



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 PM UTC

PDB ID : 6ZIB / pdb_00006zib
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE-1 (RPMFE1) COMPLEXED WITH ACETOACETYL-COA AND NADH
Authors : Wierenga, R.K.; Sridhar, S.; Kiema, T.R.
Deposited on : 2020-06-25
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

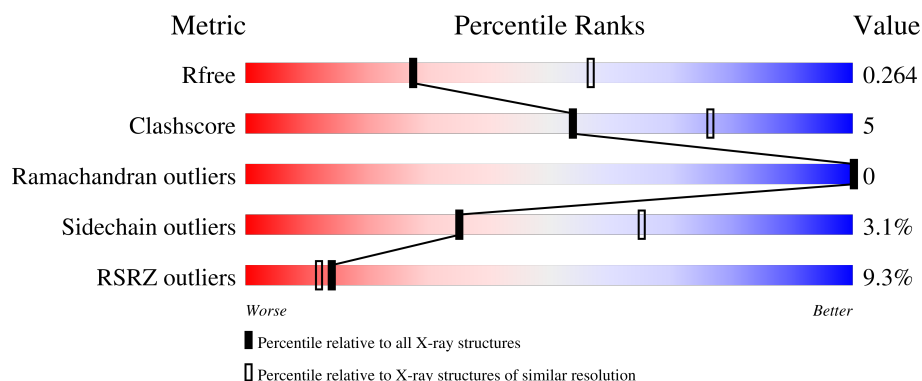
1 Overall quality at a glance

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	AAA	742	6% 84% 13% ..
1	BBB	742	12% 84% 13% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11379 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 Peroxisomal bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	723	Total	C	N	O	S	0	5	0
			5583	3567	982	1011	23			
1	BBB	719	Total	C	N	O	S	0	0	0
			5523	3531	967	1002	23			

There are 40 discrepancies between the modelled and reference sequences:

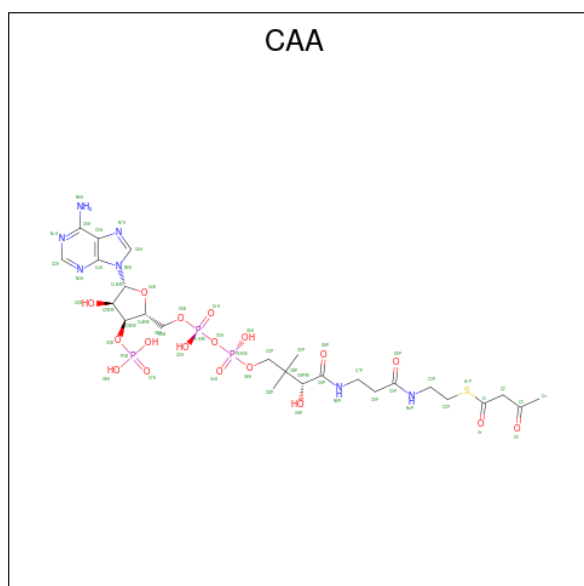
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP P07896
AAA	-18	GLY	-	expression tag	UNP P07896
AAA	-17	SER	-	expression tag	UNP P07896
AAA	-16	SER	-	expression tag	UNP P07896
AAA	-15	HIS	-	expression tag	UNP P07896
AAA	-14	HIS	-	expression tag	UNP P07896
AAA	-13	HIS	-	expression tag	UNP P07896
AAA	-12	HIS	-	expression tag	UNP P07896
AAA	-11	HIS	-	expression tag	UNP P07896
AAA	-10	HIS	-	expression tag	UNP P07896
AAA	-9	SER	-	expression tag	UNP P07896
AAA	-8	SER	-	expression tag	UNP P07896
AAA	-7	GLY	-	expression tag	UNP P07896
AAA	-6	LEU	-	expression tag	UNP P07896
AAA	-5	VAL	-	expression tag	UNP P07896
AAA	-4	PRO	-	expression tag	UNP P07896
AAA	-3	ARG	-	expression tag	UNP P07896
AAA	-2	GLY	-	expression tag	UNP P07896
AAA	-1	SER	-	expression tag	UNP P07896
AAA	0	HIS	-	expression tag	UNP P07896
BBB	-19	MET	-	initiating methionine	UNP P07896
BBB	-18	GLY	-	expression tag	UNP P07896
BBB	-17	SER	-	expression tag	UNP P07896
BBB	-16	SER	-	expression tag	UNP P07896
BBB	-15	HIS	-	expression tag	UNP P07896

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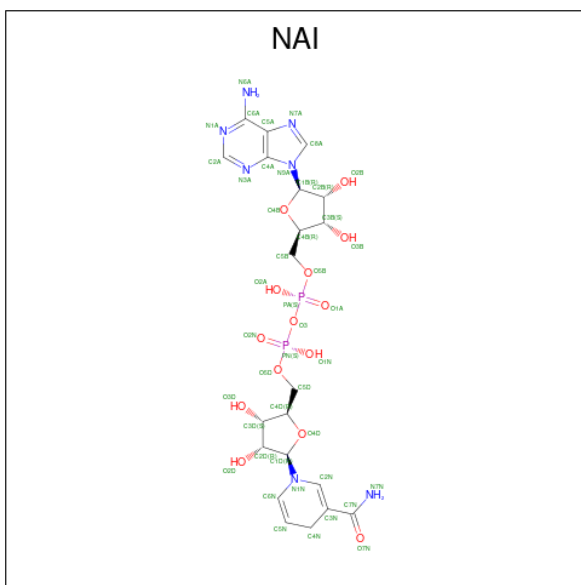
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-14	HIS	-	expression tag	UNP P07896
BBB	-13	HIS	-	expression tag	UNP P07896
BBB	-12	HIS	-	expression tag	UNP P07896
BBB	-11	HIS	-	expression tag	UNP P07896
BBB	-10	HIS	-	expression tag	UNP P07896
BBB	-9	SER	-	expression tag	UNP P07896
BBB	-8	SER	-	expression tag	UNP P07896
BBB	-7	GLY	-	expression tag	UNP P07896
BBB	-6	LEU	-	expression tag	UNP P07896
BBB	-5	VAL	-	expression tag	UNP P07896
BBB	-4	PRO	-	expression tag	UNP P07896
BBB	-3	ARG	-	expression tag	UNP P07896
BBB	-2	GLY	-	expression tag	UNP P07896
BBB	-1	SER	-	expression tag	UNP P07896
BBB	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



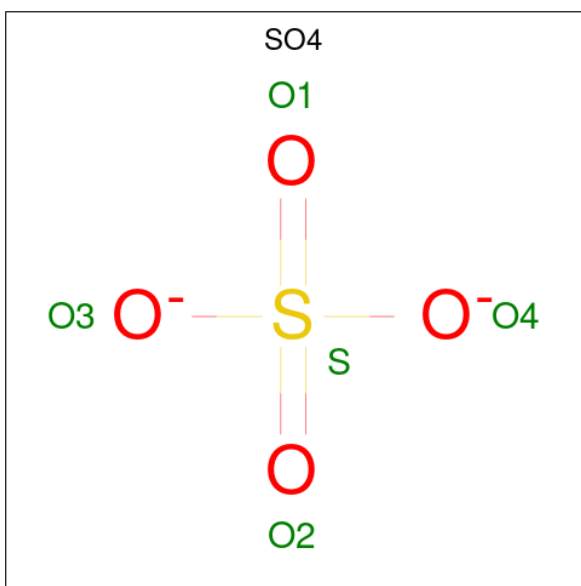
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	BBB	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	BBB	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total 5	O 4	S 1	0	0
4	BBB	1	Total 5	O 4	S 1	0	0

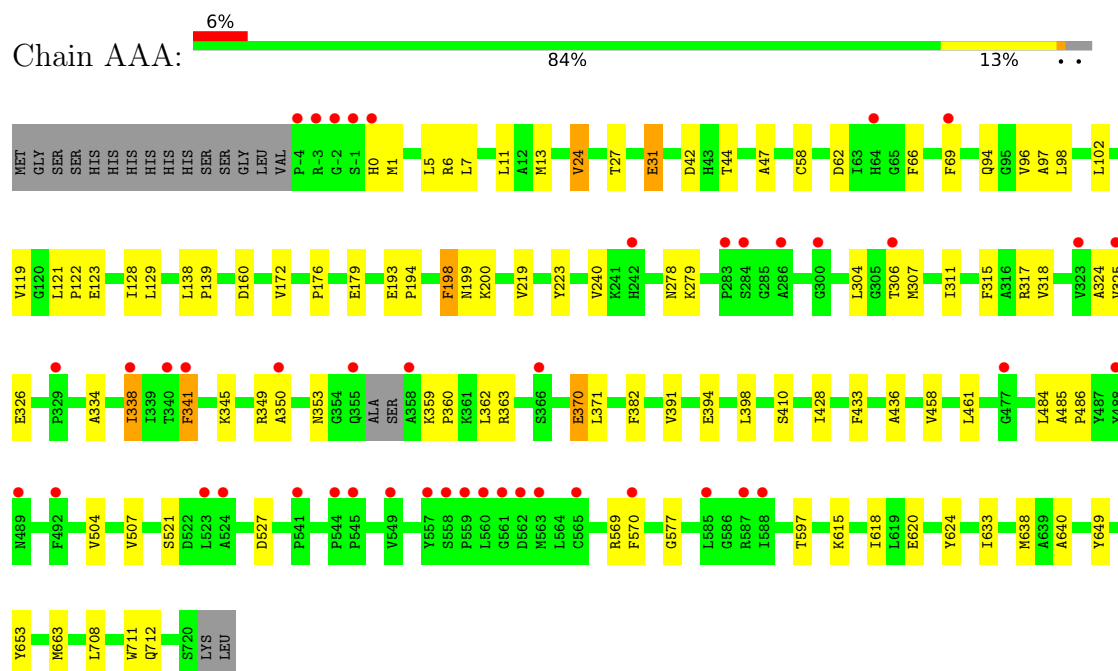
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	48	Total 48	O 48	0	0
5	BBB	19	Total 19	O 19	0	0

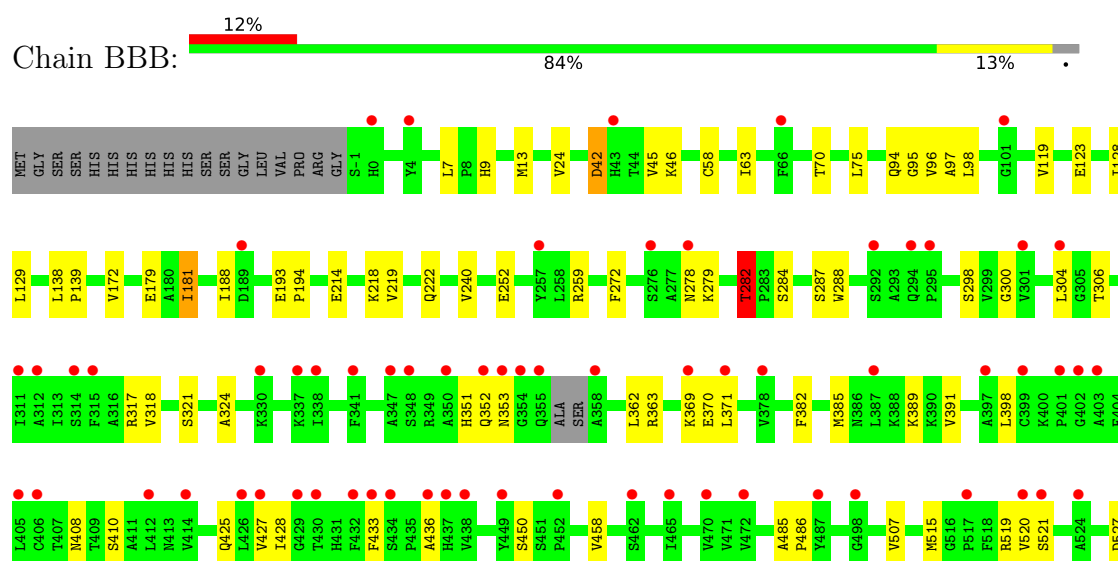
3 Residue-property plots [i](#)

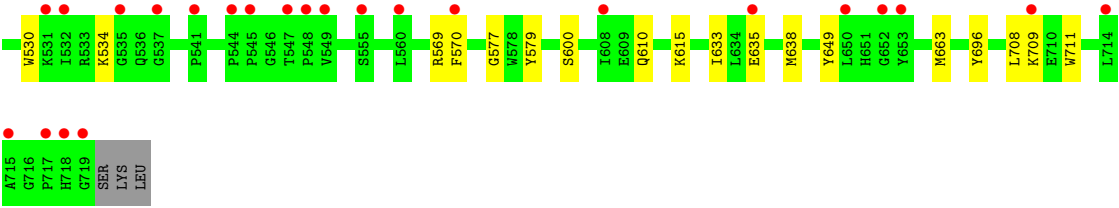
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Peroxisomal bifunctional enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.94Å 127.39Å 228.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.70 48.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (48.88-2.70) 94.6 (48.88-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.232 , 0.273 (Not available) , 0.264	Depositor DCC
R_{free} test set	2555 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11379	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: SO4, NAI, CAA

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	AAA	0.50	0/5726	0.99	4/7753 (0.1%)
1	BBB	0.48	0/5650	0.98	4/7653 (0.1%)
All	All	0.49	0/11376	0.98	8/15406 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	649	TYR	CB-CA-C	5.70	120.54	110.85
1	AAA	341	PHE	CA-CB-CG	5.67	119.47	113.80
1	BBB	282	THR	CB-CA-C	5.52	117.13	108.63
1	AAA	66	PHE	CA-CB-CG	5.40	119.20	113.80
1	BBB	649	TYR	CB-CA-C	5.33	119.90	110.85
1	BBB	353	ASN	CB-CA-C	5.29	119.67	110.94
1	AAA	31	GLU	CB-CG-CD	5.15	121.35	112.60
1	BBB	9	HIS	CB-CA-C	5.02	118.58	111.86

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	AAA	5583	0	5700	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	5523	0	5628	48	0
2	AAA	54	0	36	3	0
2	BBB	54	0	36	1	0
3	AAA	44	0	27	3	0
3	BBB	44	0	27	1	0
4	AAA	5	0	0	0	0
4	BBB	5	0	0	0	0
5	AAA	48	0	0	0	0
5	BBB	19	0	0	0	0
All	All	11379	0	11454	111	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 5.

All (111) 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:AAA:96:VAL:HG21	2:AAA:901:CAA:H133	1.51	0.93
1:BBB:172:VAL:HG11	1:BBB:179:GLU:HG3	1.54	0.90
1:AAA:325:VAL:HG21	1:AAA:371:LEU:HD11	1.60	0.82
1:AAA:6:ARG:HH12	1:AAA:44:THR:CG2	1.94	0.81
1:AAA:6:ARG:HH12	1:AAA:44:THR:HG22	1.48	0.79
1:BBB:369:LYS:HG2	1:BBB:398:LEU:HD22	1.66	0.77
1:BBB:663:MET:HA	1:BBB:663:MET:HE2	1.72	0.71
1:AAA:325:VAL:CG2	1:AAA:371:LEU:HD11	2.22	0.70
1:AAA:663:MET:HA	1:AAA:663:MET:HE2	1.71	0.70
1:AAA:96:VAL:HG13	1:AAA:98:LEU:HG	1.76	0.67
1:BBB:96:VAL:HG13	1:BBB:98:LEU:HG	1.77	0.67
1:AAA:507:VAL:HG21	1:AAA:618:ILE:CG2	2.28	0.64
1:BBB:70:THR:O	1:BBB:259:ARG:NH2	2.20	0.64
1:AAA:325:VAL:HG21	1:AAA:371:LEU:CD1	2.30	0.62
1:AAA:507:VAL:HG21	1:AAA:618:ILE:HG21	1.83	0.61
1:AAA:198:PHE:HD1	1:AAA:199:ASN:N	1.99	0.60
1:BBB:7:LEU:HD13	1:BBB:181:ILE:HD11	1.81	0.60
1:BBB:94:GLN:HE21	1:BBB:95:GLY:H	1.48	0.60
1:AAA:97:ALA:HB3	1:AAA:119:VAL:HG12	1.83	0.60
1:AAA:6:ARG:NH2	1:AAA:42:ASP:OD2	2.35	0.60
1:BBB:24:VAL:HG11	1:BBB:75:LEU:HD13	1.83	0.60
1:BBB:97:ALA:HB3	1:BBB:119:VAL:HG12	1.84	0.59
1:BBB:385:MET:HG3	1:BBB:389:LYS:HE2	1.83	0.59
1:AAA:307:MET:HG2	3:AAA:902:NAI:O2N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:597:THR:HB	1:BBB:382:PHE:HZ	1.68	0.57
1:AAA:42:ASP:OD1	1:AAA:44:THR:HB	2.04	0.57
1:AAA:597:THR:HB	1:BBB:382:PHE:CZ	2.41	0.55
1:BBB:485:ALA:HB3	1:BBB:486:PRO:HD3	1.90	0.54
1:AAA:485:ALA:HB3	1:AAA:486:PRO:HD3	1.90	0.54
1:AAA:315:PHE:HE2	1:AAA:461:LEU:HD21	1.73	0.53
1:AAA:11:LEU:HD22	1:AAA:47:ALA:HB3	1.89	0.53
1:AAA:7:LEU:HD11	1:AAA:13:MET:HE3	1.89	0.53
1:AAA:311:ILE:O	1:AAA:315:PHE:HD1	1.91	0.52
1:BBB:129:LEU:HD12	1:BBB:129:LEU:C	2.34	0.52
1:AAA:129:LEU:C	1:AAA:129:LEU:HD12	2.36	0.51
1:BBB:218:LYS:HE3	1:BBB:222:GLN:NE2	2.25	0.51
1:AAA:6:ARG:HH12	1:AAA:44:THR:HG21	1.71	0.51
1:BBB:507:VAL:HG22	1:BBB:615:LYS:HG3	1.93	0.51
1:AAA:326:GLU:OE1	3:AAA:902:NAI:H1B	2.11	0.51
1:BBB:7:LEU:HD11	1:BBB:13:MET:HE3	1.91	0.50
1:AAA:428:ILE:HG21	1:AAA:458:VAL:HG21	1.94	0.50
1:BBB:428:ILE:HG21	1:BBB:458:VAL:HG21	1.93	0.49
1:AAA:27:THR:O	1:AAA:31:GLU:HG3	2.12	0.49
1:BBB:63:ILE:HG22	1:BBB:272:PHE:CE2	2.48	0.48
1:BBB:530:TRP:CE2	1:BBB:534:LYS:HE3	2.48	0.48
1:BBB:300:GLY:HA3	1:BBB:371:LEU:HD22	1.95	0.48
1:AAA:172:VAL:HG11	1:AAA:179:GLU:HG2	1.95	0.48
1:AAA:382:PHE:CD2	3:AAA:902:NAI:H8A	2.49	0.48
1:BBB:279:LYS:HD2	1:BBB:288:TRP:CZ2	2.48	0.48
1:BBB:708:LEU:HA	1:BBB:711:TRP:CE2	2.48	0.47
1:BBB:304:LEU:HD11	1:BBB:324:ALA:HB1	1.94	0.47
1:AAA:6:ARG:NH1	1:AAA:44:THR:HG22	2.24	0.47
1:AAA:193:GLU:HB3	1:AAA:194:PRO:HD3	1.96	0.47
1:AAA:433:PHE:O	1:AAA:436:ALA:HA	2.15	0.47
1:BBB:427:VAL:O	1:BBB:450:SER:HB3	2.14	0.47
1:BBB:46:LYS:HB3	1:BBB:188:ILE:HD11	1.97	0.46
1:AAA:317:ARG:HG3	1:AAA:318:VAL:HG13	1.97	0.46
1:BBB:193:GLU:HB3	1:BBB:194:PRO:HD3	1.97	0.46
1:AAA:334:ALA:O	1:AAA:338:ILE:HG23	2.16	0.46
1:AAA:708:LEU:HA	1:AAA:711:TRP:CE2	2.51	0.46
1:BBB:279:LYS:HD2	1:BBB:288:TRP:CE2	2.51	0.46
1:AAA:24:VAL:HG12	1:AAA:58:CYS:SG	2.56	0.46
1:AAA:123:GLU:HB3	1:AAA:128:ILE:HG13	1.96	0.46
1:AAA:198:PHE:HE1	1:AAA:199:ASN:ND2	2.14	0.46
1:BBB:515:MET:HB3	1:BBB:520:VAL:HG23	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:425:GLN:HA	1:BBB:450:SER:HA	1.97	0.45
1:BBB:24:VAL:HG23	1:BBB:58:CYS:SG	2.56	0.45
1:BBB:363:ARG:HH21	1:BBB:370:GLU:HG3	1.82	0.45
1:AAA:172:VAL:CG1	1:AAA:179:GLU:HG2	2.48	0.44
1:BBB:282:THR:HG23	1:BBB:284:SER:H	1.83	0.44
1:BBB:569:ARG:HB3	1:BBB:577:GLY:HA2	2.00	0.44
1:AAA:507:VAL:HG12	1:AAA:615:LYS:HG3	1.99	0.44
1:AAA:304:LEU:HD11	1:AAA:324:ALA:HB1	1.99	0.43
1:BBB:433:PHE:O	1:BBB:436:ALA:HA	2.16	0.43
1:AAA:122:PRO:HG2	2:AAA:901:CAA:H32	1.99	0.43
1:BBB:63:ILE:HG22	1:BBB:272:PHE:HE2	1.83	0.43
1:BBB:633:ILE:HG23	1:BBB:638:MET:HB2	1.99	0.43
1:AAA:507:VAL:CG2	1:AAA:618:ILE:HG21	2.48	0.43
1:BBB:42:ASP:HB3	1:BBB:45:VAL:HG23	2.00	0.43
1:AAA:569:ARG:HB3	1:AAA:577:GLY:HA2	2.01	0.43
1:AAA:200:LYS:HB2	1:AAA:200:LYS:HE3	1.73	0.43
1:BBB:123:GLU:HB3	1:BBB:128:ILE:HG13	2.01	0.42
1:AAA:527:ASP:HB3	1:AAA:570:PHE:CD1	2.54	0.42
1:AAA:94[B]:GLN:HG3	1:AAA:176:PRO:HG2	2.01	0.42
1:AAA:345:LYS:O	1:AAA:349:ARG:HB2	2.20	0.42
1:BBB:635:GLU:HB3	1:BBB:696:TYR:HB2	2.02	0.42
1:AAA:484:LEU:HD22	1:AAA:653:TYR:CE2	2.54	0.42
1:AAA:484:LEU:HD22	1:AAA:653:TYR:HE2	1.85	0.41
1:AAA:198:PHE:CD1	1:AAA:198:PHE:C	2.98	0.41
1:BBB:96:VAL:HG21	2:BBB:801:CAA:H133	2.02	0.41
1:AAA:363:ARG:HH21	1:AAA:370:GLU:HG2	1.85	0.41
1:AAA:620:GLU:HG2	1:AAA:624:TYR:CE2	2.55	0.41
1:BBB:527:ASP:HB3	1:BBB:570:PHE:CD1	2.53	0.41
1:BBB:408:ASN:O	3:BBB:802:NAI:H1D	2.20	0.41
1:AAA:504:VAL:O	1:AAA:507:VAL:HG22	2.20	0.41
1:AAA:96:VAL:HG21	2:AAA:901:CAA:CDP	2.38	0.41
1:BBB:298:SER:HA	1:BBB:321:SER:O	2.21	0.41
1:AAA:278:ASN:HD21	1:AAA:279:LYS:HE3	1.85	0.41
1:AAA:350:ALA:HA	1:AAA:353:ASN:HB3	2.03	0.41
1:AAA:633:ILE:HG23	1:AAA:638:MET:HB2	2.03	0.41
1:AAA:640:ALA:O	1:AAA:712:GLN:NE2	2.54	0.41
1:AAA:102:LEU:HD23	1:AAA:121:LEU:HG	2.03	0.41
1:AAA:359:LYS:HA	1:AAA:360:PRO:HD3	1.95	0.40
1:BBB:138:LEU:N	1:BBB:139:PRO:CD	2.85	0.40
1:BBB:519:ARG:HG3	1:BBB:579:TYR:HE2	1.86	0.40
1:AAA:138:LEU:N	1:AAA:139:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:218:LYS:HE3	1:BBB:222:GLN:HE21	1.86	0.40
1:BBB:317:ARG:HG3	1:BBB:318:VAL:HG13	2.02	0.40
1:AAA:350:ALA:HA	1:AAA:353:ASN:CB	2.52	0.40
1:AAA:394:GLU:O	1:AAA:398:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	724/742 (98%)	687 (95%)	37 (5%)	0	100	100
1	BBB	715/742 (96%)	684 (96%)	31 (4%)	0	100	100
All	All	1439/1484 (97%)	1371 (95%)	68 (5%)	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	AAA	598/609 (98%)	580 (97%)	18 (3%)	36	66
1	BBB	590/609 (97%)	571 (97%)	19 (3%)	34	64
All	All	1188/1218 (98%)	1151 (97%)	37 (3%)	35	65

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	0	HIS
1	AAA	1	MET
1	AAA	5	LEU
1	AAA	24	VAL
1	AAA	69	PHE
1	AAA	160	ASP
1	AAA	198	PHE
1	AAA	219	VAL
1	AAA	223	TYR
1	AAA	240	VAL
1	AAA	306	THR
1	AAA	338	ILE
1	AAA	341	PHE
1	AAA	362	LEU
1	AAA	370	GLU
1	AAA	391	VAL
1	AAA	410	SER
1	AAA	521	SER
1	BBB	42	ASP
1	BBB	181	ILE
1	BBB	214	GLU
1	BBB	219	VAL
1	BBB	240	VAL
1	BBB	252	GLU
1	BBB	278	ASN
1	BBB	282	THR
1	BBB	287	SER
1	BBB	306	THR
1	BBB	351	HIS
1	BBB	352	GLN
1	BBB	362	LEU
1	BBB	391	VAL
1	BBB	410	SER
1	BBB	521	SER
1	BBB	600	SER
1	BBB	610	GLN
1	BBB	709	LYS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	CAA	AAA	901	-	53,56,56	0.52	0	77,83,83	0.81	2 (2%)
4	SO4	AAA	903	-	4,4,4	0.31	0	6,6,6	0.10	0
4	SO4	BBB	803	-	4,4,4	0.34	0	6,6,6	0.09	0
3	NAI	AAA	902	-	47,48,48	1.31	6 (12%)	64,73,73	1.57	11 (17%)
3	NAI	BBB	802	-	47,48,48	1.34	8 (17%)	64,73,73	1.61	12 (18%)
2	CAA	BBB	801	-	53,56,56	0.45	0	77,83,83	0.72	1 (1%)

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	NAI	BBB	802	-	-	5/29/72/72	0/5/5/5
2	CAA	AAA	901	-	-	8/55/71/71	0/3/3/3
2	CAA	BBB	801	-	-	16/55/71/71	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	AAA	902	-	-	12/29/72/72	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	902	NAI	C5A-C4A	4.78	1.47	1.39
3	BBB	802	NAI	C5A-C4A	4.77	1.47	1.39
3	BBB	802	NAI	C5A-C6A	2.89	1.49	1.41
3	BBB	802	NAI	PN-O3	2.69	1.62	1.59
3	AAA	902	NAI	C5A-C6A	2.65	1.48	1.41
3	BBB	802	NAI	PA-O3	2.57	1.62	1.59
3	BBB	802	NAI	C8A-N7A	2.43	1.36	1.31
3	AAA	902	NAI	PA-O3	2.41	1.62	1.59
3	AAA	902	NAI	C5A-N7A	-2.40	1.34	1.39
3	AAA	902	NAI	C8A-N7A	2.37	1.36	1.31
3	AAA	902	NAI	C6N-C5N	2.26	1.40	1.33
3	BBB	802	NAI	C5A-N7A	-2.19	1.35	1.39
3	BBB	802	NAI	C6N-C5N	2.15	1.39	1.33
3	BBB	802	NAI	C2N-C3N	2.02	1.40	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	802	NAI	C5A-C4A-N3A	-5.42	119.25	126.72
3	AAA	902	NAI	C5A-C4A-N3A	-5.40	119.28	126.72
2	AAA	901	CAA	P3B-O3B-C3B	-4.56	111.25	123.43
3	AAA	902	NAI	N3A-C4A-N9A	4.31	134.50	127.17
3	BBB	802	NAI	N3A-C4A-N9A	4.28	134.45	127.17
2	BBB	801	CAA	P3B-O3B-C3B	-3.95	112.88	123.43
3	BBB	802	NAI	C2A-N3A-C4A	3.80	121.11	111.83
3	BBB	802	NAI	N3A-C2A-N1A	-3.68	123.01	128.58
3	AAA	902	NAI	C2A-N3A-C4A	3.65	120.75	111.83
3	AAA	902	NAI	N3A-C2A-N1A	-3.52	123.25	128.58
3	BBB	802	NAI	C4A-C5A-N7A	-3.39	106.71	110.58
3	AAA	902	NAI	O4B-C1B-N9A	3.38	114.58	108.09
3	AAA	902	NAI	C4A-C5A-N7A	-3.10	107.03	110.58
3	BBB	802	NAI	O4B-C1B-N9A	2.79	113.45	108.09
3	BBB	802	NAI	C4A-N9A-C8A	2.74	108.62	105.74
3	AAA	902	NAI	C4A-N9A-C8A	2.49	108.35	105.74
3	BBB	802	NAI	C5A-N7A-C8A	2.48	107.34	103.45
3	BBB	802	NAI	C6A-C5A-N7A	2.41	136.73	132.09
3	BBB	802	NAI	O4D-C1D-N1N	2.36	112.58	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	901	CAA	C3B-C2B-C1B	2.31	104.98	99.89
3	AAA	902	NAI	C5A-N7A-C8A	2.28	107.04	103.45
3	AAA	902	NAI	C6A-C5A-N7A	2.10	136.14	132.09
3	BBB	802	NAI	C2A-N1A-C6A	2.09	122.16	118.73
3	BBB	802	NAI	N9A-C8A-N7A	-2.05	111.03	113.94
3	AAA	902	NAI	O3-PN-O2N	-2.01	104.66	110.70
3	AAA	902	NAI	C2A-N1A-C6A	2.00	122.02	118.73

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	901	CAA	C1-C2-C3-O3
2	AAA	901	CAA	C1-C2-C3-C4
2	BBB	801	CAA	C5B-O5B-P1A-O1A
2	BBB	801	CAA	C5B-O5B-P1A-O3A
2	BBB	801	CAA	CCP-O6A-P2A-O5A
2	BBB	801	CAA	C9P-CAP-CBP-CCP
2	BBB	801	CAA	C1-C2-C3-O3
2	BBB	801	CAA	C1-C2-C3-C4
3	AAA	902	NAI	C3B-C4B-C5B-O5B
3	AAA	902	NAI	C5D-O5D-PN-O3
3	AAA	902	NAI	C5D-O5D-PN-O1N
3	AAA	902	NAI	O4D-C4D-C5D-O5D
3	AAA	902	NAI	C3D-C4D-C5D-O5D
3	AAA	902	NAI	O4B-C4B-C5B-O5B
3	BBB	802	NAI	O4B-C4B-C5B-O5B
3	BBB	802	NAI	C3B-C4B-C5B-O5B
3	BBB	802	NAI	O4D-C4D-C5D-O5D
2	BBB	801	CAA	O5P-C5P-N4P-C3P
2	AAA	901	CAA	P2A-O3A-P1A-O1A
3	AAA	902	NAI	PA-O3-PN-O2N
3	BBB	802	NAI	C3D-C4D-C5D-O5D
2	BBB	801	CAA	C9P-CAP-CBP-CDP
2	BBB	801	CAA	C6P-C5P-N4P-C3P
2	AAA	901	CAA	CEP-CBP-CCP-O6A
2	BBB	801	CAA	CDP-CBP-CCP-O6A
2	BBB	801	CAA	CEP-CBP-CCP-O6A
2	AAA	901	CAA	C3P-C2P-S1P-C1
2	BBB	801	CAA	C3P-C2P-S1P-C1
2	AAA	901	CAA	CAP-CBP-CCP-O6A
2	BBB	801	CAA	C5B-O5B-P1A-O2A

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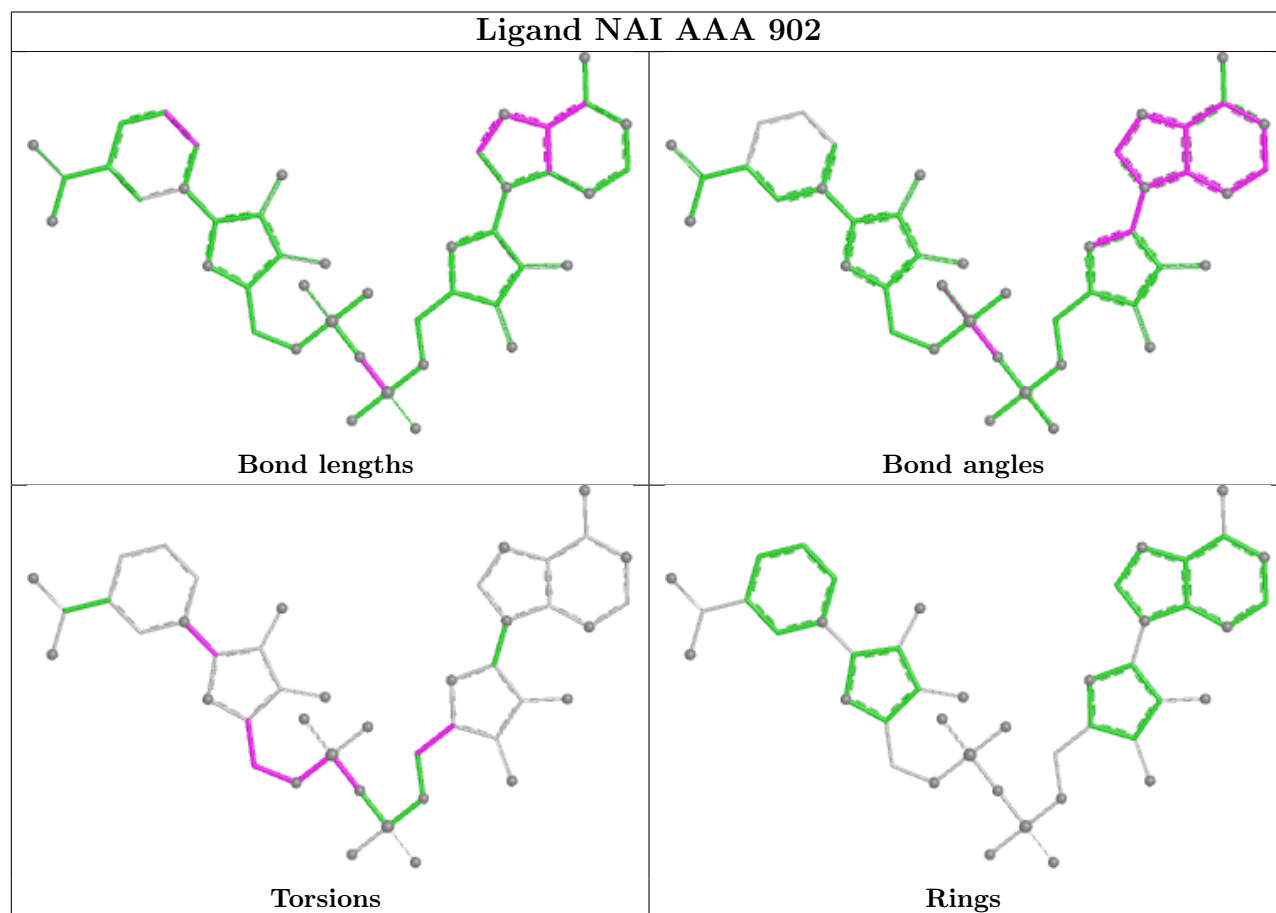
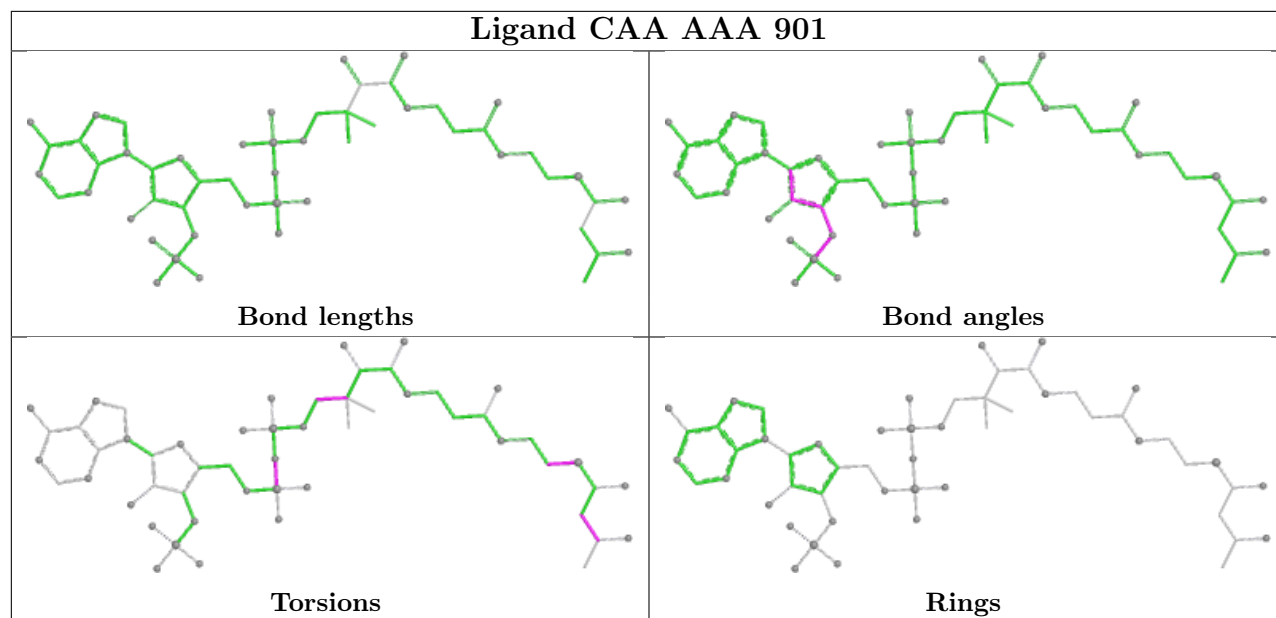
Mol	Chain	Res	Type	Atoms
3	AAA	902	NAI	C5D-O5D-PN-O2N
2	AAA	901	CAA	P2A-O3A-P1A-O2A
3	BBB	802	NAI	O4D-C1D-N1N-C6N
3	AAA	902	NAI	O4D-C1D-N1N-C6N
2	BBB	801	CAA	C3B-O3B-P3B-O7A
3	AAA	902	NAI	C4D-C5D-O5D-PN
3	AAA	902	NAI	C2D-C1D-N1N-C6N
2	BBB	801	CAA	C9P-CAP-CBP-CEP
2	BBB	801	CAA	P2A-O3A-P1A-O2A
3	AAA	902	NAI	PA-O3-PN-O1N
2	AAA	901	CAA	CDP-CBP-CCP-O6A

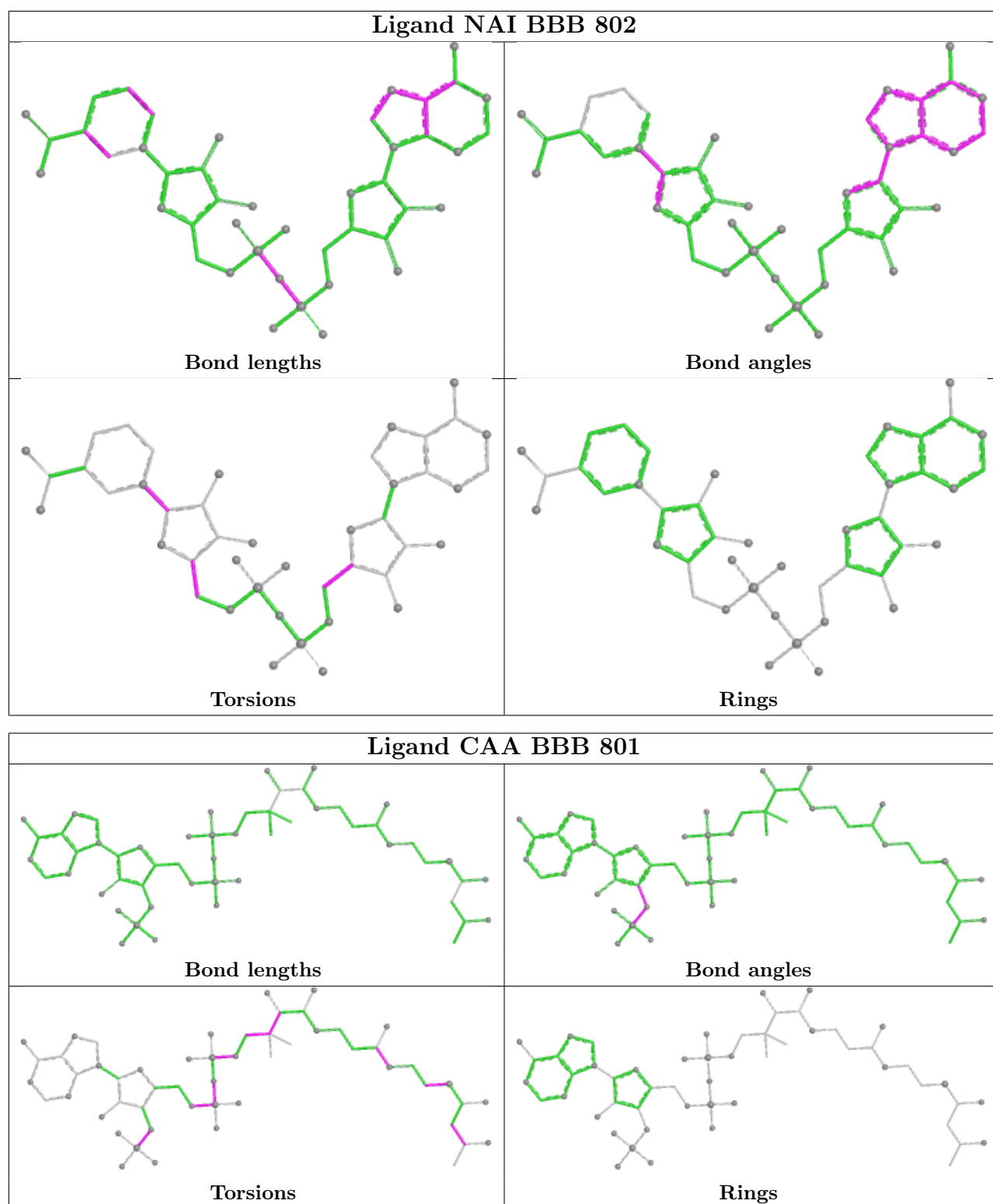
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	901	CAA	3	0
3	AAA	902	NAI	3	0
3	BBB	802	NAI	1	0
2	BBB	801	CAA	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.





5.7 Other polymers ⓘ

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, 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	AAA	723/742 (97%)	0.64	45 (6%) 26 23	24, 54, 109, 170	5 (0%)
1	BBB	719/742 (96%)	1.01	89 (12%) 8 7	40, 79, 135, 176	0
All	All	1442/1484 (97%)	0.82	134 (9%) 14 12	24, 67, 125, 176	5 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	69	PHE	4.5
1	BBB	437	HIS	4.4
1	BBB	430	THR	4.3
1	AAA	565	CYS	4.1
1	AAA	-4	PRO	4.0
1	BBB	531	LYS	4.0
1	BBB	535	GLY	3.9
1	BBB	434	SER	3.8
1	BBB	545	PRO	3.8
1	BBB	717	PRO	3.7
1	AAA	-1	SER	3.7
1	AAA	545	PRO	3.7
1	AAA	492	PHE	3.6
1	AAA	350	ALA	3.5
1	BBB	462	SER	3.5
1	BBB	355	GLN	3.5
1	BBB	470	VAL	3.5
1	BBB	718	HIS	3.4
1	BBB	438	VAL	3.4
1	BBB	719	GLY	3.4
1	AAA	558	SER	3.4
1	AAA	541	PRO	3.4
1	BBB	403	ALA	3.3
1	BBB	354	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	585	LEU	3.3
1	AAA	-3	ARG	3.2
1	BBB	401	PRO	3.2
1	BBB	402	GLY	3.2
1	AAA	560	LEU	3.1
1	AAA	-2	GLY	3.1
1	BBB	570	PHE	3.1
1	BBB	436	ALA	3.1
1	BBB	517	PRO	3.0
1	BBB	330	LYS	3.0
1	AAA	561	GLY	2.9
1	BBB	714	LEU	2.9
1	BBB	353	ASN	2.9
1	BBB	544	PRO	2.8
1	AAA	477	GLY	2.8
1	AAA	557	TYR	2.8
1	AAA	358	ALA	2.8
1	BBB	426	LEU	2.8
1	BBB	524	ALA	2.8
1	BBB	429	GLY	2.8
1	AAA	0	HIS	2.8
1	AAA	325	VAL	2.8
1	BBB	709	LYS	2.8
1	BBB	276	SER	2.8
1	BBB	66	PHE	2.8
1	BBB	257	TYR	2.7
1	BBB	414	VAL	2.7
1	AAA	64	HIS	2.7
1	AAA	338	ILE	2.6
1	AAA	355	GLN	2.6
1	AAA	323	VAL	2.6
1	AAA	329	PRO	2.6
1	BBB	541	PRO	2.6
1	BBB	387	LEU	2.5
1	BBB	452	PRO	2.5
1	BBB	472	VAL	2.5
1	BBB	548	PRO	2.5
1	AAA	524	ALA	2.5
1	BBB	312	ALA	2.5
1	AAA	286	ALA	2.5
1	AAA	306	THR	2.4
1	BBB	295	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	341	PHE	2.4
1	BBB	358	ALA	2.4
1	BBB	433	PHE	2.4
1	AAA	523	LEU	2.4
1	BBB	278	ASN	2.4
1	AAA	549	VAL	2.4
1	BBB	4	TYR	2.4
1	AAA	587	ARG	2.4
1	BBB	348	SER	2.4
1	BBB	189	ASP	2.4
1	BBB	537	GLY	2.4
1	BBB	653	TYR	2.4
1	BBB	520	VAL	2.3
1	BBB	315	PHE	2.3
1	BBB	338	ILE	2.3
1	AAA	242	HIS	2.3
1	AAA	283	PRO	2.3
1	BBB	347	ALA	2.3
1	AAA	588	ILE	2.3
1	BBB	427	VAL	2.3
1	BBB	341	PHE	2.3
1	AAA	284	SER	2.2
1	AAA	366	SER	2.2
1	BBB	314	SER	2.2
1	BBB	498	GLY	2.2
1	BBB	432	PHE	2.2
1	BBB	532	ILE	2.2
1	AAA	562	ASP	2.2
1	BBB	369	LYS	2.2
1	BBB	43	HIS	2.2
1	BBB	465	ILE	2.2
1	AAA	559	PRO	2.2
1	BBB	412	LEU	2.2
1	BBB	311	ILE	2.2
1	BBB	635	GLU	2.2
1	BBB	294	GLN	2.2
1	BBB	101	GLY	2.2
1	BBB	521	SER	2.2
1	BBB	549	VAL	2.2
1	BBB	487	TYR	2.1
1	BBB	608	ILE	2.1
1	BBB	715	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	340	THR	2.1
1	BBB	399	CYS	2.1
1	BBB	371	LEU	2.1
1	BBB	301	VAL	2.1
1	BBB	350	ALA	2.1
1	BBB	337	LYS	2.1
1	BBB	304	LEU	2.1
1	AAA	489	ASN	2.1
1	AAA	488	TYR	2.1
1	BBB	292	SER	2.1
1	BBB	555	SER	2.1
1	AAA	544	PRO	2.1
1	BBB	352	GLN	2.1
1	BBB	405	LEU	2.1
1	AAA	300	GLY	2.1
1	BBB	0	HIS	2.1
1	BBB	547	THR	2.0
1	BBB	560	LEU	2.0
1	BBB	650	LEU	2.0
1	BBB	406	CYS	2.0
1	AAA	570	PHE	2.0
1	BBB	397	ALA	2.0
1	AAA	563	MET	2.0
1	BBB	652	GLY	2.0
1	BBB	378	VAL	2.0
1	BBB	449	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

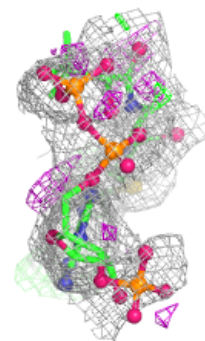
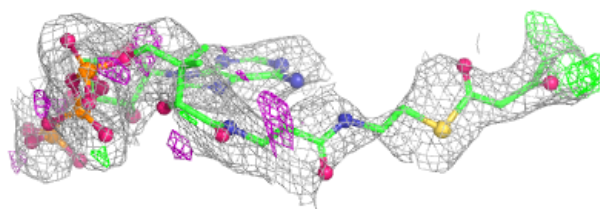
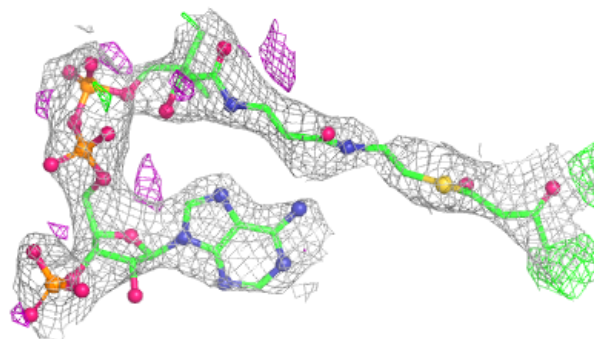
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CAA	AAA	901	54/54	0.75	0.18	70,106,146,149	0
4	SO4	BBB	803	5/5	0.77	0.15	85,89,91,93	0
3	NAI	BBB	802	44/44	0.81	0.13	89,104,113,115	0
2	CAA	BBB	801	54/54	0.84	0.14	63,79,89,95	0
4	SO4	AAA	903	5/5	0.89	0.12	59,60,64,67	0
3	NAI	AAA	902	44/44	0.89	0.12	76,84,101,108	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.

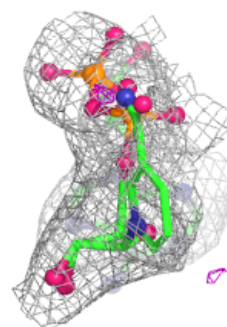
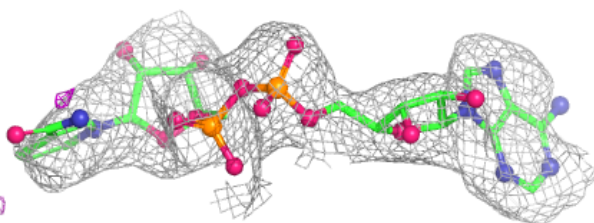
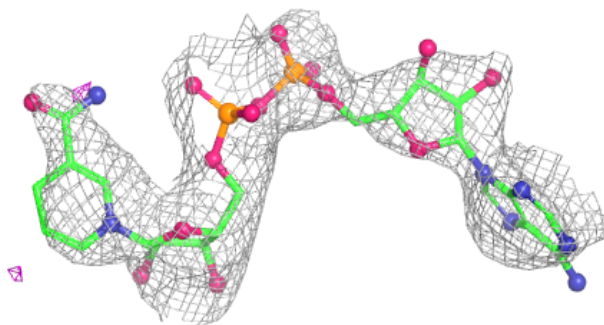
Electron density around CAA AAA 901:

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

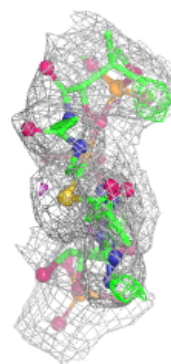
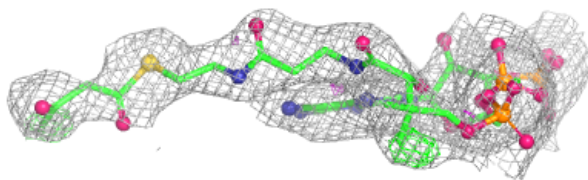
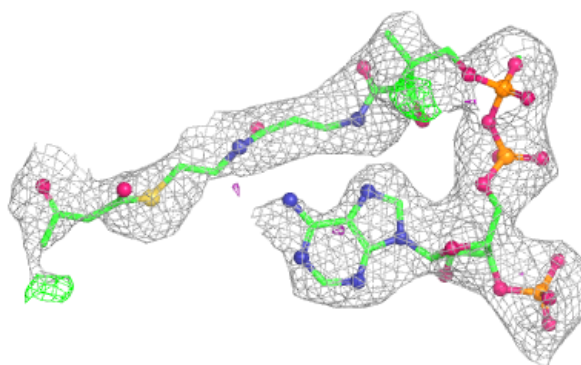


Electron density around NAI BBB 802:

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

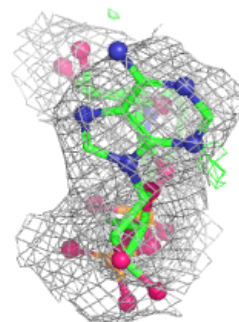
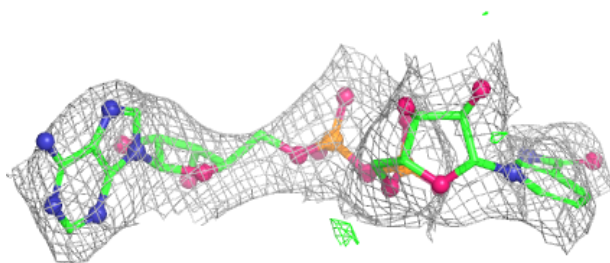
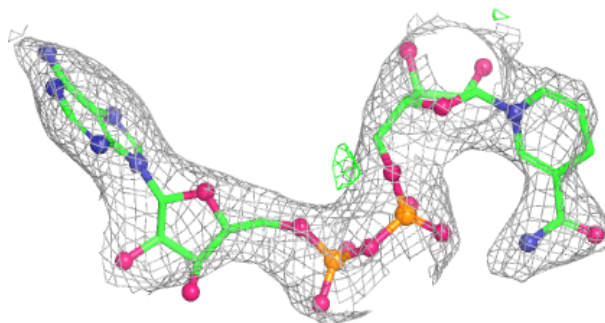
**Electron density around CAA BBB 801:**

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



Electron density around NAI AAA 902:

$2mF_o - DF_c$ (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.