



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:19 PM UTC

PDB ID : 7Q9Z / pdb_00007q9z
Title : Crystal structure of Chromobacterium violaceum aminotransferase in complex with PLP-pyruvate adduct
Authors : Isupov, M.N.; Mitchell, D.; Sayer, C.; Littlechild, J.A.
Deposited on : 2021-11-15
Resolution : 1.95 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

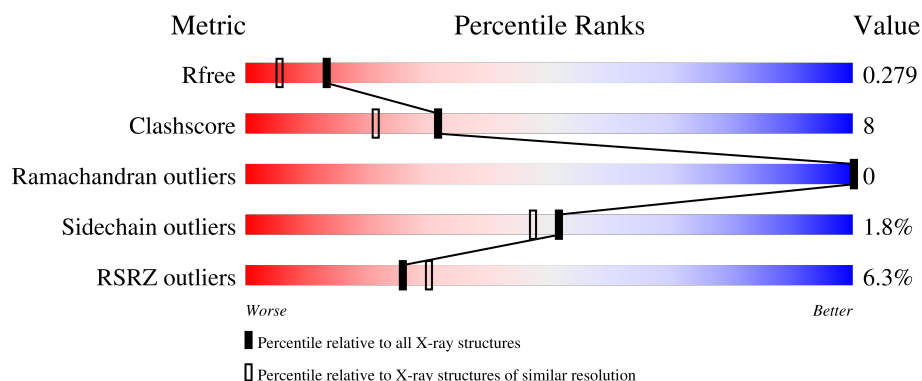
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	493	3% 72% 14% 13%
1	BBB	493	8% 74% 13% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AN7	AAA	501	-	-	X	-
3	EDO	AAA	503	-	-	X	-
3	EDO	BBB	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6881 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 Probable aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	427	Total	C	N	O	S	0	5	0
			3381	2159	592	609	21			
1	BBB	427	Total	C	N	O	S	0	2	0
			3359	2145	586	607	21			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-33	MET	-	initiating methionine	UNP Q7N WG4
AAA	-32	GLY	-	expression tag	UNP Q7N WG4
AAA	-31	SER	-	expression tag	UNP Q7N WG4
AAA	-30	SER	-	expression tag	UNP Q7N WG4
AAA	-29	HIS	-	expression tag	UNP Q7N WG4
AAA	-28	HIS	-	expression tag	UNP Q7N WG4
AAA	-27	HIS	-	expression tag	UNP Q7N WG4
AAA	-26	HIS	-	expression tag	UNP Q7N WG4
AAA	-25	HIS	-	expression tag	UNP Q7N WG4
AAA	-24	HIS	-	expression tag	UNP Q7N WG4
AAA	-23	SER	-	expression tag	UNP Q7N WG4
AAA	-22	SER	-	expression tag	UNP Q7N WG4
AAA	-21	GLY	-	expression tag	UNP Q7N WG4
AAA	-20	LEU	-	expression tag	UNP Q7N WG4
AAA	-19	VAL	-	expression tag	UNP Q7N WG4
AAA	-18	PRO	-	expression tag	UNP Q7N WG4
AAA	-17	ARG	-	expression tag	UNP Q7N WG4
AAA	-16	GLY	-	expression tag	UNP Q7N WG4
AAA	-15	SER	-	expression tag	UNP Q7N WG4
AAA	-14	HIS	-	expression tag	UNP Q7N WG4
AAA	-13	MET	-	expression tag	UNP Q7N WG4
AAA	-12	ALA	-	expression tag	UNP Q7N WG4
AAA	-11	SER	-	expression tag	UNP Q7N WG4
AAA	-10	MET	-	expression tag	UNP Q7N WG4
AAA	-9	THR	-	expression tag	UNP Q7N WG4

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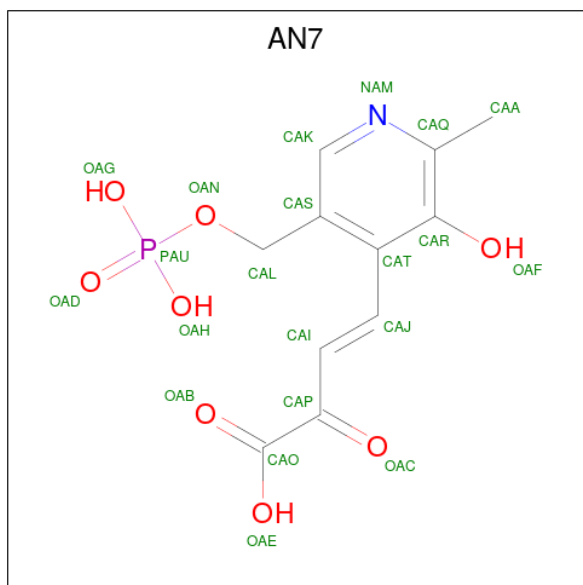
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-8	GLY	-	expression tag	UNP Q7NWX4
AAA	-7	GLY	-	expression tag	UNP Q7NWX4
AAA	-6	GLN	-	expression tag	UNP Q7NWX4
AAA	-5	GLN	-	expression tag	UNP Q7NWX4
AAA	-4	MET	-	expression tag	UNP Q7NWX4
AAA	-3	GLY	-	expression tag	UNP Q7NWX4
AAA	-2	ARG	-	expression tag	UNP Q7NWX4
AAA	-1	GLY	-	expression tag	UNP Q7NWX4
AAA	0	SER	-	expression tag	UNP Q7NWX4
BBB	-33	MET	-	initiating methionine	UNP Q7NWX4
BBB	-32	GLY	-	expression tag	UNP Q7NWX4
BBB	-31	SER	-	expression tag	UNP Q7NWX4
BBB	-30	SER	-	expression tag	UNP Q7NWX4
BBB	-29	HIS	-	expression tag	UNP Q7NWX4
BBB	-28	HIS	-	expression tag	UNP Q7NWX4
BBB	-27	HIS	-	expression tag	UNP Q7NWX4
BBB	-26	HIS	-	expression tag	UNP Q7NWX4
BBB	-25	HIS	-	expression tag	UNP Q7NWX4
BBB	-24	HIS	-	expression tag	UNP Q7NWX4
BBB	-23	SER	-	expression tag	UNP Q7NWX4
BBB	-22	SER	-	expression tag	UNP Q7NWX4
BBB	-21	GLY	-	expression tag	UNP Q7NWX4
BBB	-20	LEU	-	expression tag	UNP Q7NWX4
BBB	-19	VAL	-	expression tag	UNP Q7NWX4
BBB	-18	PRO	-	expression tag	UNP Q7NWX4
BBB	-17	ARG	-	expression tag	UNP Q7NWX4
BBB	-16	GLY	-	expression tag	UNP Q7NWX4
BBB	-15	SER	-	expression tag	UNP Q7NWX4
BBB	-14	HIS	-	expression tag	UNP Q7NWX4
BBB	-13	MET	-	expression tag	UNP Q7NWX4
BBB	-12	ALA	-	expression tag	UNP Q7NWX4
BBB	-11	SER	-	expression tag	UNP Q7NWX4
BBB	-10	MET	-	expression tag	UNP Q7NWX4
BBB	-9	THR	-	expression tag	UNP Q7NWX4
BBB	-8	GLY	-	expression tag	UNP Q7NWX4
BBB	-7	GLY	-	expression tag	UNP Q7NWX4
BBB	-6	GLN	-	expression tag	UNP Q7NWX4
BBB	-5	GLN	-	expression tag	UNP Q7NWX4
BBB	-4	MET	-	expression tag	UNP Q7NWX4
BBB	-3	GLY	-	expression tag	UNP Q7NWX4
BBB	-2	ARG	-	expression tag	UNP Q7NWX4
BBB	-1	GLY	-	expression tag	UNP Q7NWX4

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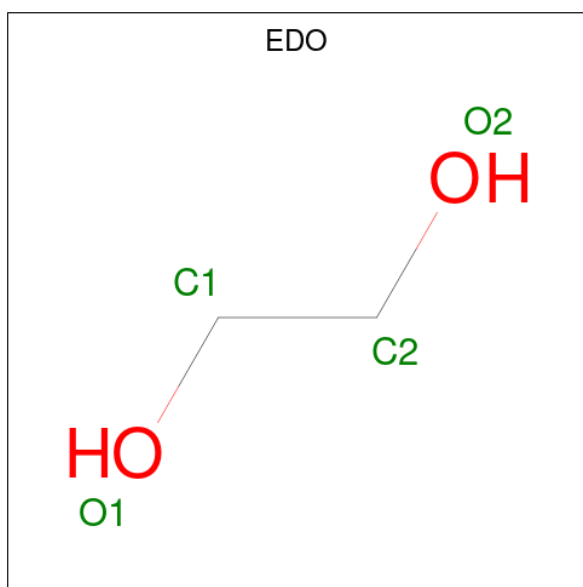
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	SER	-	expression tag	UNP Q7NWX4

- Molecule 2 is (3E)-4-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}-2-oxobut-3-enoic acid (CCD ID: AN7) (formula: C₁₁H₁₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			21	11	1	8	1		
2	BBB	1	Total	C	N	O	P	0	0
			21	11	1	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Cl 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Na 1 1	0	0
5	BBB	1	Total Na 1 1	0	0

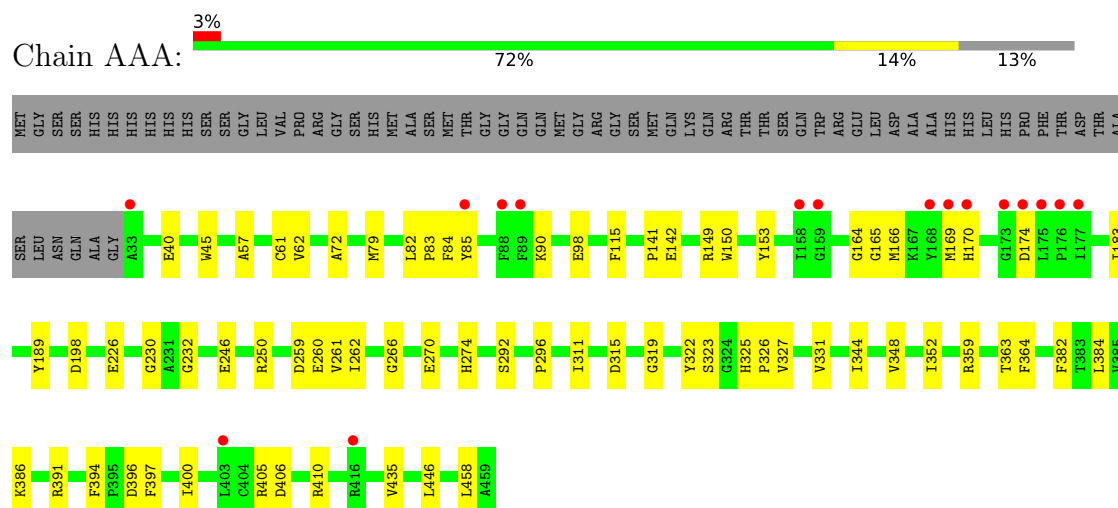
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	44	Total 44	O 44	0	0
6	BBB	32	Total 32	O 32	0	0

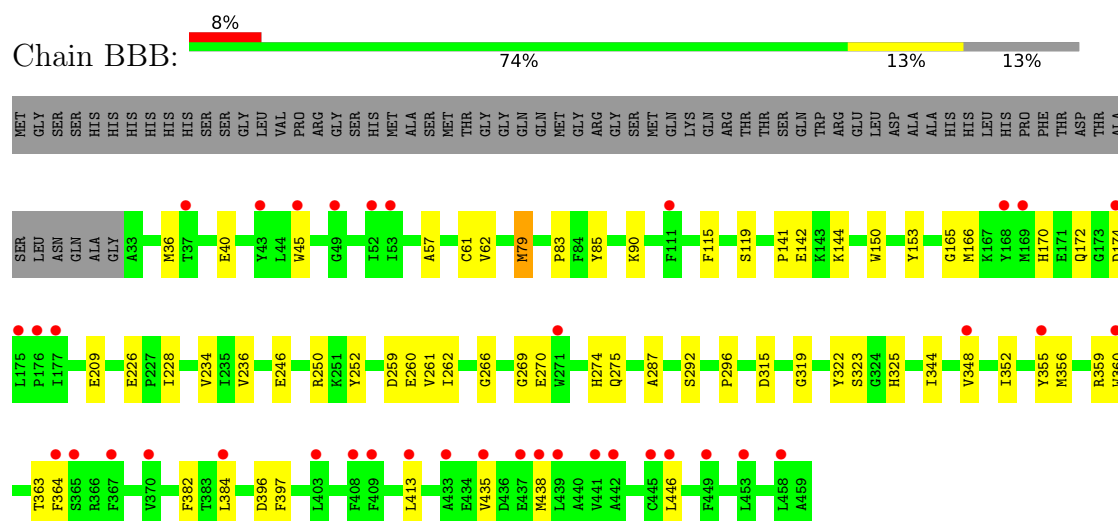
3 Residue-property plots

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: Probable aminotransferase



- Molecule 1: Probable aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.15Å 60.72Å 61.80Å 71.30° 75.94° 85.73°	Depositor
Resolution (Å)	56.41 – 1.95 56.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (56.41-1.95) 97.7 (56.41-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.243 , 0.279 0.243 , 0.279	Depositor DCC
R_{free} test set	2759 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, EDO, AN7

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	0/3483	1.03	0/4708
1	BBB	0.50	0/3452	1.03	0/4668
All	All	0.50	0/6935	1.03	0/9376

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	3381	0	3311	57	0
1	BBB	3359	0	3279	56	0
2	AAA	21	0	8	8	0
2	BBB	21	0	8	6	0
3	AAA	8	0	12	5	0
3	BBB	12	0	18	8	0
4	AAA	1	0	0	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
6	AAA	44	0	0	3	0
6	BBB	32	0	0	1	0
All	All	6881	0	6636	109	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 8.

All (109) 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:153:TYR:HE1	1:AAA:169:MET:HE1	1.29	0.97
1:AAA:261:VAL:HG11	2:AAA:501:AN7:CAQ	1.94	0.96
1:BBB:261:VAL:HG11	2:BBB:501:AN7:NAM	1.89	0.86
1:BBB:261:VAL:HG11	2:BBB:501:AN7:CAQ	2.08	0.82
1:AAA:261:VAL:HG11	2:AAA:501:AN7:NAM	1.97	0.80
1:AAA:261:VAL:HG11	2:AAA:501:AN7:CAA	2.15	0.77
1:BBB:226:GLU:OE1	3:BBB:503:EDO:O1	2.05	0.73
1:AAA:153:TYR:CE1	1:AAA:169:MET:HE1	2.21	0.71
2:AAA:501:AN7:OAD	6:AAA:601:HOH:O	2.11	0.69
1:BBB:262:ILE:HB	3:BBB:503:EDO:H12	1.76	0.67
1:AAA:262:ILE:HB	3:AAA:503:EDO:H22	1.77	0.66
1:AAA:261:VAL:HG11	2:AAA:501:AN7:HAA	1.80	0.64
1:AAA:40[A]:GLU:HB3	1:AAA:45:TRP:HZ3	1.62	0.64
1:AAA:226:GLU:HB3	3:AAA:503:EDO:H12	1.79	0.63
1:AAA:226:GLU:OE1	3:AAA:503:EDO:O2	2.16	0.63
1:AAA:325:HIS:CD2	1:BBB:296:PRO:HD3	2.35	0.61
1:AAA:153:TYR:O	2:AAA:501:AN7:HAAA	2.00	0.61
1:BBB:261:VAL:HG13	3:BBB:503:EDO:H21	1.83	0.60
1:BBB:115:PHE:CE2	1:BBB:319:GLY:HA3	2.37	0.60
1:AAA:405:ARG:NH1	1:AAA:406:ASP:OD1	2.35	0.60
1:AAA:115:PHE:CE2	1:AAA:319:GLY:HA3	2.37	0.59
1:AAA:261:VAL:CG1	2:AAA:501:AN7:HAA	2.34	0.57
1:BBB:236:VAL:HG11	3:BBB:504:EDO:H11	1.86	0.57
1:BBB:356:MET:HE3	1:BBB:360:TRP:CE3	2.39	0.57
1:BBB:40:GLU:HB3	1:BBB:45:TRP:HZ3	1.70	0.56
1:BBB:261:VAL:HG11	2:BBB:501:AN7:CAA	2.33	0.56
1:AAA:40[B]:GLU:HB3	1:AAA:45:TRP:HZ3	1.71	0.56
1:BBB:356:MET:CE	1:BBB:360:TRP:CE3	2.88	0.56
1:BBB:413:LEU:HD11	1:BBB:438:MET:HG3	1.88	0.56
1:AAA:364:PHE:CE1	1:AAA:446:LEU:HD12	2.41	0.55
1:BBB:228:ILE:O	3:BBB:503:EDO:H11	2.07	0.55
1:AAA:261:VAL:CG1	2:AAA:501:AN7:CAA	2.84	0.54
1:AAA:262:ILE:HB	3:AAA:503:EDO:C2	2.37	0.53
1:AAA:141:PRO:HD2	1:AAA:142:GLU:OE1	2.07	0.53
1:BBB:142:GLU:CD	1:BBB:142:GLU:H	2.16	0.53
1:AAA:164:GLY:O	1:AAA:170:HIS:NE2	2.26	0.53
1:BBB:246:GLU:O	1:BBB:250:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:153:TYR:HB2	1:BBB:166:MET:HE2	1.91	0.53
1:AAA:40[A]:GLU:HB3	1:AAA:45:TRP:CZ3	2.42	0.52
1:BBB:261:VAL:HG11	2:BBB:501:AN7:HAA	1.91	0.52
1:AAA:246:GLU:O	1:AAA:250:ARG:HG2	2.09	0.52
1:BBB:356:MET:CE	1:BBB:360:TRP:HE3	2.23	0.51
1:BBB:266:GLY:HA2	1:BBB:270:GLU:O	2.11	0.50
1:AAA:153:TYR:HB2	1:AAA:166:MET:HE2	1.92	0.50
1:BBB:356:MET:HE3	1:BBB:360:TRP:HE3	1.77	0.50
1:AAA:266:GLY:HA2	1:AAA:270:GLU:O	2.11	0.50
1:AAA:406:ASP:O	1:AAA:410[B]:ARG:HD3	2.11	0.49
1:BBB:262:ILE:HB	3:BBB:503:EDO:C1	2.41	0.49
1:AAA:352:ILE:HD11	1:AAA:435:VAL:HG21	1.93	0.49
1:BBB:319:GLY:O	1:BBB:323:SER:HB3	2.13	0.49
1:BBB:226:GLU:HB3	3:BBB:503:EDO:C1	2.43	0.49
1:BBB:57:ALA:O	1:BBB:62:VAL:HG23	2.13	0.49
1:AAA:189:TYR:CZ	1:AAA:391:ARG:HG2	2.48	0.49
1:BBB:40:GLU:HB3	1:BBB:45:TRP:CZ3	2.48	0.49
1:BBB:261:VAL:CG1	2:BBB:501:AN7:HAA	2.43	0.48
1:BBB:209:GLU:OE2	1:BBB:252:TYR:OH	2.29	0.48
1:AAA:57:ALA:O	1:AAA:62:VAL:HG23	2.14	0.47
1:BBB:260:GLU:OE2	1:BBB:274:HIS:ND1	2.43	0.47
1:BBB:359:ARG:O	1:BBB:363:THR:OG1	2.30	0.47
1:AAA:364:PHE:HE1	1:AAA:446:LEU:HD12	1.79	0.46
1:AAA:40[B]:GLU:HB3	1:AAA:45:TRP:CZ3	2.49	0.46
1:AAA:344:ILE:O	1:AAA:348:VAL:HG23	2.16	0.46
1:BBB:352:ILE:HD11	1:BBB:435:VAL:HG21	1.97	0.46
1:BBB:79:MET:HA	1:BBB:83:PRO:HB3	1.98	0.46
1:BBB:344:ILE:O	1:BBB:348:VAL:HG23	2.16	0.45
1:BBB:119:SER:HB2	2:BBB:501:AN7:OAD	2.16	0.45
1:AAA:319:GLY:O	1:AAA:323:SER:HB3	2.15	0.45
1:AAA:230:GLY:H	3:AAA:503:EDO:HO2	1.64	0.45
1:BBB:226:GLU:HB3	3:BBB:503:EDO:H11	1.98	0.45
1:AAA:79:MET:HA	1:AAA:83:PRO:HB3	1.99	0.45
1:BBB:364:PHE:CE1	1:BBB:446:LEU:HD12	2.52	0.45
1:AAA:259:ASP:OD1	1:AAA:261:VAL:HG12	2.18	0.44
1:BBB:150:TRP:HA	1:BBB:165:GLY:HA3	1.99	0.44
1:BBB:259:ASP:OD1	1:BBB:261:VAL:HG12	2.17	0.44
1:BBB:287:ALA:HB1	6:BBB:601:HOH:O	2.15	0.44
1:BBB:270:GLU:HG2	1:BBB:275:GLN:HB3	1.99	0.44
1:BBB:355:TYR:CZ	1:BBB:359:ARG:HG3	2.53	0.44
1:AAA:61:CYS:O	1:AAA:292:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:150:TRP:HA	1:AAA:165:GLY:HA3	2.00	0.43
1:AAA:296:PRO:HD3	1:BBB:325:HIS:CD2	2.53	0.43
1:AAA:331:VAL:HG21	1:BBB:79:MET:HE1	2.00	0.43
1:BBB:364:PHE:HE1	1:BBB:446:LEU:HD12	1.83	0.43
1:AAA:396:ASP:N	6:AAA:604:HOH:O	2.52	0.43
1:BBB:90:LYS:HA	1:BBB:322:TYR:OH	2.19	0.43
1:AAA:382:PHE:HE1	1:AAA:384:LEU:HD21	1.84	0.43
1:BBB:61:CYS:O	1:BBB:292:SER:HA	2.19	0.43
1:AAA:232:GLY:N	6:AAA:602:HOH:O	2.46	0.42
1:AAA:359:ARG:O	1:AAA:363:THR:OG1	2.31	0.42
1:AAA:352:ILE:HD11	1:AAA:435:VAL:CG2	2.49	0.42
1:AAA:386:LYS:NZ	1:AAA:458:LEU:O	2.52	0.42
1:AAA:90:LYS:HA	1:AAA:322:TYR:OH	2.20	0.42
1:AAA:396:ASP:O	1:AAA:397:PHE:C	2.63	0.42
1:BBB:319:GLY:O	1:BBB:323:SER:CB	2.67	0.42
1:BBB:396:ASP:O	1:BBB:397:PHE:C	2.64	0.41
1:AAA:394:PHE:CG	1:AAA:400:ILE:HG13	2.55	0.41
1:BBB:269:GLY:HA2	1:BBB:348:VAL:HB	2.02	0.41
1:AAA:79:MET:HG2	1:AAA:327:VAL:HG21	2.02	0.41
1:BBB:352:ILE:HD11	1:BBB:435:VAL:CG2	2.51	0.41
1:AAA:149:ARG:HA	1:AAA:183:ILE:O	2.21	0.41
1:BBB:382:PHE:HE1	1:BBB:384:LEU:HD21	1.86	0.41
1:AAA:260:GLU:OE2	1:AAA:274:HIS:ND1	2.45	0.41
1:BBB:141:PRO:O	1:BBB:144:LYS:HE2	2.21	0.40
1:AAA:82:LEU:HD11	1:BBB:36:MET:HE2	2.03	0.40
1:AAA:83:PRO:HG2	1:AAA:84:PHE:CD2	2.57	0.40
1:AAA:325:HIS:HA	1:AAA:326:PRO:HD3	1.97	0.40
1:BBB:270:GLU:HG2	1:BBB:275:GLN:CB	2.51	0.40
1:AAA:72:ALA:HB2	1:BBB:79:MET:HB3	2.04	0.40
1:AAA:319:GLY:O	1:AAA:323:SER:CB	2.68	0.40
1:BBB:234:VAL:O	1:BBB:234:VAL:HG12	2.22	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	430/493 (87%)	411 (96%)	19 (4%)	0	100	100
1	BBB	427/493 (87%)	405 (95%)	22 (5%)	0	100	100
All	All	857/986 (87%)	816 (95%)	41 (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	346/394 (88%)	340 (98%)	6 (2%)	53	49
1	BBB	343/394 (87%)	337 (98%)	6 (2%)	53	49
All	All	689/788 (87%)	677 (98%)	12 (2%)	51	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	85	TYR
1	AAA	98	GLU
1	AAA	174	ASP
1	AAA	198	ASP
1	AAA	311	ILE
1	AAA	315	ASP
1	BBB	79	MET
1	BBB	85	TYR
1	BBB	170	HIS
1	BBB	172	GLN
1	BBB	174	ASP
1	BBB	315	ASP

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AN7	BBB	501	-	20,21,21	0.76	1 (5%)	24,30,30	0.67	0
3	EDO	AAA	503	-	3,3,3	0.21	0	2,2,2	0.43	0
3	EDO	AAA	502	-	3,3,3	0.11	0	2,2,2	0.14	0
2	AN7	AAA	501	-	20,21,21	0.79	1 (5%)	24,30,30	0.73	0
3	EDO	BBB	503	-	3,3,3	0.23	0	2,2,2	0.46	0
3	EDO	BBB	502	-	3,3,3	0.07	0	2,2,2	0.14	0
3	EDO	BBB	504	-	3,3,3	0.14	0	2,2,2	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AN7	BBB	501	-	-	6/15/15/15	0/1/1/1
3	EDO	AAA	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	502	-	-	1/1/1/1	-
2	AN7	AAA	501	-	-	7/15/15/15	0/1/1/1
3	EDO	BBB	503	-	-	0/1/1/1	-
3	EDO	BBB	502	-	-	1/1/1/1	-
3	EDO	BBB	504	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	AN7	OAE-CAO	-2.94	1.22	1.30
2	BBB	501	AN7	OAE-CAO	-2.84	1.22	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	AN7	CAP-CAI-CAJ-CAT
2	AAA	501	AN7	OAB-CAO-CAP-OAC
2	AAA	501	AN7	OAB-CAO-CAP-CAI
2	AAA	501	AN7	OAE-CAO-CAP-OAC
2	AAA	501	AN7	OAE-CAO-CAP-CAI
2	BBB	501	AN7	CAP-CAI-CAJ-CAT
2	BBB	501	AN7	CAL-OAN-PAU-OAD
2	BBB	501	AN7	CAL-OAN-PAU-OAG
2	BBB	501	AN7	OAB-CAO-CAP-CAI
3	AAA	502	EDO	O1-C1-C2-O2
3	BBB	504	EDO	O1-C1-C2-O2
2	BBB	501	AN7	OAB-CAO-CAP-OAC
2	BBB	501	AN7	OAE-CAO-CAP-OAC
3	BBB	502	EDO	O1-C1-C2-O2
2	AAA	501	AN7	CAJ-CAI-CAP-CAO
2	AAA	501	AN7	CAI-CAJ-CAT-CAR

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	501	AN7	6	0
3	AAA	503	EDO	5	0

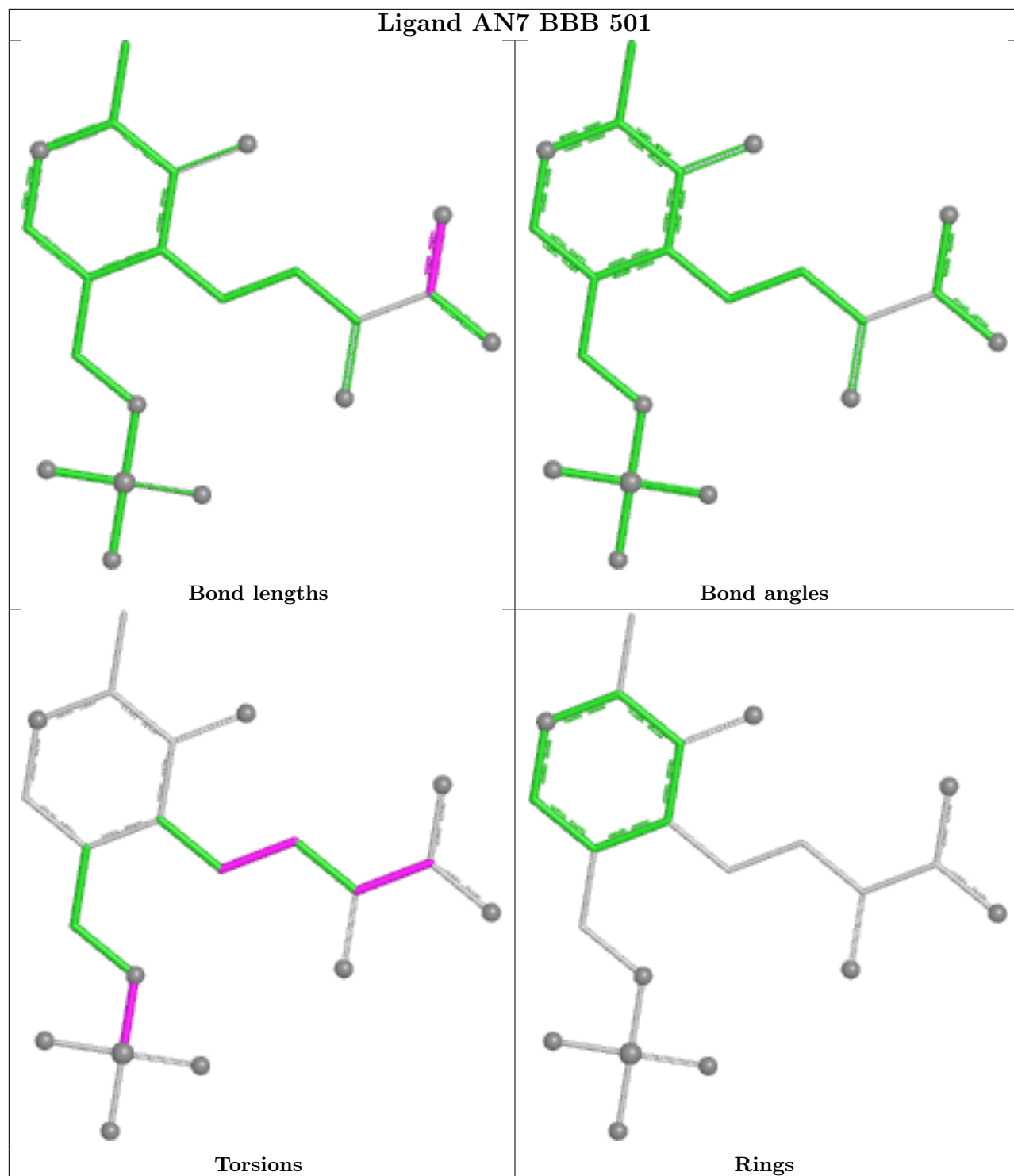
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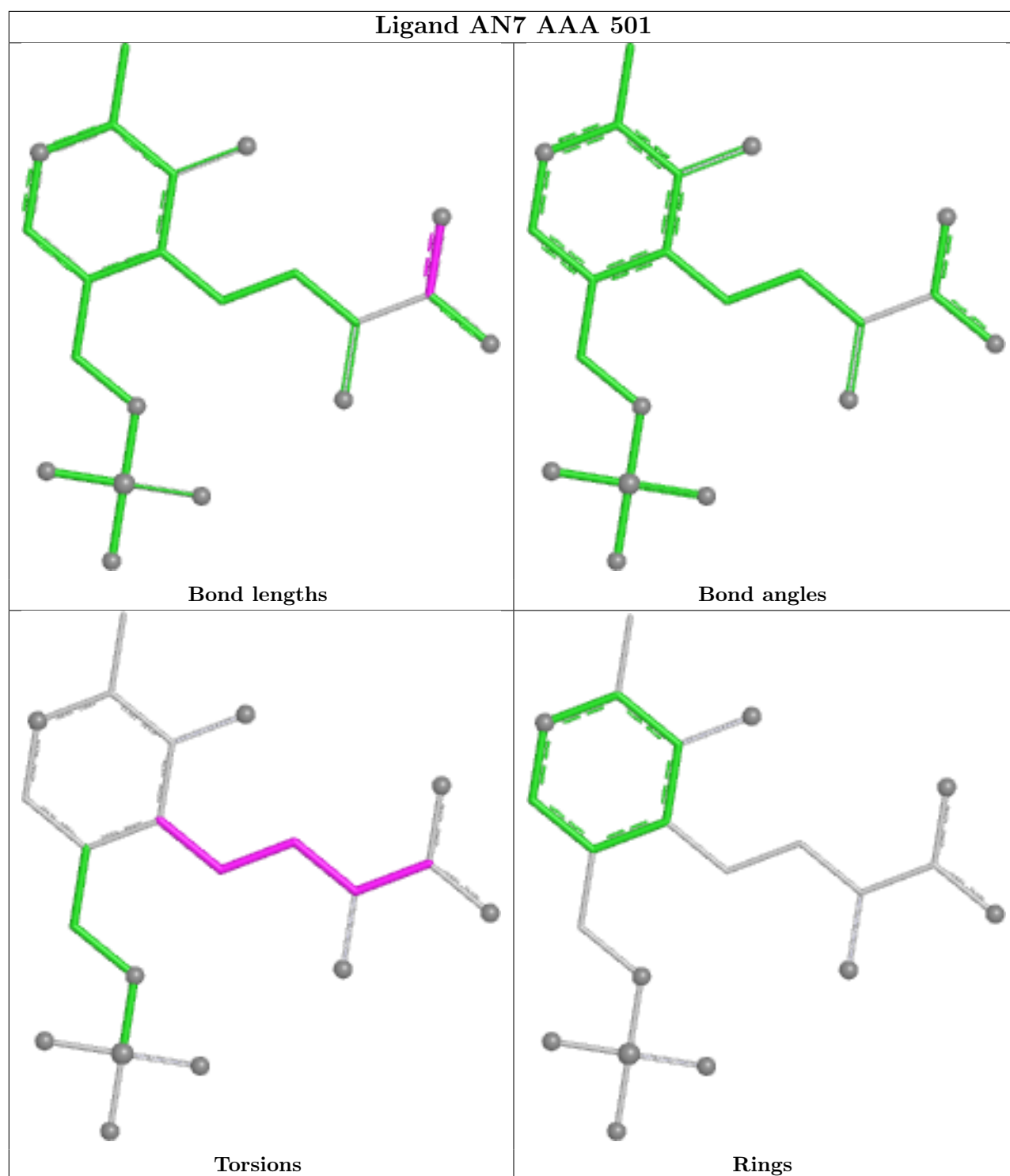
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	501	AN7	8	0
3	BBB	503	EDO	7	0
3	BBB	504	EDO	1	0

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

Ligand AN7 BBB 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	427/493 (86%)	0.26	16 (3%)	45 52	32, 55, 90, 162	5 (1%)
1	BBB	427/493 (86%)	0.64	38 (8%)	15 17	33, 62, 111, 166	2 (0%)
All	All	854/986 (86%)	0.45	54 (6%)	26 30	32, 59, 101, 166	7 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	53	ILE	4.4
1	BBB	364	PHE	4.1
1	BBB	360	TRP	3.9
1	AAA	175	LEU	3.5
1	AAA	169	MET	3.5
1	BBB	45	TRP	3.3
1	BBB	446	LEU	3.3
1	AAA	88	PHE	3.1
1	BBB	441	VAL	3.0
1	BBB	43	TYR	3.0
1	BBB	175	LEU	2.9
1	AAA	168	TYR	2.8
1	BBB	408	PHE	2.8
1	BBB	174	ASP	2.8
1	BBB	169	MET	2.7
1	BBB	177	ILE	2.7
1	BBB	413	LEU	2.7
1	BBB	453	LEU	2.7
1	BBB	348	VAL	2.7
1	BBB	435	VAL	2.7
1	AAA	173	GLY	2.6
1	AAA	158	ILE	2.6
1	BBB	49	GLY	2.6
1	BBB	271	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	174	ASP	2.5
1	BBB	37	THR	2.5
1	BBB	168	TYR	2.5
1	BBB	111	PHE	2.5
1	AAA	403	LEU	2.4
1	BBB	409	PHE	2.4
1	AAA	177	ILE	2.4
1	BBB	52	ILE	2.4
1	AAA	33	ALA	2.4
1	BBB	438	MET	2.4
1	AAA	416[A]	ARG	2.4
1	BBB	384	LEU	2.3
1	BBB	403	LEU	2.3
1	BBB	355	TYR	2.3
1	BBB	442	ALA	2.3
1	BBB	370	VAL	2.3
1	BBB	445	CYS	2.3
1	BBB	458	LEU	2.3
1	AAA	159	GLY	2.2
1	BBB	439	LEU	2.2
1	BBB	367	PHE	2.2
1	BBB	449	PHE	2.2
1	AAA	170	HIS	2.2
1	BBB	437	GLU	2.2
1	AAA	176	PRO	2.2
1	BBB	365	SER	2.2
1	BBB	176	PRO	2.1
1	AAA	89	PHE	2.1
1	AAA	85	TYR	2.1
1	BBB	433	ALA	2.1

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

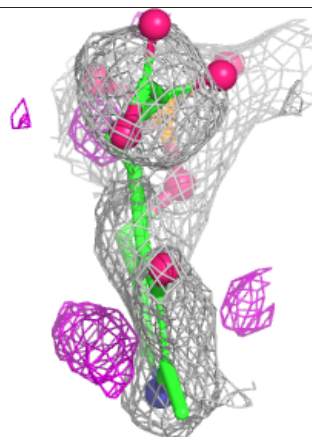
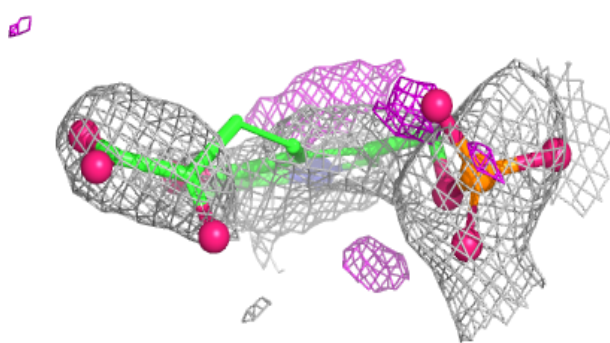
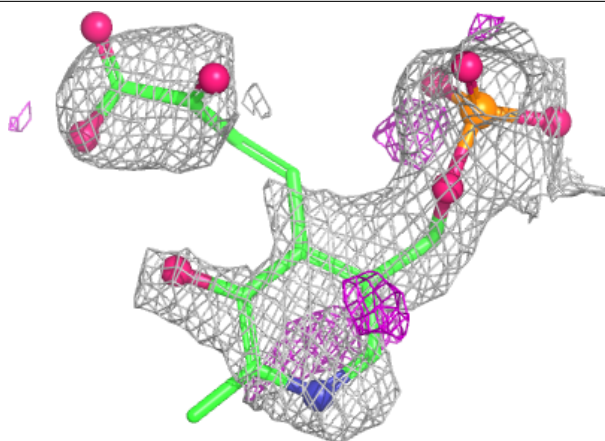
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	BBB	505	1/1	0.77	0.12	84,84,84,84	0
2	AN7	AAA	501	21/21	0.81	0.14	90,102,111,119	0
3	EDO	BBB	504	4/4	0.82	0.11	67,67,67,68	0
2	AN7	BBB	501	21/21	0.86	0.11	89,98,107,110	0
5	NA	AAA	505	1/1	0.89	0.16	65,65,65,65	0
3	EDO	AAA	502	4/4	0.89	0.09	73,76,76,78	0
4	CL	AAA	504	1/1	0.90	0.09	76,76,76,76	0
3	EDO	AAA	503	4/4	0.91	0.09	54,56,63,66	0
3	EDO	BBB	502	4/4	0.92	0.10	76,77,77,79	0
3	EDO	BBB	503	4/4	0.92	0.08	53,60,60,61	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.

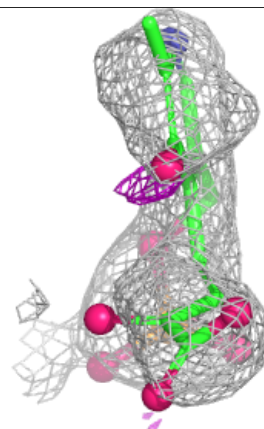
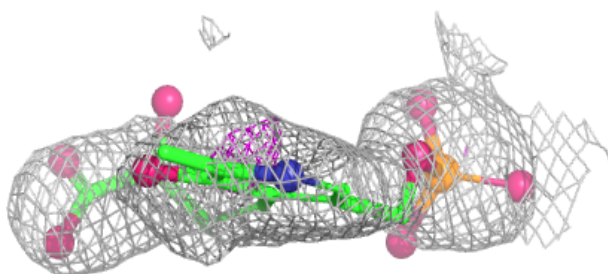
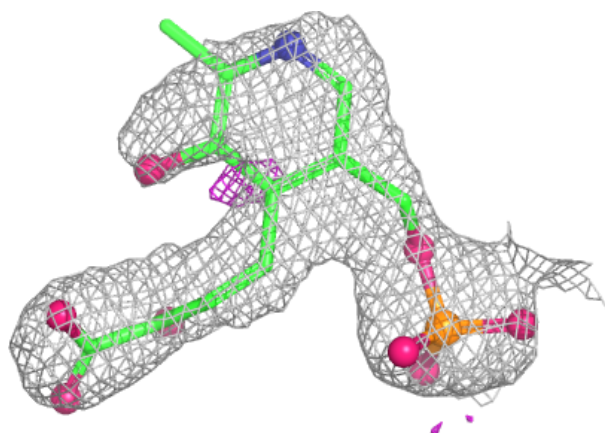
Electron density around AN7 AAA 501:

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



Electron density around AN7 BBB 501:

$2mF_o-DF_c$ (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.