



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2021 – 12:03 am BST

PDB ID : 6ZIB
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
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) : 2.22

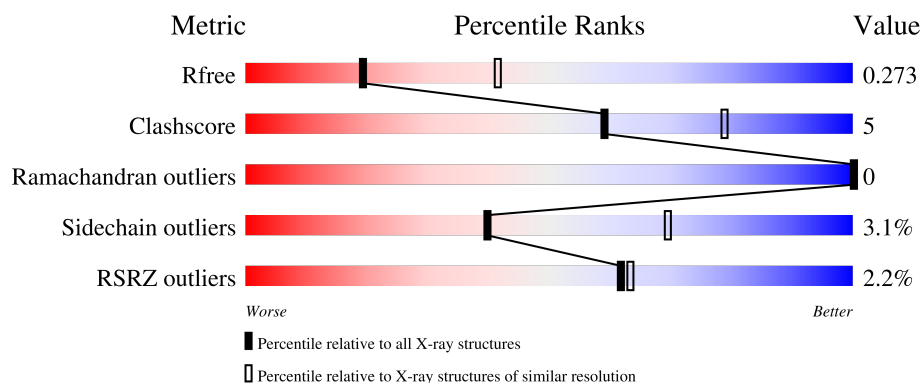
1 Overall quality at a glance

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 ≥ 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	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	BBB	742	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>

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:

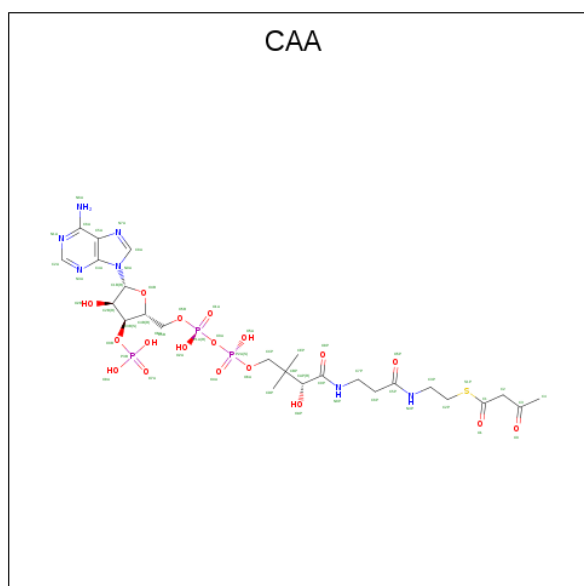
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP P07896
AAA	-18	GLY	-	expression tag	UNP P07896
AAA	-17	SER	-	expression tag	UNP P07896
AAA	-16	SER	-	expression tag	UNP P07896
AAA	-15	HIS	-	expression tag	UNP P07896
AAA	-14	HIS	-	expression tag	UNP P07896
AAA	-13	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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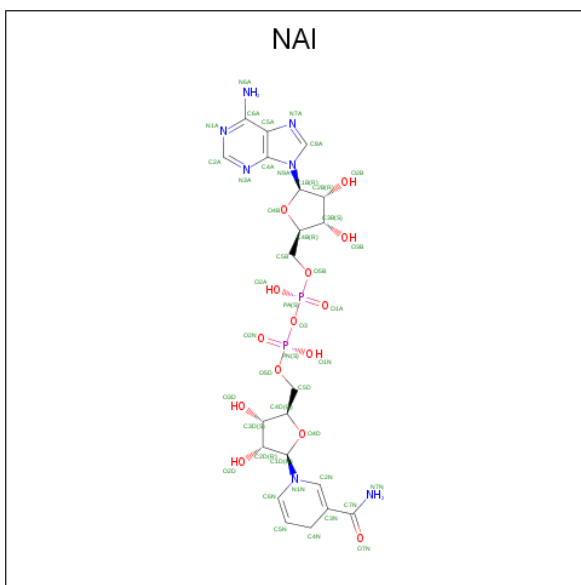
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-14	HIS	-	expression tag	UNP P07896
BBB	-13	HIS	-	expression tag	UNP P07896
BBB	-12	HIS	-	expression tag	UNP P07896
BBB	-11	HIS	-	expression tag	UNP P07896
BBB	-10	HIS	-	expression tag	UNP P07896
BBB	-9	SER	-	expression tag	UNP P07896
BBB	-8	SER	-	expression 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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

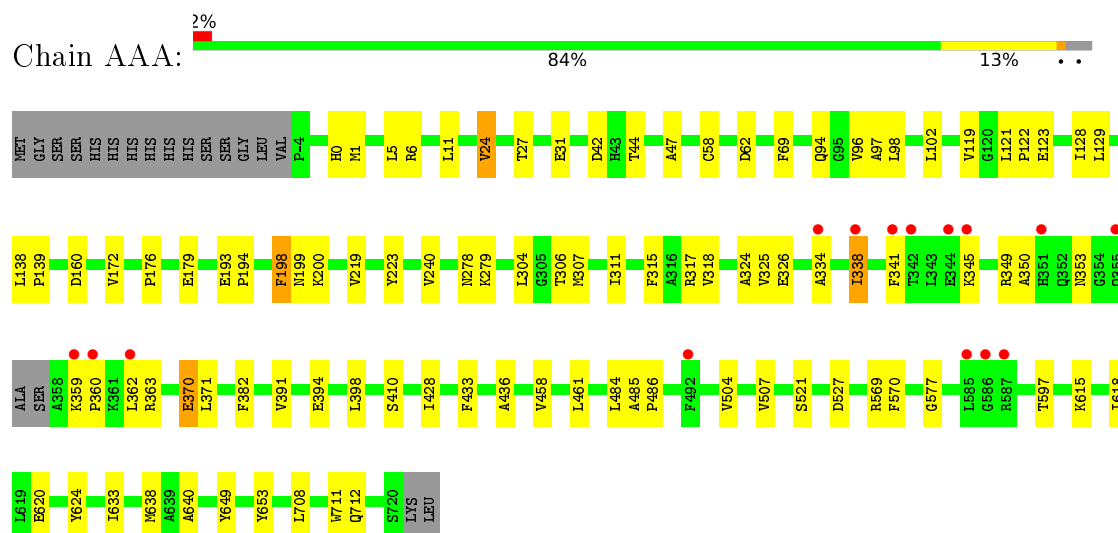
- Molecule 5 is water.

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

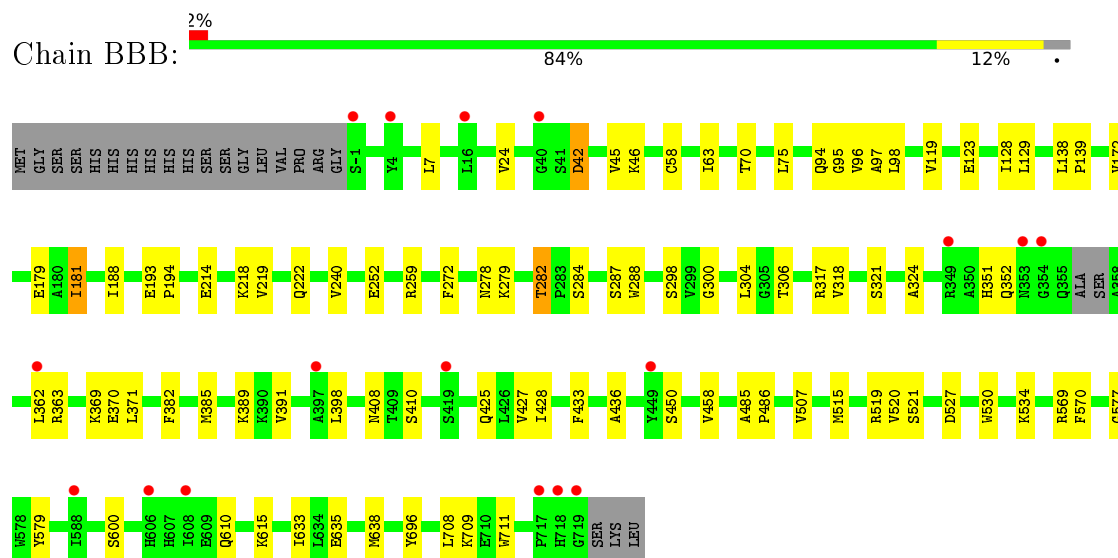
3 Residue-property plots [i](#)

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 48.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (48.88-2.70) 94.6 (48.83-2.70)	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 0.231 , 0.273	Depositor DCC
R_{free} test set	2555 reflections (4.99%)	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)	0.29 , 29.0	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: NAI, SO4, 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	0.33	0/5726	0.61	1/7753 (0.0%)
1	BBB	0.30	0/5650	0.60	0/7653
All	All	0.31	0/11376	0.61	1/15406 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	649	TYR	CB-CA-C	5.07	120.54	110.40

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	63	0
1	BBB	5523	0	5628	46	0
2	AAA	54	0	36	3	0
2	BBB	54	0	36	1	0
3	AAA	44	0	27	4	0
3	BBB	44	0	27	1	0
4	AAA	5	0	0	0	0
4	BBB	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	48	0	0	0	0
5	BBB	19	0	0	0	0
All	All	11379	0	11454	107	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 (107) 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:AAA:325:VAL:CG2	1:AAA:371:LEU:HD11	2.22	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
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:311:ILE:O	1:AAA:315:PHE:HD1	1.91	0.52
1:BBB:218:LYS:HE3	1:BBB:222:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:129:LEU:HD12	1:BBB:129:LEU:C	2.34	0.47
1:BBB:427:VAL:O	1:BBB:450:SER:HB3	2.14	0.47
1:AAA:129:LEU:C	1:AAA:129:LEU:HD12	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:326:GLU:OE2	3:AAA:902:NAI:O2B	2.29	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: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
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

5.3.1 Protein backbone

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

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%)	41	70
1	BBB	590/609 (97%)	571 (97%)	19 (3%)	39	68
All	All	1188/1218 (98%)	1151 (97%)	37 (3%)	40	69

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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

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

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](#)

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$
4	SO4	AAA	903	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	BBB	803	-	4,4,4	0.38	0	6,6,6	0.07	0
2	CAA	AAA	901	-	47,56,56	0.57	0	60,83,83	0.74	2 (3%)
3	NAI	BBB	802	-	42,48,48	1.05	3 (7%)	47,73,73	1.22	4 (8%)
2	CAA	BBB	801	-	47,56,56	0.53	0	60,83,83	0.66	1 (1%)
3	NAI	AAA	902	-	42,48,48	1.08	4 (9%)	47,73,73	1.13	3 (6%)

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	-	-	5/25/72/72	0/5/5/5
2	CAA	BBB	801	-	-	18/50/71/71	0/3/3/3
2	CAA	AAA	901	-	-	8/50/71/71	0/3/3/3
3	NAI	AAA	902	-	-	12/25/72/72	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	902	NAI	C6N-C5N	3.73	1.40	1.33
3	BBB	802	NAI	C6N-C5N	3.53	1.39	1.33
3	AAA	902	NAI	C5A-C4A	2.53	1.47	1.40
3	BBB	802	NAI	C5A-C4A	2.52	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	802	NAI	C2N-C3N	2.07	1.40	1.34
3	AAA	902	NAI	O4B-C1B	2.05	1.43	1.41
3	AAA	902	NAI	C2N-C3N	2.00	1.40	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	802	NAI	N3A-C2A-N1A	-3.63	123.01	128.68
3	AAA	902	NAI	N3A-C2A-N1A	-3.47	123.25	128.68
3	BBB	802	NAI	PN-O3-PA	-2.61	123.88	132.83
3	BBB	802	NAI	C4A-C5A-N7A	-2.58	106.71	109.40
2	AAA	901	CAA	C5A-C6A-N6A	2.42	124.03	120.35
2	BBB	801	CAA	C5A-C6A-N6A	2.33	123.90	120.35
3	BBB	802	NAI	O4D-C1D-N1N	2.32	112.58	108.06
2	AAA	901	CAA	C3B-C2B-C1B	2.30	104.98	99.89
3	AAA	902	NAI	C4A-C5A-N7A	-2.27	107.03	109.40
3	AAA	902	NAI	PN-O3-PA	-2.18	125.36	132.83

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	901	CAA	C3P-C2P-S1P-C1
2	AAA	901	CAA	C1-C2-C3-O3
2	AAA	901	CAA	C1-C2-C3-C4
2	BBB	801	CAA	C3B-O3B-P3B-O7A
2	BBB	801	CAA	C5B-O5B-P1A-O1A
2	BBB	801	CAA	CCP-O6A-P2A-O5A
2	BBB	801	CAA	C9P-CAP-CBP-CCP
2	BBB	801	CAA	C3P-C2P-S1P-C1
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-O1N
3	AAA	902	NAI	O4D-C4D-C5D-O5D
3	AAA	902	NAI	C3D-C4D-C5D-O5D
3	BBB	802	NAI	O4B-C4B-C5B-O5B
3	AAA	902	NAI	O4B-C4B-C5B-O5B
3	BBB	802	NAI	C3B-C4B-C5B-O5B
2	BBB	801	CAA	O5P-C5P-N4P-C3P
3	BBB	802	NAI	O4D-C4D-C5D-O5D
3	BBB	802	NAI	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	AAA	901	CAA	P2A-O3A-P1A-O1A
3	AAA	902	NAI	PA-O3-PN-O2N
2	BBB	801	CAA	C6P-C5P-N4P-C3P
2	BBB	801	CAA	CDP-CBP-CCP-O6A
2	BBB	801	CAA	C9P-CAP-CBP-CDP
3	AAA	902	NAI	C5D-O5D-PN-O3
2	BBB	801	CAA	C5B-O5B-P1A-O2A
3	AAA	902	NAI	C5D-O5D-PN-O2N
2	AAA	901	CAA	CAP-CBP-CCP-O6A
2	BBB	801	CAA	CEP-CBP-CCP-O6A
2	AAA	901	CAA	P2A-O3A-P1A-O2A
3	AAA	902	NAI	C4D-C5D-O5D-PN
3	AAA	902	NAI	O4D-C1D-N1N-C6N
3	BBB	802	NAI	O4D-C1D-N1N-C6N
2	AAA	901	CAA	CDP-CBP-CCP-O6A
2	AAA	901	CAA	CEP-CBP-CCP-O6A
3	AAA	902	NAI	C2D-C1D-N1N-C6N
2	BBB	801	CAA	C9P-CAP-CBP-CEP
2	BBB	801	CAA	C5B-O5B-P1A-O3A
2	BBB	801	CAA	CCP-O6A-P2A-O3A
2	BBB	801	CAA	P2A-O3A-P1A-O2A
3	AAA	902	NAI	PA-O3-PN-O1N
2	BBB	801	CAA	CCP-O6A-P2A-O4A

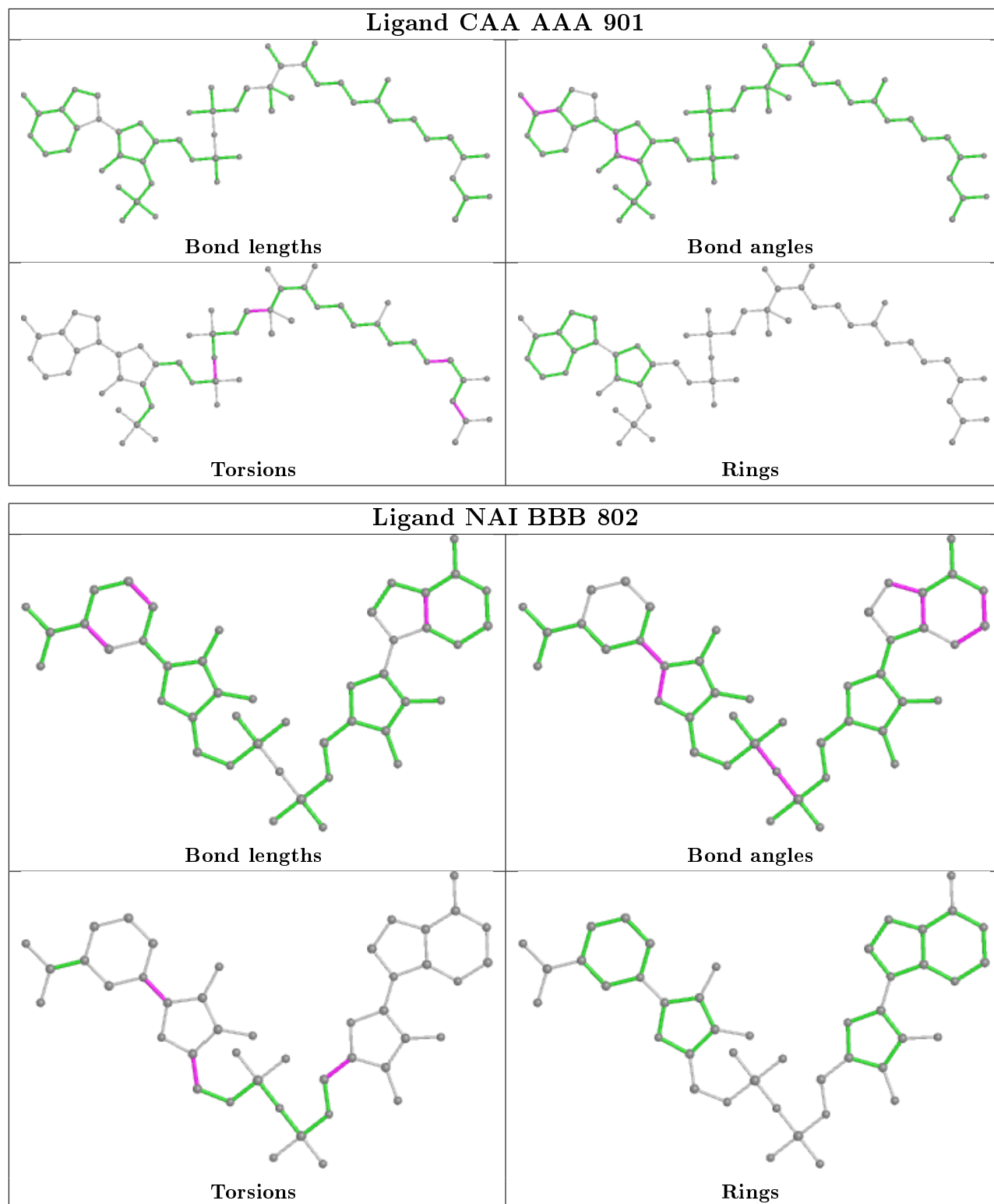
There are no ring outliers.

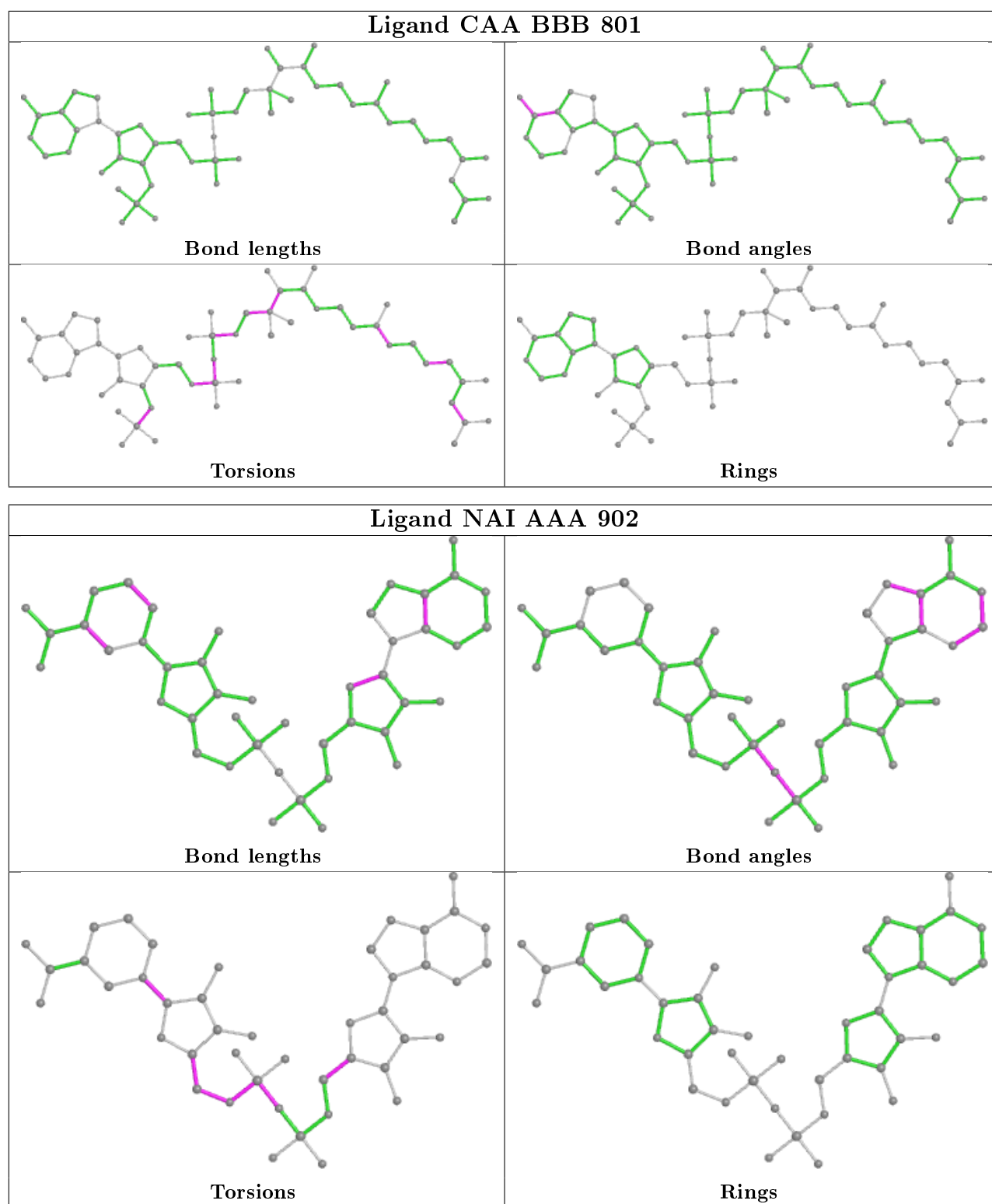
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	901	CAA	3	0
3	BBB	802	NAI	1	0
2	BBB	801	CAA	1	0
3	AAA	902	NAI	4	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%)	0.07	15 (2%) 63 65	32, 55, 109, 170	0
1	BBB	719/742 (96%)	0.22	17 (2%) 59 60	40, 79, 135, 176	0
All	All	1442/1484 (97%)	0.15	32 (2%) 62 63	32, 67, 125, 176	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	351	HIS	4.2
1	AAA	585	LEU	3.9
1	BBB	719	GLY	3.6
1	AAA	338	ILE	3.6
1	BBB	4	TYR	3.4
1	BBB	718	HIS	3.3
1	AAA	355	GLN	3.1
1	BBB	419	SER	3.1
1	AAA	587	ARG	3.0
1	BBB	362	LEU	2.8
1	BBB	717	PRO	2.8
1	AAA	334	ALA	2.7
1	BBB	588	ILE	2.7
1	BBB	608	ILE	2.7
1	AAA	359	LYS	2.7
1	AAA	341	PHE	2.6
1	BBB	353	ASN	2.6
1	AAA	586	GLY	2.5
1	BBB	40	GLY	2.5
1	BBB	-1	SER	2.5
1	AAA	492	PHE	2.4
1	AAA	360	PRO	2.4
1	AAA	362	LEU	2.3
1	BBB	606	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	342	THR	2.3
1	BBB	449	TYR	2.2
1	BBB	16	LEU	2.1
1	BBB	397	ALA	2.1
1	BBB	354	GLY	2.1
1	AAA	344	GLU	2.1
1	AAA	345	LYS	2.1
1	BBB	349	ARG	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 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, 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(\AA^2)	Q<0.9
2	CAA	AAA	901	54/54	0.78	0.29	70,106,146,149	0
4	SO4	BBB	803	5/5	0.86	0.17	85,89,91,93	0
3	NAI	BBB	802	44/44	0.87	0.19	89,104,113,115	0
2	CAA	BBB	801	54/54	0.87	0.20	63,79,89,95	0
3	NAI	AAA	902	44/44	0.91	0.18	76,84,101,108	0
4	SO4	AAA	903	5/5	0.95	0.14	59,60,64,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.