



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 AM UTC

PDB ID : 6EQO / pdb_00006eqo
Title : Tri-functional propionyl-CoA synthase of Erythrobacter sp. NAP1 with bound NADP⁺ 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

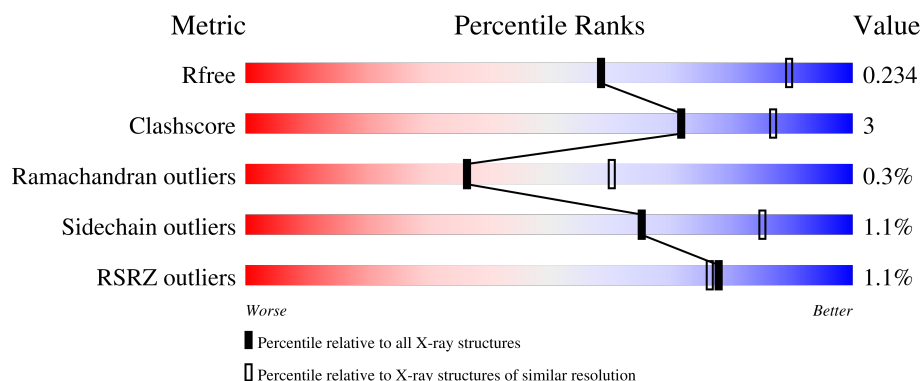
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	% 89% 8% .
1	B	1850	% 90% 7% .

2 Entry composition [i](#)

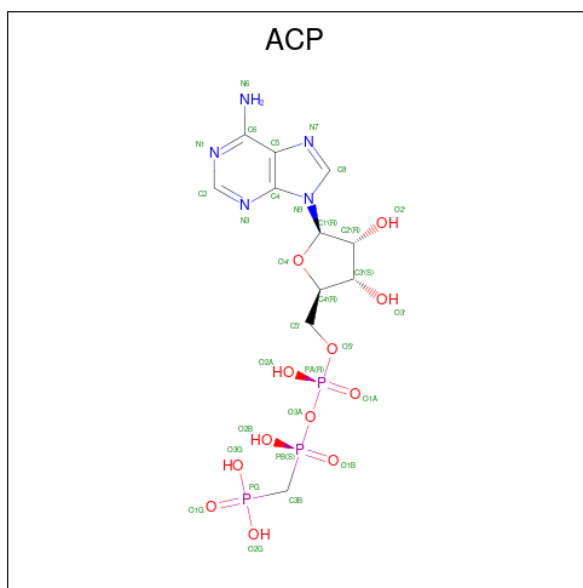
There are 4 unique types of molecules in this entry. The entry contains 28218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



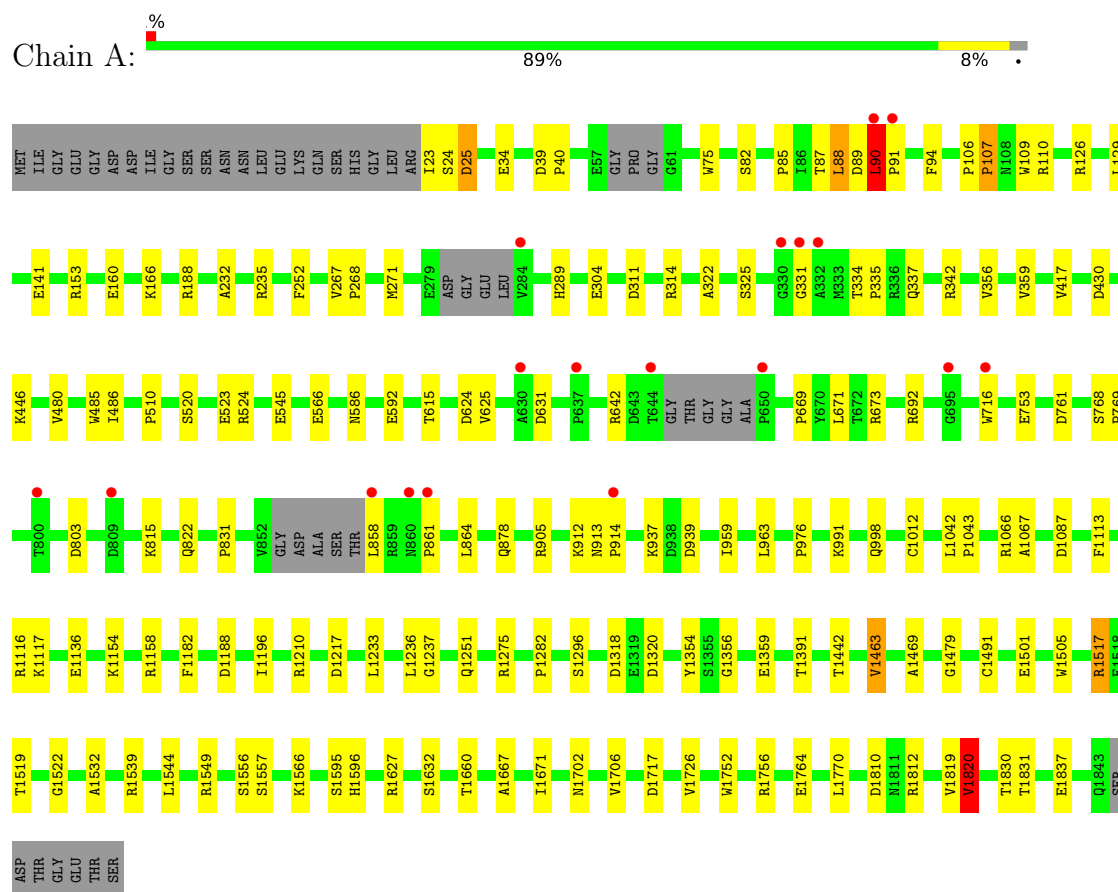
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

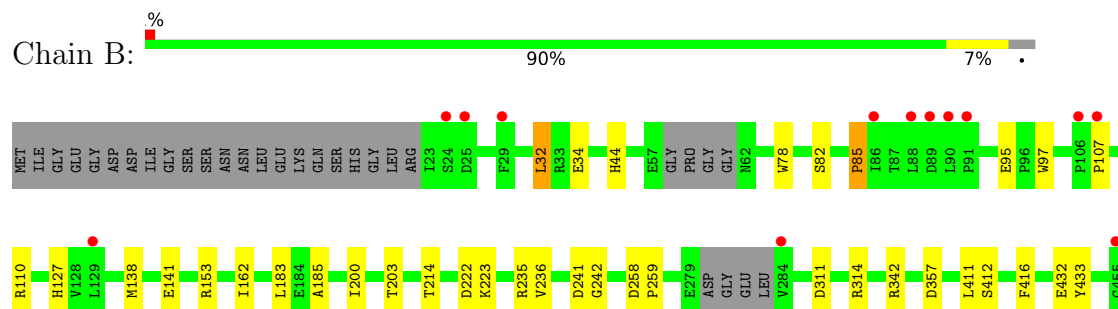
3 Residue-property plots

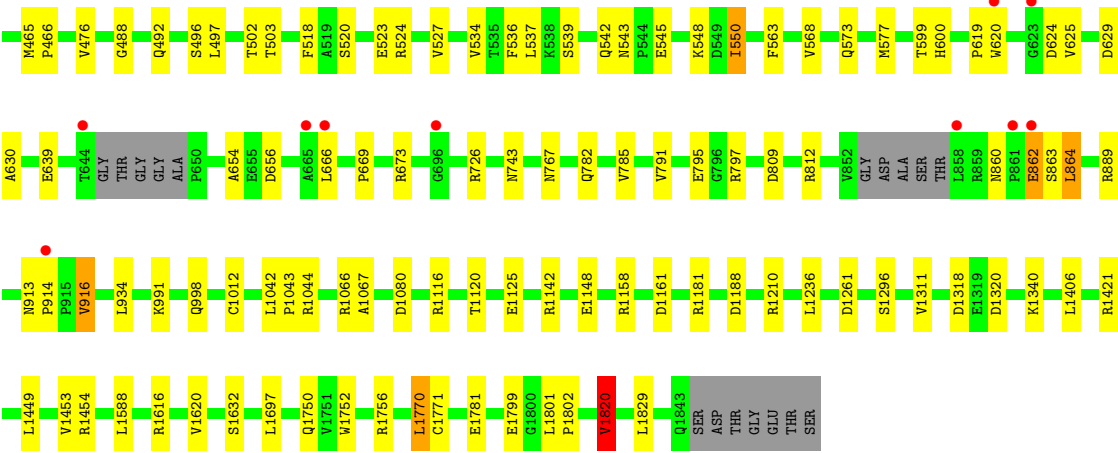
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.229 0.199 , 0.234	Depositor DCC
R_{free} test set	2009 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.34	6/14138 (0.0%)	0.46	9/19223 (0.0%)
1	B	0.32	5/14134 (0.0%)	0.43	7/19218 (0.0%)
All	All	0.33	11/28272 (0.0%)	0.45	16/38441 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LEU	CA-C	-7.31	1.47	1.53
1	A	90	LEU	C-O	-7.05	1.20	1.23
1	A	913	ASN	C-O	-6.78	1.18	1.25
1	B	913	ASN	C-O	-6.67	1.19	1.25
1	A	1819	VAL	C-O	-6.55	1.17	1.24
1	B	914	PRO	CA-C	-6.15	1.46	1.52
1	B	1820	VAL	C-O	-5.88	1.17	1.24
1	A	359	VAL	C-O	-5.71	1.18	1.24
1	A	1820	VAL	C-O	-5.66	1.17	1.24
1	B	791	VAL	C-O	-5.38	1.18	1.24
1	B	1311	VAL	C-O	-5.37	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	914	PRO	N-CA-C	15.16	129.19	110.70
1	B	862	GLU	N-CA-C	12.85	128.59	108.67
1	B	914	PRO	N-CA-C	12.43	125.86	110.70
1	A	914	PRO	CA-C-O	-9.69	106.52	120.56
1	A	914	PRO	CA-C-N	-9.33	109.27	118.97
1	A	914	PRO	C-N-CA	-9.33	109.27	118.97
1	A	90	LEU	CA-C-N	-9.17	109.43	118.97
1	A	90	LEU	C-N-CA	-9.17	109.43	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	PRO	N-CA-C	8.19	125.18	113.47
1	B	914	PRO	CA-C-O	-8.05	108.88	120.56
1	B	914	PRO	CA-C-N	-7.18	111.50	118.97
1	B	914	PRO	C-N-CA	-7.18	111.50	118.97
1	B	913	ASN	N-CA-C	-5.82	96.72	109.11
1	A	912	LYS	N-CA-C	5.76	116.82	107.32
1	A	91	PRO	CA-C-O	-5.62	111.88	120.03
1	B	863	SER	N-CA-C	5.03	119.10	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13820	0	13424	92	0
1	B	13816	0	13421	87	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	7	0
4	B	231	0	0	4	0
All	All	28218	0	26918	178	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 (178) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:32:LEU:HD13	1:B:32:LEU:C	2.21	0.65
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1154:LYS:NZ	4:A:2026:HOH:O	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:545:GLU:OE1	1:A:937:LYS:NZ	2.31	0.48
1:B:32:LEU:C	1:B:32:LEU:CD1	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1660:THR:OG1	1:A:1717:ASP:OD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:573:GLN:HG2	1:B:577:MET:HE2	1.99	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:753:GLU:OE1	1:A:815:LYS:NZ	2.50	0.42
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:334:THR:O	1:A:335:PRO:C	2.63	0.42
1:A:23:ILE:O	1:A:24:SER:OG	2.38	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
1:A:976:PRO:HG3	1:A:1182:PHE:HD2	1.85	0.41
1:A:39:ASP:O	1:A:40:PRO:C	2.62	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:B:127:HIS:NE2	1:B:497:LEU:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	60
1	B	1793/1850 (97%)	1703 (95%)	86 (5%)	4 (0%)	43	68
All	All	3587/3700 (97%)	3405 (95%)	173 (5%)	9 (0%)	36	60

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

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Mol	Chain	Res	Type
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%)	65	85
1	B	1416/1448 (98%)	1402 (99%)	14 (1%)	68	86
All	All	2832/2896 (98%)	2802 (99%)	30 (1%)	65	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	34	GLU
1	A	88	LEU
1	A	90	LEU
1	A	252	PHE
1	A	566	GLU
1	A	631	ASP
1	A	858	LEU
1	A	864	LEU
1	A	998	GLN
1	A	1463	VAL
1	A	1517	ARG
1	A	1557	SER
1	A	1752	TRP
1	A	1770	LEU
1	A	1820	VAL
1	B	32	LEU
1	B	550	ILE
1	B	785	VAL
1	B	862	GLU
1	B	864	LEU
1	B	916	VAL

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Mol	Chain	Res	Type
1	B	998	GLN
1	B	1080	ASP
1	B	1236	LEU
1	B	1752	TRP
1	B	1770	LEU
1	B	1781	GLU
1	B	1799	GLU
1	B	1820	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	ASN
1	A	579	HIS
1	A	681	ASN
1	A	686	HIS
1	A	1346	GLN
1	A	1580	ASN
1	B	192	ASN
1	B	199	GLN
1	B	546	ASN
1	B	747	HIS
1	B	1843	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 oligosaccharides 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$
3	NAP	B	1902	-	50,52,52	3.64	20 (40%)	71,80,80	1.83	17 (23%)
3	NAP	A	1902	-	50,52,52	3.70	18 (36%)	71,80,80	1.80	15 (21%)
2	ACP	B	1901	-	25,25,33	3.64	12 (48%)	37,38,52	2.12	10 (27%)
2	ACP	A	1901	-	31,33,33	3.50	14 (45%)	47,52,52	2.35	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	1902	-	-	4/35/67/67	0/5/5/5
3	NAP	A	1902	-	-	4/35/67/67	0/5/5/5
2	ACP	B	1901	-	-	3/10/26/38	0/3/3/3
2	ACP	A	1901	-	-	9/19/38/38	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1902	NAP	O4D-C1D	16.14	1.62	1.40
3	B	1902	NAP	O4D-C1D	15.16	1.60	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
3	A	1902	NAP	O4B-C1B	8.81	1.62	1.42
2	B	1901	ACP	O4'-C4'	-8.68	1.25	1.45
3	B	1902	NAP	O4B-C1B	8.45	1.61	1.42
2	A	1901	ACP	O4'-C4'	-8.40	1.26	1.45
3	A	1902	NAP	C2B-C1B	-8.33	1.32	1.53
3	B	1902	NAP	C2B-C1B	-8.23	1.32	1.53
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
3	A	1902	NAP	O4B-C4B	-6.60	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	ACP	O4'-C1'	6.48	1.57	1.42
2	A	1901	ACP	O4'-C1'	6.44	1.56	1.42
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	B	1901	ACP	C6-N6	5.03	1.47	1.34
2	A	1901	ACP	C1'-N9	-4.86	1.32	1.46
2	A	1901	ACP	PB-O2B	-4.76	1.44	1.56
2	B	1901	ACP	C1'-N9	-4.61	1.33	1.46
3	A	1902	NAP	C6A-N6A	4.54	1.45	1.34
2	A	1901	ACP	PG-O3G	-4.48	1.44	1.55
2	A	1901	ACP	C8-N9	-4.46	1.30	1.37
2	B	1901	ACP	C3'-C4'	4.40	1.64	1.53
2	A	1901	ACP	C6-N6	4.36	1.45	1.34
3	B	1902	NAP	C6A-N6A	4.28	1.45	1.34
2	A	1901	ACP	C3'-C4'	4.23	1.63	1.53
2	B	1901	ACP	C8-N9	-3.99	1.30	1.37
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
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	P2B-O2B	3.24	1.65	1.59
3	A	1902	NAP	PA-O3	3.17	1.62	1.59
3	B	1902	NAP	C5A-C4A	-3.09	1.33	1.39
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	C5A-N7A	-2.94	1.33	1.39
3	A	1902	NAP	C5A-N7A	-2.94	1.33	1.39
3	B	1902	NAP	O3B-C3B	-2.88	1.35	1.43
3	A	1902	NAP	O3D-C3D	-2.85	1.35	1.43
2	B	1901	ACP	C5-N7	-2.85	1.33	1.39
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	C5A-C4A	-2.71	1.34	1.39
3	A	1902	NAP	O2D-C2D	2.69	1.49	1.43
3	A	1902	NAP	O3B-C3B	-2.63	1.36	1.43
2	A	1901	ACP	C6-N1	-2.57	1.28	1.35
2	B	1901	ACP	C2-N3	-2.55	1.29	1.33
3	B	1902	NAP	C8A-N9A	-2.49	1.33	1.37
3	B	1902	NAP	O2D-C2D	2.49	1.49	1.43
3	B	1902	NAP	C3N-C7N	2.45	1.54	1.50
2	B	1901	ACP	C5-C4	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	ACP	C6-N1	-2.25	1.29	1.35
2	A	1901	ACP	C5-C4	-2.20	1.35	1.39
3	B	1902	NAP	O2B-C2B	2.17	1.51	1.44
3	B	1902	NAP	O3D-C3D	-2.10	1.37	1.43
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	B	1901	ACP	C4-N9	-2.03	1.33	1.37
3	A	1902	NAP	C8A-N9A	-2.01	1.34	1.37

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1901	ACP	C5-C4-N3	-6.72	117.46	126.72
3	A	1902	NAP	N3A-C2A-N1A	-6.08	119.38	128.58
3	B	1902	NAP	C5A-C4A-N3A	-5.74	118.81	126.72
3	B	1902	NAP	N3A-C2A-N1A	-5.42	120.37	128.58
3	A	1902	NAP	C5A-C4A-N3A	-5.35	119.35	126.72
2	A	1901	ACP	C4-C5-N7	-5.29	104.54	110.58
2	B	1901	ACP	N3-C2-N1	-5.16	120.77	128.58
2	B	1901	ACP	C5-C4-N3	-4.71	120.22	126.72
2	B	1901	ACP	C4-C5-N7	-4.66	105.25	110.58
3	B	1902	NAP	N9A-C8A-N7A	-4.47	107.59	113.94
2	A	1901	ACP	C5-N7-C8	4.31	110.22	103.45
2	A	1901	ACP	C2-N3-C4	4.28	122.28	111.83
2	A	1901	ACP	N3-C2-N1	-4.23	122.18	128.58
2	A	1901	ACP	N3-C4-N9	4.08	134.10	127.17
3	A	1902	NAP	N9A-C8A-N7A	-3.88	108.44	113.94
2	B	1901	ACP	C2-N3-C4	3.78	121.06	111.83
3	B	1902	NAP	N3A-C4A-N9A	3.77	133.59	127.17
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
3	B	1902	NAP	C2A-N3A-C4A	3.64	120.71	111.83
3	A	1902	NAP	C2A-N3A-C4A	3.61	120.66	111.83
2	A	1901	ACP	O1G-PG-C3B	-3.56	103.60	111.37
2	A	1901	ACP	N9-C8-N7	-3.55	108.90	113.94
3	A	1902	NAP	C6N-N1N-C2N	-3.53	118.87	121.88
2	B	1901	ACP	C5-N7-C8	3.47	108.90	103.45
3	A	1902	NAP	N3A-C4A-N9A	3.37	132.90	127.17
3	B	1902	NAP	C4A-N9A-C1B	-3.32	118.86	126.63
3	B	1902	NAP	C5A-N7A-C8A	3.31	108.64	103.45
3	A	1902	NAP	C4A-N9A-C1B	-3.27	119.00	126.63
2	B	1901	ACP	C5-C4-N9	3.25	109.35	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	B	1901	ACP	C6-C5-N7	2.98	137.83	132.09
2	B	1901	ACP	N9-C8-N7	-2.93	109.78	113.94
3	A	1902	NAP	C1B-N9A-C8A	2.87	133.46	127.09
3	A	1902	NAP	C4D-O4D-C1D	-2.86	107.30	109.92
3	A	1902	NAP	C5A-N7A-C8A	2.80	107.86	103.45
2	A	1901	ACP	C6-C5-N7	2.61	137.13	132.09
3	B	1902	NAP	C1B-N9A-C8A	2.60	132.87	127.09
3	B	1902	NAP	N6A-C6A-N1A	-2.57	112.66	118.38
3	A	1902	NAP	C2N-C3N-C4N	2.49	121.15	118.26
3	B	1902	NAP	O4B-C1B-N9A	-2.47	103.34	108.09
3	B	1902	NAP	C6A-C5A-C4A	2.43	120.49	117.18
2	A	1901	ACP	C5-C4-N9	2.39	108.42	105.81
3	B	1902	NAP	C4A-N9A-C8A	2.38	108.24	105.74
3	A	1902	NAP	P2B-O2B-C2B	-2.38	117.08	123.43
3	B	1902	NAP	C4A-C5A-N7A	-2.33	107.92	110.58
3	A	1902	NAP	C6A-C5A-C4A	2.30	120.32	117.18
3	B	1902	NAP	C4B-O4B-C1B	-2.26	104.47	109.47
3	A	1902	NAP	N6A-C6A-N1A	-2.25	113.37	118.38
2	B	1901	ACP	O2'-C2'-C1'	-2.17	102.64	110.10
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
2	B	1901	ACP	O4'-C1'-C2'	-2.05	102.22	106.62
2	A	1901	ACP	C4-N9-C8	2.05	107.89	105.74
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

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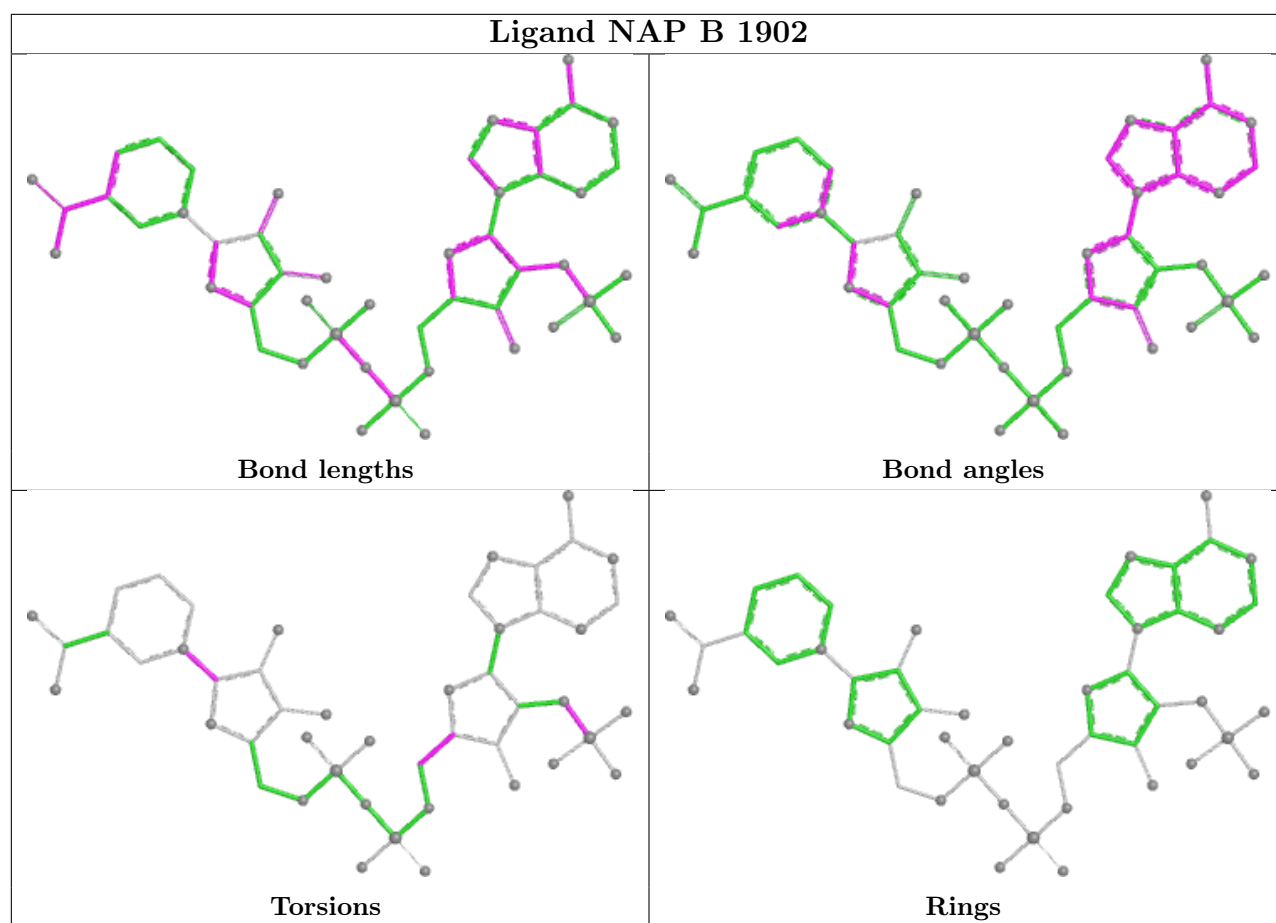
Mol	Chain	Res	Type	Atoms
2	A	1901	ACP	PB-O3A-PA-O1A
2	A	1901	ACP	C5'-O5'-PA-O1A
2	A	1901	ACP	C5'-O5'-PA-O2A
2	A	1901	ACP	C5'-O5'-PA-O3A
3	A	1902	NAP	O4D-C1D-N1N-C2N
3	B	1902	NAP	O4D-C1D-N1N-C2N
3	B	1902	NAP	C2B-O2B-P2B-O1X
2	A	1901	ACP	PB-O3A-PA-O2A
3	A	1902	NAP	O4B-C4B-C5B-O5B
3	B	1902	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

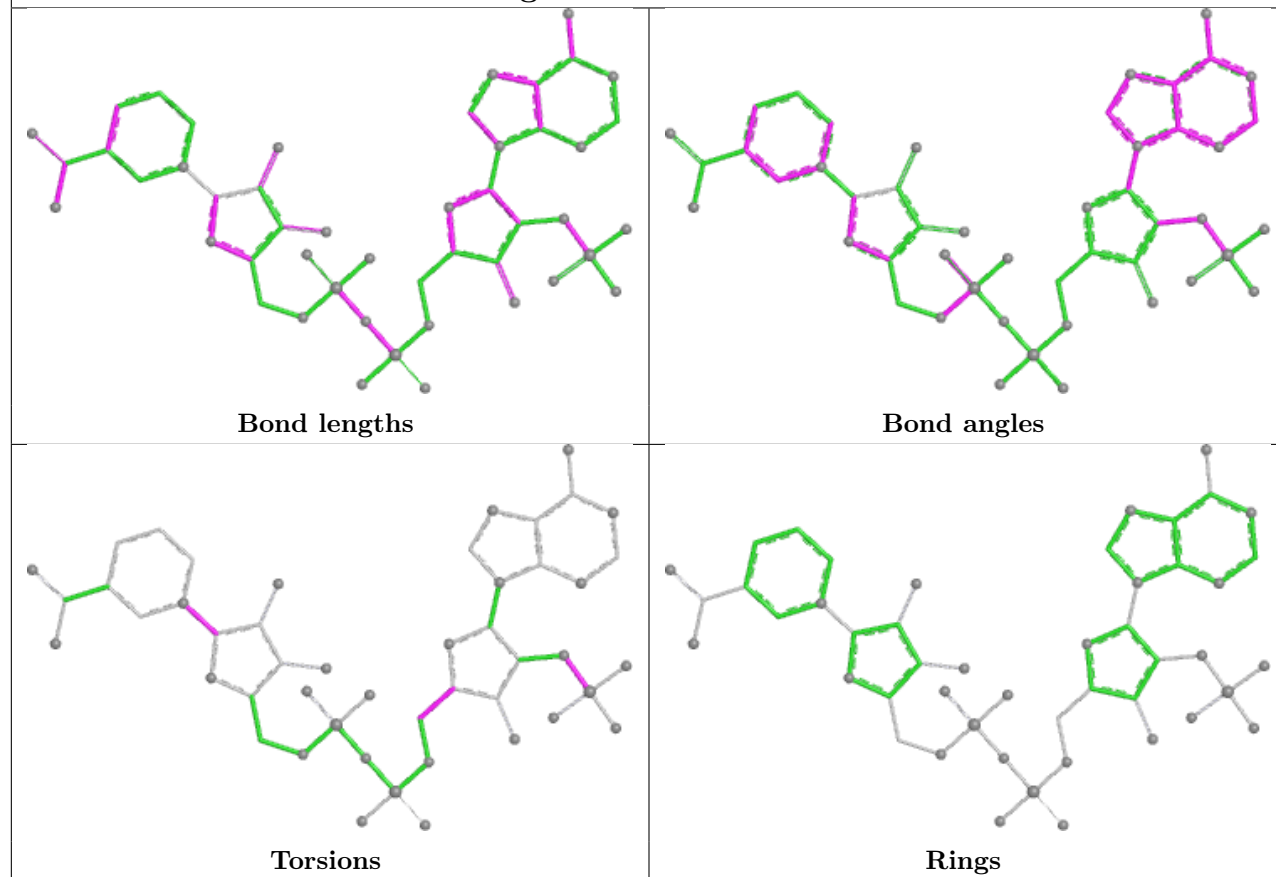
3 monomers are involved in 5 short contacts:

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

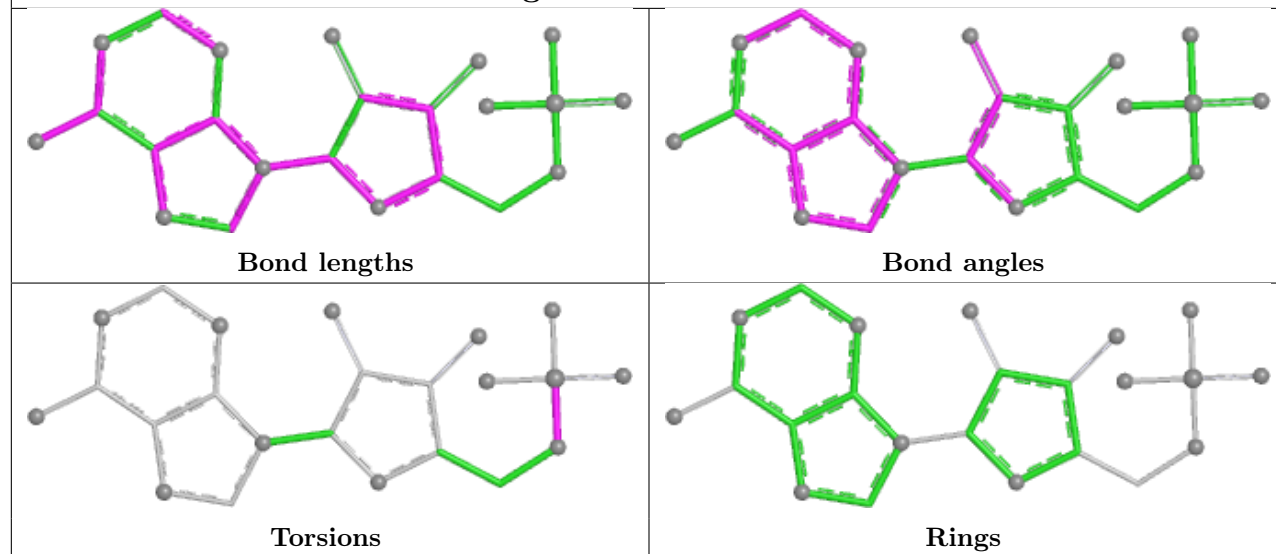
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

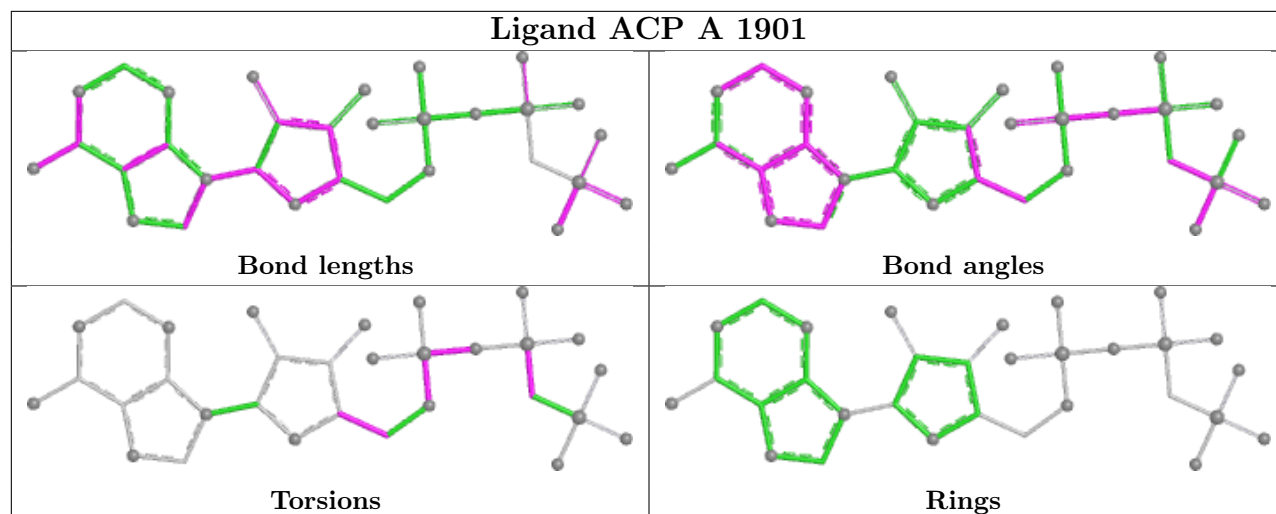


Ligand NAP A 1902



Ligand ACP B 1901





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1804/1850 (97%)	-0.38	18 (0%) 79 78	21, 46, 80, 125	0
1	B	1803/1850 (97%)	-0.27	23 (1%) 75 73	23, 50, 94, 152	0
All	All	3607/3700 (97%)	-0.33	41 (1%) 78 76	21, 48, 90, 152	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	696	GLY	3.7
1	A	861	PRO	3.4
1	A	284	VAL	3.3
1	A	858	LEU	3.3
1	A	637	PRO	3.1
1	B	106	PRO	2.9
1	B	858	LEU	2.9
1	A	800	THR	2.9
1	B	666	LEU	2.9
1	B	862	GLU	2.8
1	A	650	PRO	2.8
1	A	331	GLY	2.8
1	A	330	GLY	2.7
1	A	860	ASN	2.6
1	B	644	THR	2.5
1	B	623	GLY	2.5
1	B	665	ALA	2.5
1	A	630	ALA	2.4
1	A	716	TRP	2.4
1	B	914	PRO	2.4
1	A	90	LEU	2.3
1	A	644	THR	2.3
1	B	24	SER	2.3
1	B	29	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	86	ILE	2.3
1	B	91	PRO	2.3
1	B	107	PRO	2.3
1	B	861	PRO	2.2
1	B	90	LEU	2.2
1	A	914	PRO	2.2
1	A	91	PRO	2.2
1	A	695	GLY	2.2
1	B	25	ASP	2.2
1	B	455	GLY	2.1
1	B	284	VAL	2.1
1	B	129	LEU	2.1
1	A	809	ASP	2.1
1	B	89	ASP	2.0
1	A	332	ALA	2.0
1	B	620	TRP	2.0
1	B	88	LEU	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 oligosaccharides in this entry.

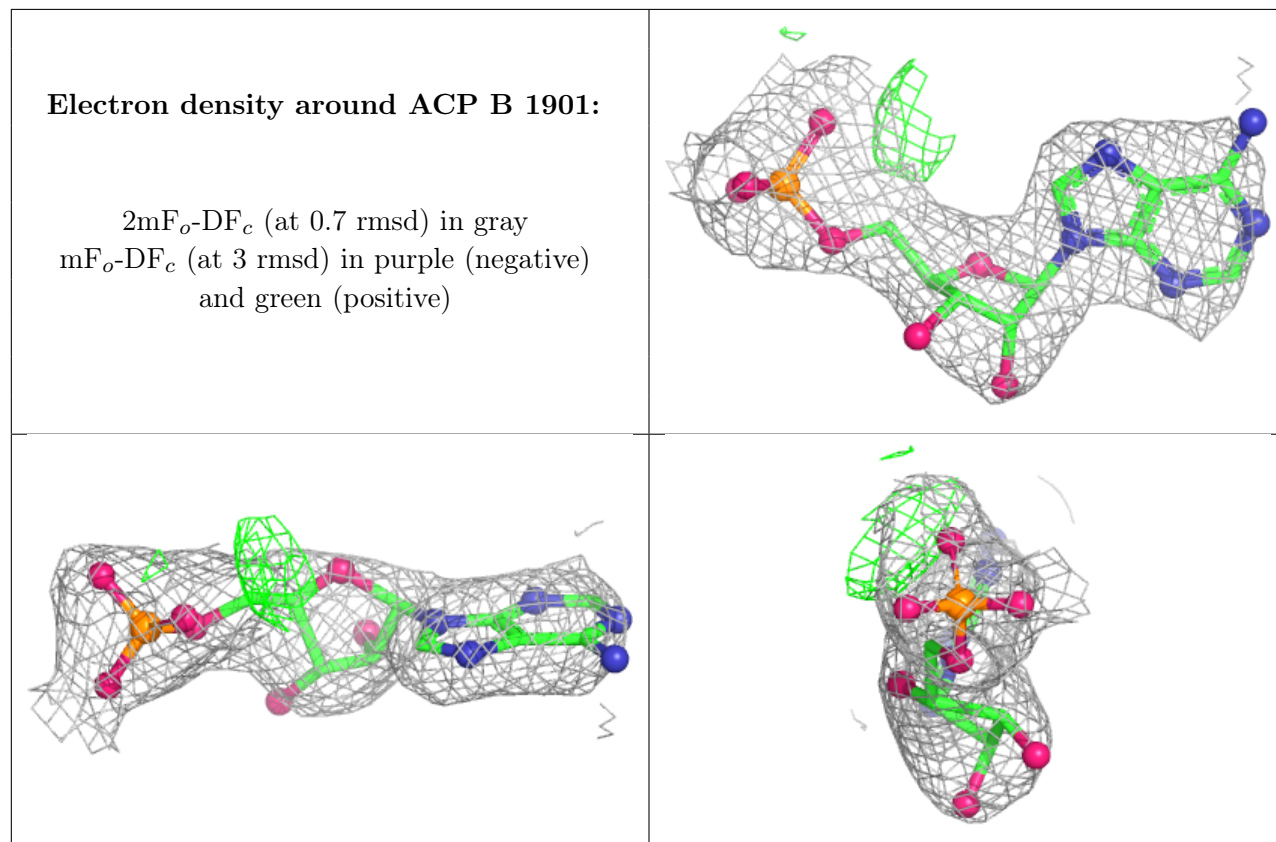
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACP	B	1901	23/31	0.89	0.11	49,80,91,93	0
2	ACP	A	1901	31/31	0.90	0.12	50,74,96,107	31
3	NAP	A	1902	48/48	0.97	0.06	25,39,51,57	0
3	NAP	B	1902	48/48	0.97	0.06	22,37,47,49	0

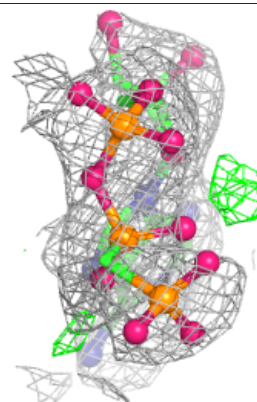
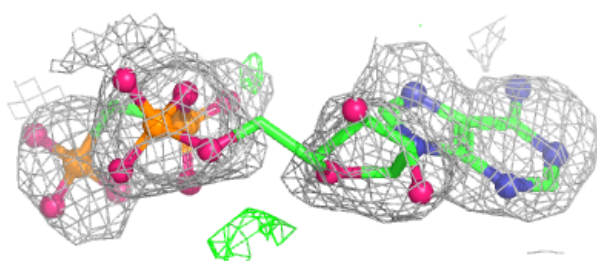
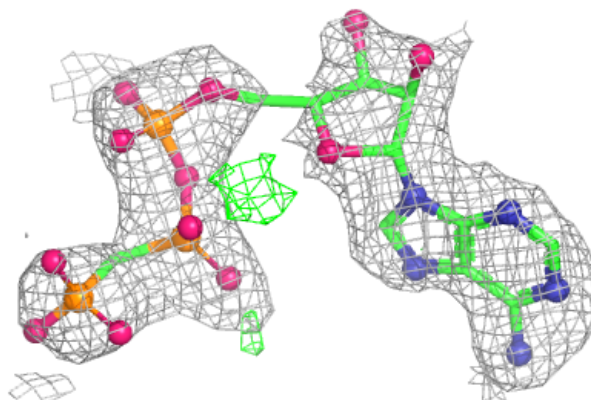
The following is a graphical depiction of the model fit to experimental electron density of all

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.

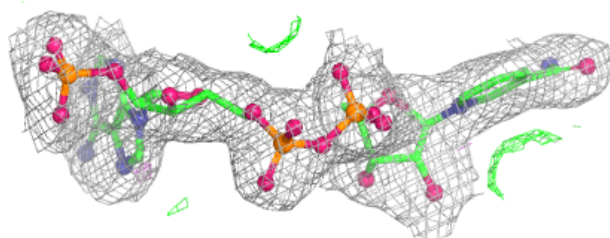
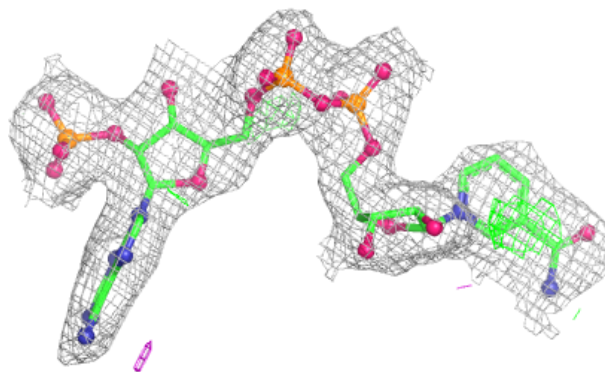


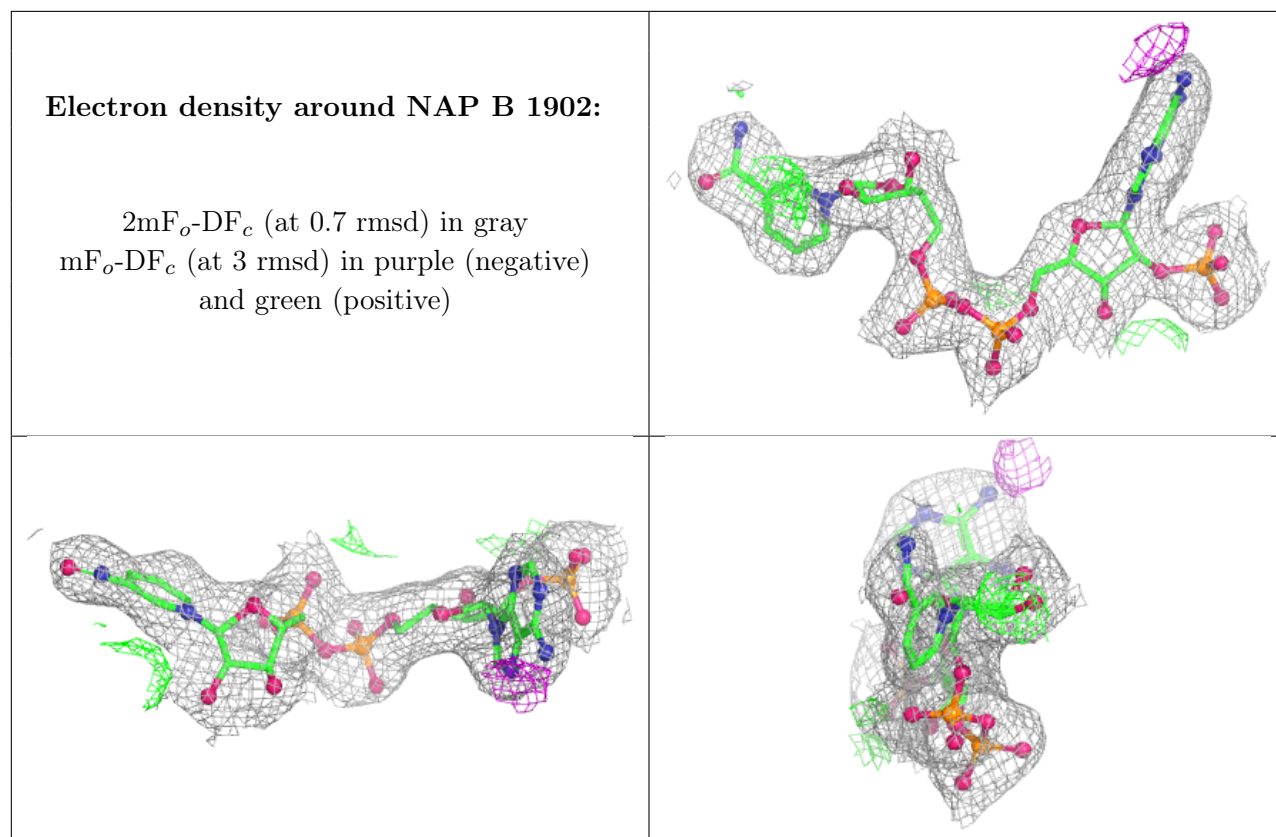
Electron density around ACP A 1901:

$2mF_o-DF_c$ (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.