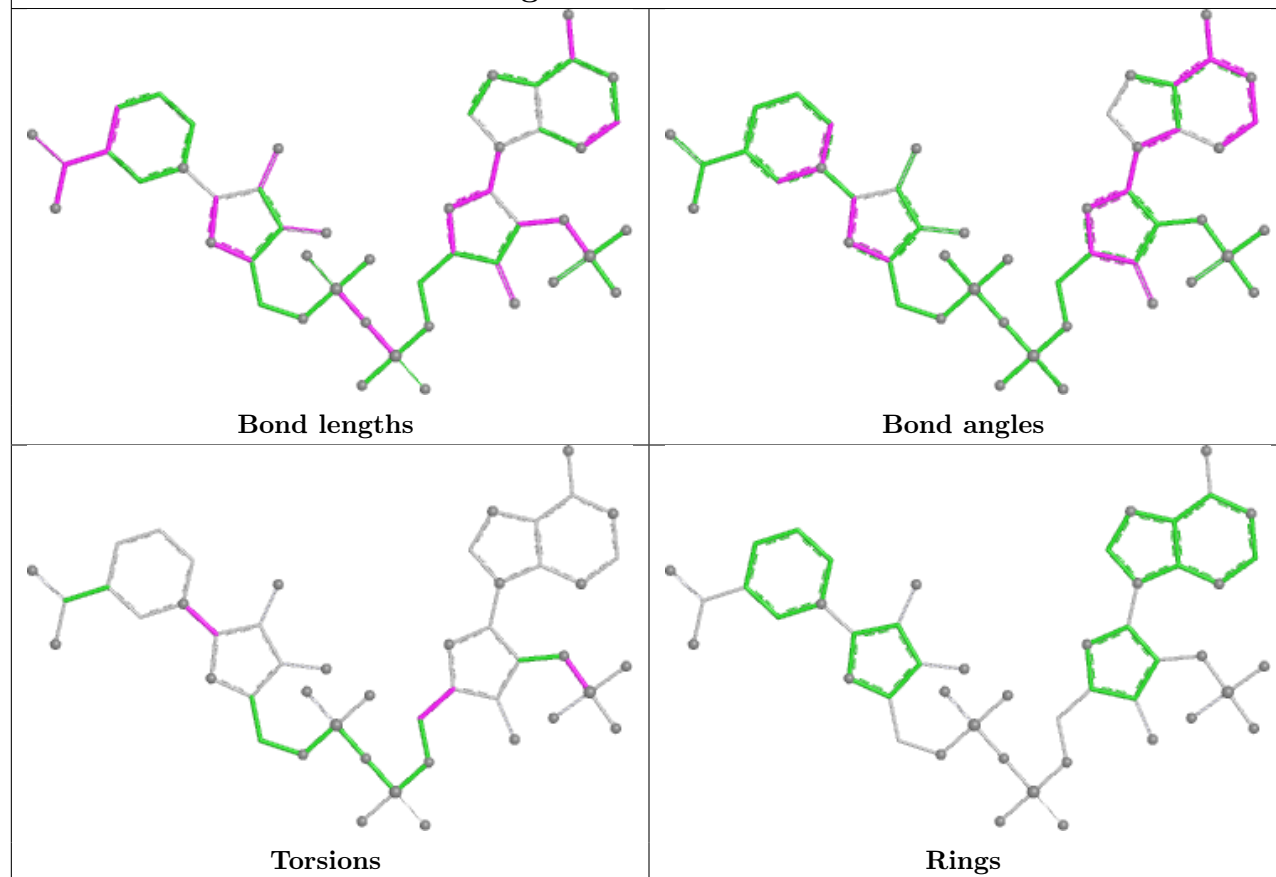
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	ACP	3	0
3	B	1902	NAP	1	0
3	A	1902	NAP	1	0

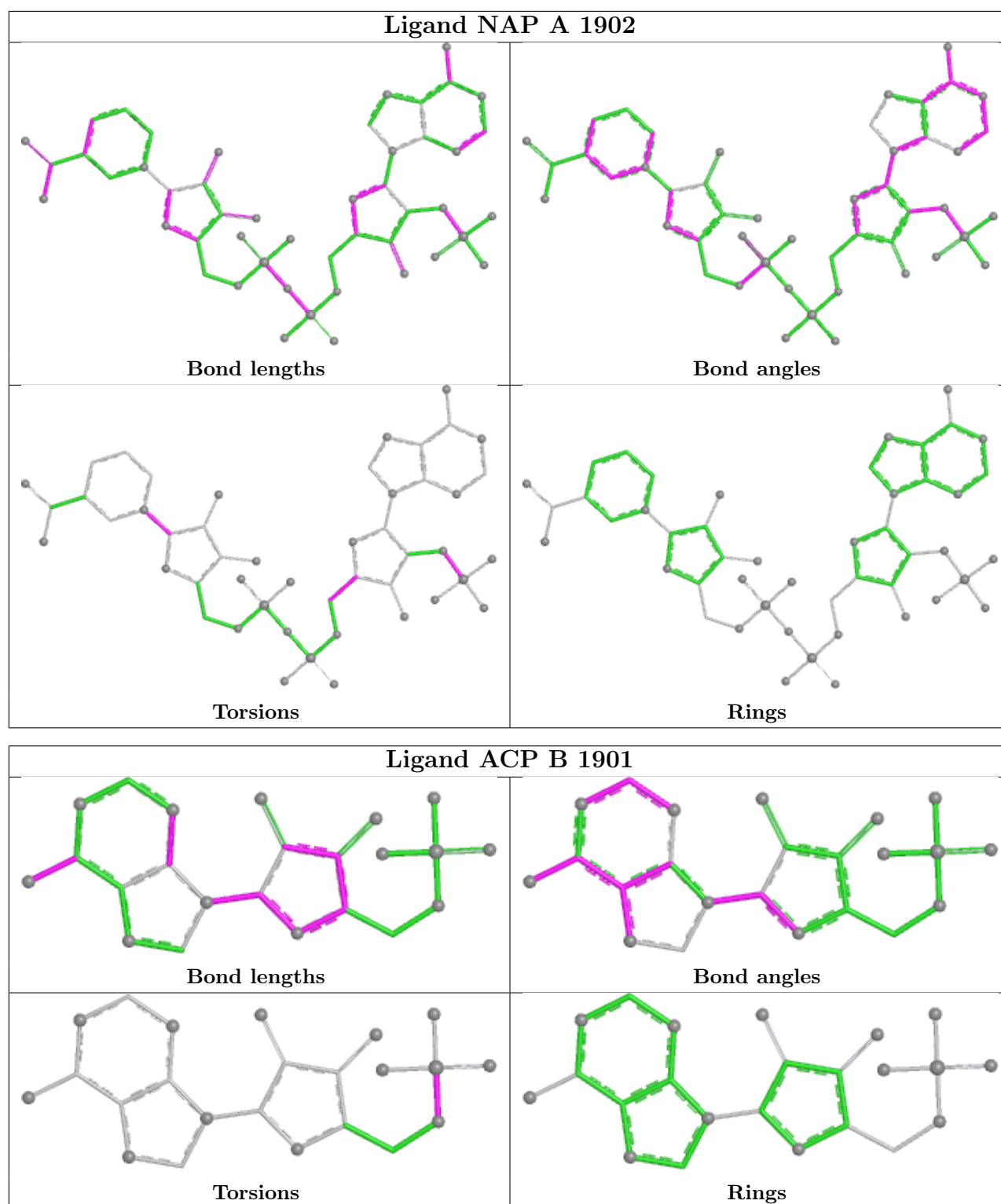
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand ACP A 1901



## Ligand NAP B 1902





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	1804/1850 (97%)	-0.26	21 (1%) 79 80	21, 46, 80, 125	0
1	B	1803/1850 (97%)	-0.16	41 (2%) 60 62	23, 50, 94, 152	0
All	All	3607/3700 (97%)	-0.21	62 (1%) 70 72	21, 48, 90, 152	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	630	ALA	5.3
1	B	91	PRO	5.0
1	A	834	ARG	4.5
1	B	611	ALA	4.3
1	B	88	LEU	4.0
1	A	637	PRO	3.7
1	B	696	GLY	3.6
1	B	87	THR	3.4
1	B	75	TRP	3.1
1	B	85	PRO	3.0
1	B	834	ARG	3.0
1	A	860	ASN	3.0
1	B	64	ALA	2.9
1	B	403	ALA	2.9
1	A	653	VAL	2.8
1	A	902	PRO	2.8
1	B	31	ARG	2.8
1	A	277	ALA	2.8
1	B	90	LEU	2.8
1	B	129	LEU	2.7
1	B	657	GLY	2.7
1	A	794	VAL	2.7
1	A	629	ASP	2.7
1	B	89	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	633	SER	2.6
1	B	836	GLY	2.6
1	A	595	GLY	2.6
1	B	73	GLU	2.5
1	A	899	LEU	2.5
1	B	631	ASP	2.5
1	A	98	GLU	2.4
1	B	553	TYR	2.4
1	B	399	GLY	2.4
1	A	490	SER	2.4
1	B	607	PHE	2.4
1	A	320	LEU	2.4
1	B	487	THR	2.3
1	A	712	TRP	2.3
1	A	716	TRP	2.3
1	B	712	TRP	2.3
1	B	68	TYR	2.3
1	B	859	ARG	2.3
1	B	106	PRO	2.3
1	B	71	ALA	2.3
1	B	400	PHE	2.2
1	B	601	PHE	2.2
1	B	86	ILE	2.2
1	A	89	ASP	2.2
1	B	637	PRO	2.1
1	B	284	VAL	2.1
1	B	76	THR	2.1
1	B	625	VAL	2.1
1	A	769	PRO	2.1
1	A	1222	ALA	2.1
1	B	767	ASN	2.1
1	B	850	GLY	2.1
1	A	837	LYS	2.0
1	B	28	HIS	2.0
1	B	33	ARG	2.0
1	B	1104	GLY	2.0
1	B	402	VAL	2.0
1	A	835	SER	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 [i](#)

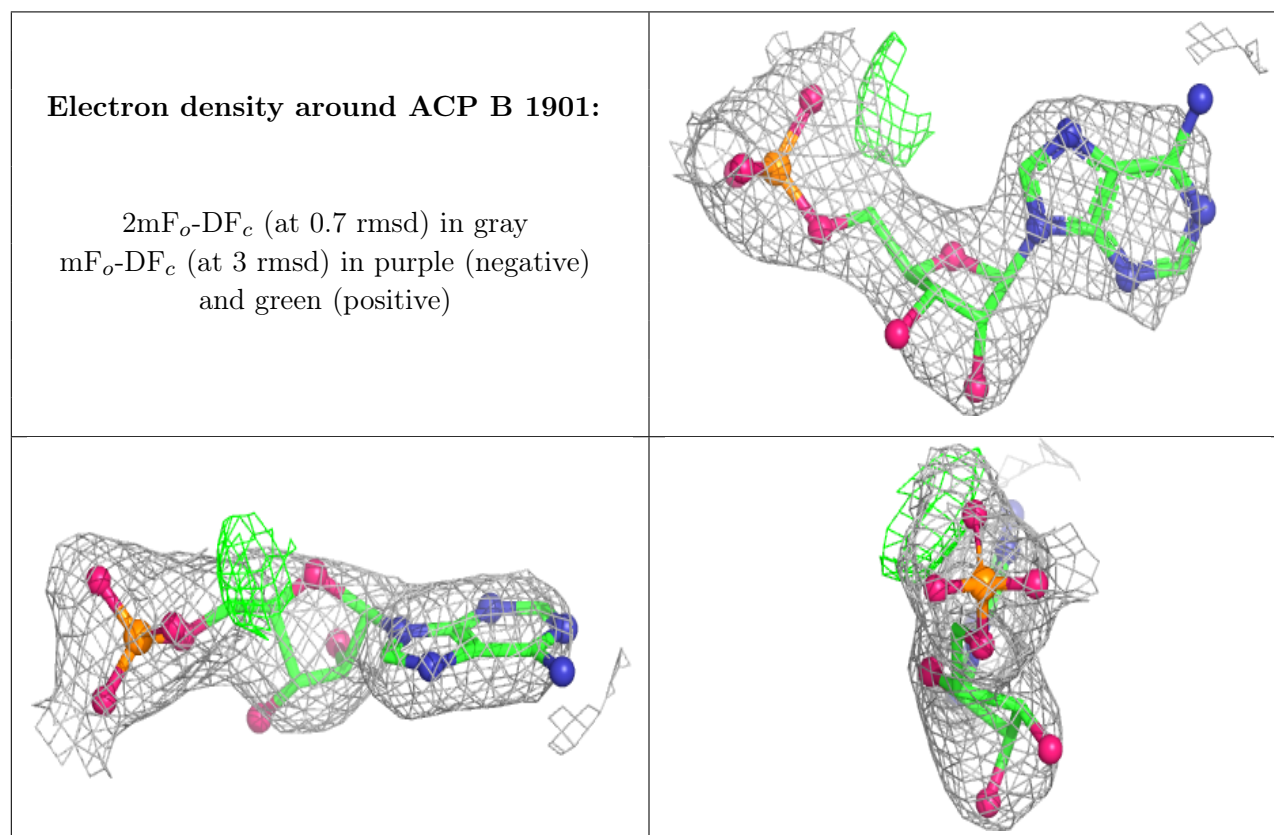
There are no monosaccharides in this entry.

## 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.

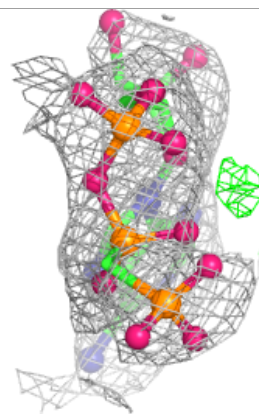
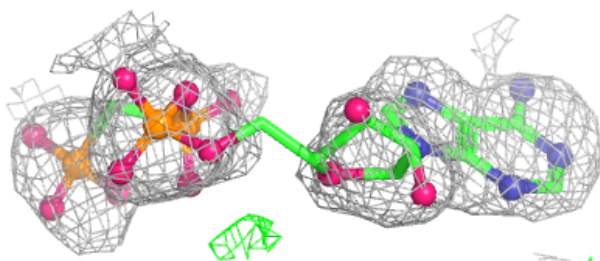
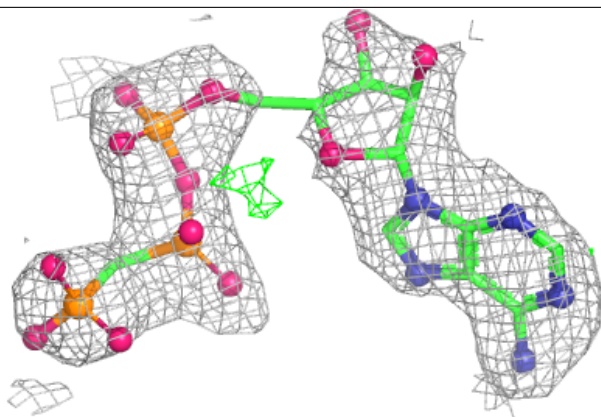
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACP	B	1901	23/31	0.85	0.27	49,80,91,93	0
2	ACP	A	1901	31/31	0.94	0.24	50,74,96,107	31
3	NAP	A	1902	48/48	0.98	0.13	25,39,51,57	0
3	NAP	B	1902	48/48	0.98	0.13	22,37,47,49	0

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.

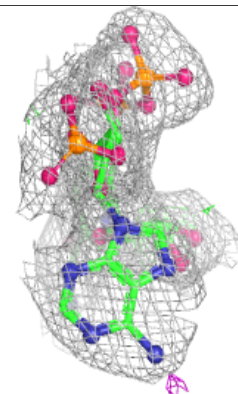
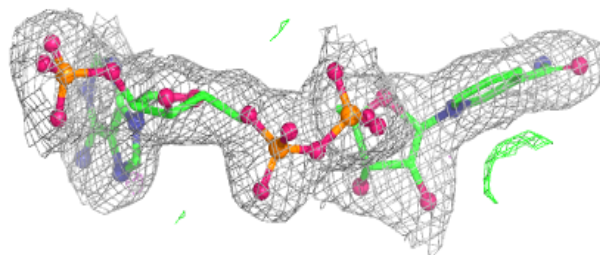
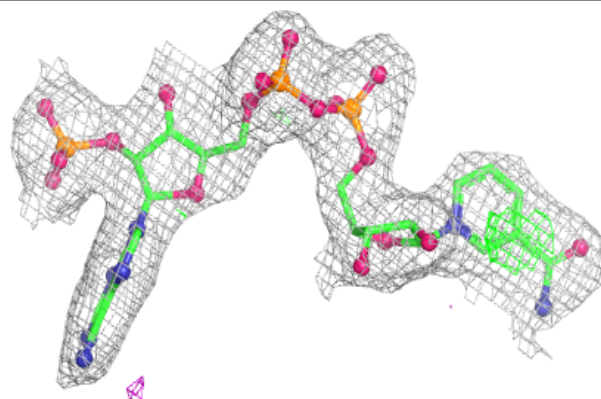


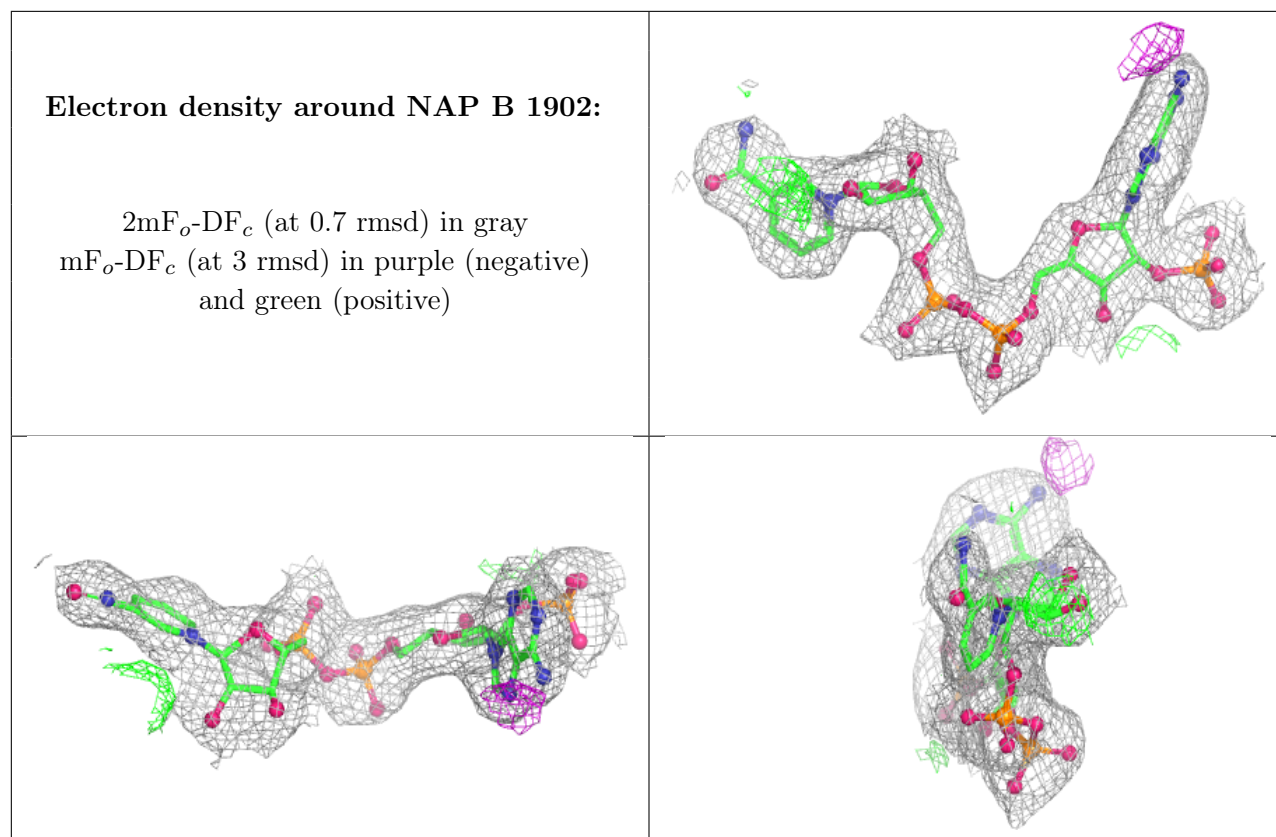
**Electron density around ACP A 1901:**

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

**Electron density around NAP A 1902:**

$2mF_o-DF_c$  (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.