wwPDB X-ray Structure Validation Summary Report (i)

Nov 18, 2022 – 03:30 am GMT

PDB ID	:	7Q9X
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	:	1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

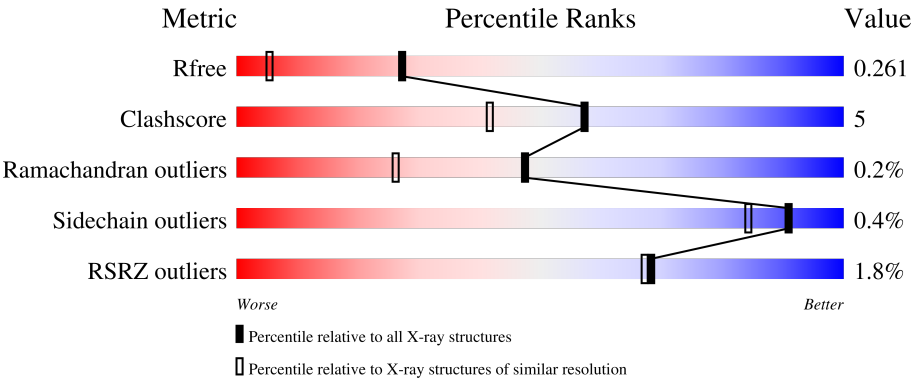
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	87% 5% 8%
1	BBB	493	85% 7% 8%
1	CCC	493	85% 8% 8%
1	DDD	493	83% 9% 8%

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	-
4	NA	DDD	505	-	-	-	X
4	NA	DDD	514	-	-	-	X
5	PLP	BBB	503[B]	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 17188 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	455	Total	C	N	O	S	0	27	0
			3728	2387	647	673	21			
1	BBB	455	Total	C	N	O	S	0	34	0
			3771	2425	647	678	21			
1	CCC	455	Total	C	N	O	S	0	29	0
			3734	2399	644	670	21			
1	DDD	455	Total	C	N	O	S	0	22	0
			3711	2378	643	669	21			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-33	MET	-	initiating methionine	UNP Q7NWG4
AAA	-32	GLY	-	expression tag	UNP Q7NWG4
AAA	-31	SER	-	expression tag	UNP Q7NWG4
AAA	-30	SER	-	expression tag	UNP Q7NWG4
AAA	-29	HIS	-	expression tag	UNP Q7NWG4
AAA	-28	HIS	-	expression tag	UNP Q7NWG4
AAA	-27	HIS	-	expression tag	UNP Q7NWG4
AAA	-26	HIS	-	expression tag	UNP Q7NWG4
AAA	-25	HIS	-	expression tag	UNP Q7NWG4
AAA	-24	HIS	-	expression tag	UNP Q7NWG4
AAA	-23	SER	-	expression tag	UNP Q7NWG4
AAA	-22	SER	-	expression tag	UNP Q7NWG4
AAA	-21	GLY	-	expression tag	UNP Q7NWG4
AAA	-20	LEU	-	expression tag	UNP Q7NWG4
AAA	-19	VAL	-	expression tag	UNP Q7NWG4
AAA	-18	PRO	-	expression tag	UNP Q7NWG4
AAA	-17	ARG	-	expression tag	UNP Q7NWG4
AAA	-16	GLY	-	expression tag	UNP Q7NWG4
AAA	-15	SER	-	expression tag	UNP Q7NWG4
AAA	-14	HIS	-	expression tag	UNP Q7NWG4
AAA	-13	MET	-	expression tag	UNP Q7NWG4

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-12	ALA	-	expression tag	UNP Q7NWG4
AAA	-11	SER	-	expression tag	UNP Q7NWG4
AAA	-10	MET	-	expression tag	UNP Q7NWG4
AAA	-9	THR	-	expression tag	UNP Q7NWG4
AAA	-8	GLY	-	expression tag	UNP Q7NWG4
AAA	-7	GLY	-	expression tag	UNP Q7NWG4
AAA	-6	GLN	-	expression tag	UNP Q7NWG4
AAA	-5	GLN	-	expression tag	UNP Q7NWG4
AAA	-4	MET	-	expression tag	UNP Q7NWG4
AAA	-3	GLY	-	expression tag	UNP Q7NWG4
AAA	-2	ARG	-	expression tag	UNP Q7NWG4
AAA	-1	GLY	-	expression tag	UNP Q7NWG4
AAA	0	SER	-	expression tag	UNP Q7NWG4
BBB	-33	MET	-	initiating methionine	UNP Q7NWG4
BBB	-32	GLY	-	expression tag	UNP Q7NWG4
BBB	-31	SER	-	expression tag	UNP Q7NWG4
BBB	-30	SER	-	expression tag	UNP Q7NWG4
BBB	-29	HIS	-	expression tag	UNP Q7NWG4
BBB	-28	HIS	-	expression tag	UNP Q7NWG4
BBB	-27	HIS	-	expression tag	UNP Q7NWG4
BBB	-26	HIS	-	expression tag	UNP Q7NWG4
BBB	-25	HIS	-	expression tag	UNP Q7NWG4
BBB	-24	HIS	-	expression tag	UNP Q7NWG4
BBB	-23	SER	-	expression tag	UNP Q7NWG4
BBB	-22	SER	-	expression tag	UNP Q7NWG4
BBB	-21	GLY	-	expression tag	UNP Q7NWG4
BBB	-20	LEU	-	expression tag	UNP Q7NWG4
BBB	-19	VAL	-	expression tag	UNP Q7NWG4
BBB	-18	PRO	-	expression tag	UNP Q7NWG4
BBB	-17	ARG	-	expression tag	UNP Q7NWG4
BBB	-16	GLY	-	expression tag	UNP Q7NWG4
BBB	-15	SER	-	expression tag	UNP Q7NWG4
BBB	-14	HIS	-	expression tag	UNP Q7NWG4
BBB	-13	MET	-	expression tag	UNP Q7NWG4
BBB	-12	ALA	-	expression tag	UNP Q7NWG4
BBB	-11	SER	-	expression tag	UNP Q7NWG4
BBB	-10	MET	-	expression tag	UNP Q7NWG4
BBB	-9	THR	-	expression tag	UNP Q7NWG4
BBB	-8	GLY	-	expression tag	UNP Q7NWG4
BBB	-7	GLY	-	expression tag	UNP Q7NWG4
BBB	-6	GLN	-	expression tag	UNP Q7NWG4
BBB	-5	GLN	-	expression tag	UNP Q7NWG4

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-4	MET	-	expression tag	UNP Q7NWG4
BBB	-3	GLY	-	expression tag	UNP Q7NWG4
BBB	-2	ARG	-	expression tag	UNP Q7NWG4
BBB	-1	GLY	-	expression tag	UNP Q7NWG4
BBB	0	SER	-	expression tag	UNP Q7NWG4
CCC	-33	MET	-	initiating methionine	UNP Q7NWG4
CCC	-32	GLY	-	expression tag	UNP Q7NWG4
CCC	-31	SER	-	expression tag	UNP Q7NWG4
CCC	-30	SER	-	expression tag	UNP Q7NWG4
CCC	-29	HIS	-	expression tag	UNP Q7NWG4
CCC	-28	HIS	-	expression tag	UNP Q7NWG4
CCC	-27	HIS	-	expression tag	UNP Q7NWG4
CCC	-26	HIS	-	expression tag	UNP Q7NWG4
CCC	-25	HIS	-	expression tag	UNP Q7NWG4
CCC	-24	HIS	-	expression tag	UNP Q7NWG4
CCC	-23	SER	-	expression tag	UNP Q7NWG4
CCC	-22	SER	-	expression tag	UNP Q7NWG4
CCC	-21	GLY	-	expression tag	UNP Q7NWG4
CCC	-20	LEU	-	expression tag	UNP Q7NWG4
CCC	-19	VAL	-	expression tag	UNP Q7NWG4
CCC	-18	PRO	-	expression tag	UNP Q7NWG4
CCC	-17	ARG	-	expression tag	UNP Q7NWG4
CCC	-16	GLY	-	expression tag	UNP Q7NWG4
CCC	-15	SER	-	expression tag	UNP Q7NWG4
CCC	-14	HIS	-	expression tag	UNP Q7NWG4
CCC	-13	MET	-	expression tag	UNP Q7NWG4
CCC	-12	ALA	-	expression tag	UNP Q7NWG4
CCC	-11	SER	-	expression tag	UNP Q7NWG4
CCC	-10	MET	-	expression tag	UNP Q7NWG4
CCC	-9	THR	-	expression tag	UNP Q7NWG4
CCC	-8	GLY	-	expression tag	UNP Q7NWG4
CCC	-7	GLY	-	expression tag	UNP Q7NWG4
CCC	-6	GLN	-	expression tag	UNP Q7NWG4
CCC	-5	GLN	-	expression tag	UNP Q7NWG4
CCC	-4	MET	-	expression tag	UNP Q7NWG4
CCC	-3	GLY	-	expression tag	UNP Q7NWG4
CCC	-2	ARG	-	expression tag	UNP Q7NWG4
CCC	-1	GLY	-	expression tag	UNP Q7NWG4
CCC	0	SER	-	expression tag	UNP Q7NWG4
DDD	-33	MET	-	initiating methionine	UNP Q7NWG4
DDD	-32	GLY	-	expression tag	UNP Q7NWG4
DDD	-31	SER	-	expression tag	UNP Q7NWG4

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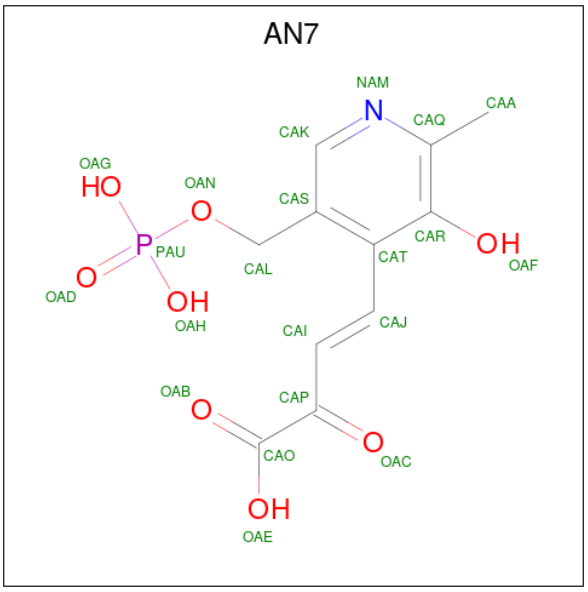
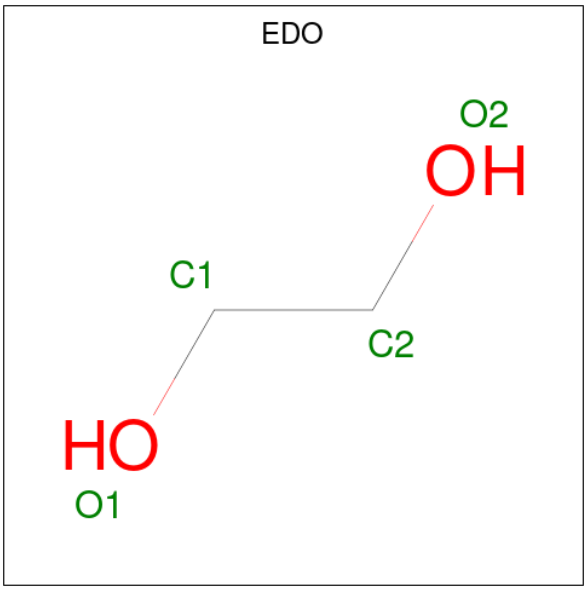
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-30	SER	-	expression tag	UNP Q7NWG4
DDD	-29	HIS	-	expression tag	UNP Q7NWG4
DDD	-28	HIS	-	expression tag	UNP Q7NWG4
DDD	-27	HIS	-	expression tag	UNP Q7NWG4
DDD	-26	HIS	-	expression tag	UNP Q7NWG4
DDD	-25	HIS	-	expression tag	UNP Q7NWG4
DDD	-24	HIS	-	expression tag	UNP Q7NWG4
DDD	-23	SER	-	expression tag	UNP Q7NWG4
DDD	-22	SER	-	expression tag	UNP Q7NWG4
DDD	-21	GLY	-	expression tag	UNP Q7NWG4
DDD	-20	LEU	-	expression tag	UNP Q7NWG4
DDD	-19	VAL	-	expression tag	UNP Q7NWG4
DDD	-18	PRO	-	expression tag	UNP Q7NWG4
DDD	-17	ARG	-	expression tag	UNP Q7NWG4
DDD	-16	GLY	-	expression tag	UNP Q7NWG4
DDD	-15	SER	-	expression tag	UNP Q7NWG4
DDD	-14	HIS	-	expression tag	UNP Q7NWG4
DDD	-13	MET	-	expression tag	UNP Q7NWG4
DDD	-12	ALA	-	expression tag	UNP Q7NWG4
DDD	-11	SER	-	expression tag	UNP Q7NWG4
DDD	-10	MET	-	expression tag	UNP Q7NWG4
DDD	-9	THR	-	expression tag	UNP Q7NWG4
DDD	-8	GLY	-	expression tag	UNP Q7NWG4
DDD	-7	GLY	-	expression tag	UNP Q7NWG4
DDD	-6	GLN	-	expression tag	UNP Q7NWG4
DDD	-5	GLN	-	expression tag	UNP Q7NWG4
DDD	-4	MET	-	expression tag	UNP Q7NWG4
DDD	-3	GLY	-	expression tag	UNP Q7NWG4
DDD	-2	ARG	-	expression tag	UNP Q7NWG4
DDD	-1	GLY	-	expression tag	UNP Q7NWG4
DDD	0	SER	-	expression tag	UNP Q7NWG4

- Molecule 2 is (3E)-4-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}-2-oxobut-3-enoic acid (three-letter code: AN7) (formula: $C_{11}H_{12}NO_8P$) (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	1
			21	11	1	8	1		
2	CCC	1	Total	C	N	O	P	0	0
			21	11	1	8	1		
2	DDD	1	Total	C	N	O	P	0	0
			21	11	1	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

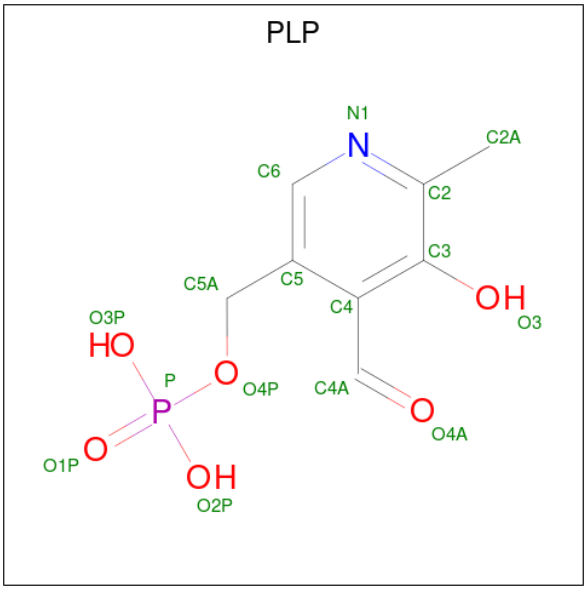


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

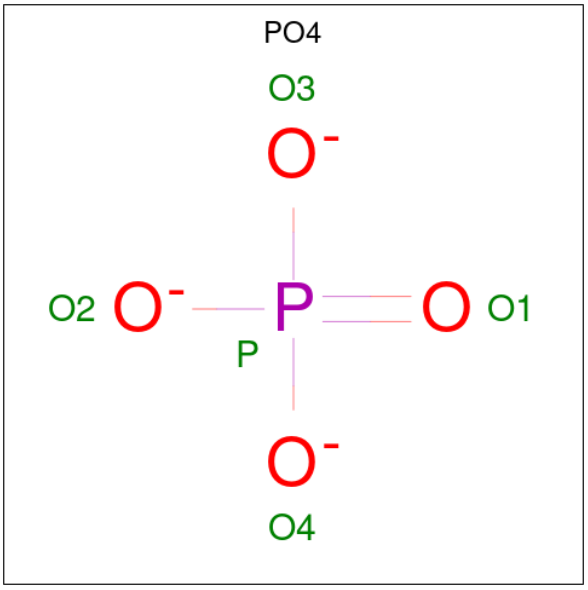
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	13	Total Na 13 13	0	0
4	BBB	26	Total Na 26 26	0	0
4	CCC	17	Total Na 17 17	0	0
4	DDD	21	Total Na 21 21	0	0

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



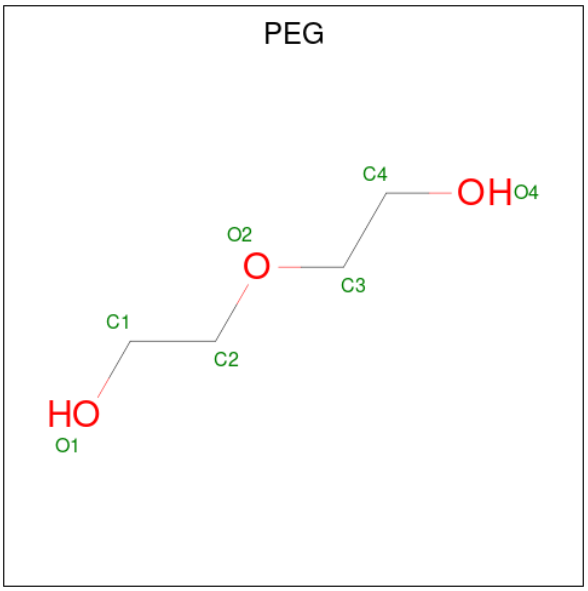
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	BBB	1	Total	C	N	O	P	0	1
			15	8	1	5	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	O	P	0	0
			5	4	1		
6	DDD	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	CCC	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

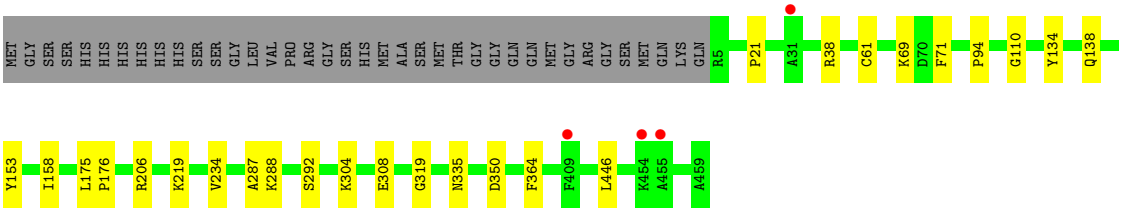
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	526	Total O 526 526	0	0
8	BBB	567	Total O 567 567	0	0
8	CCC	453	Total O 453 453	0	0
8	DDD	485	Total O 485 485	0	0

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.

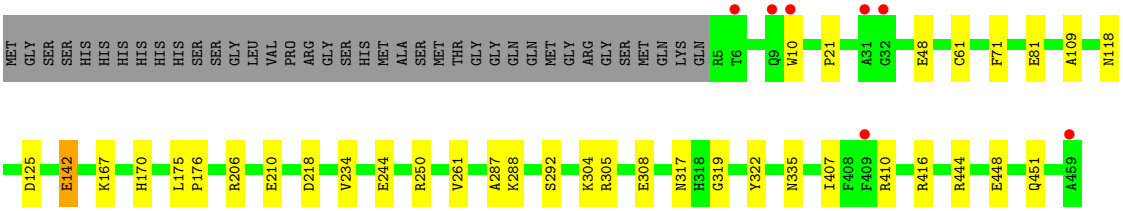
• Molecule 1: Probable aminotransferase

Chain AAA:



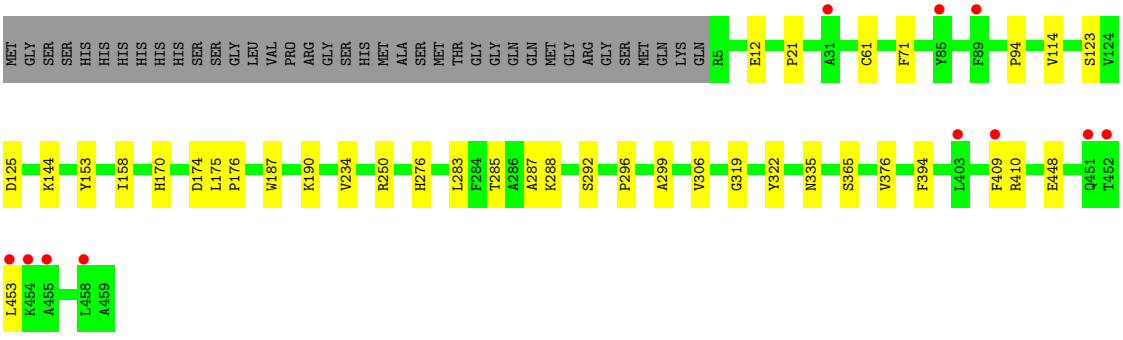
• Molecule 1: Probable aminotransferase

Chain BBB:



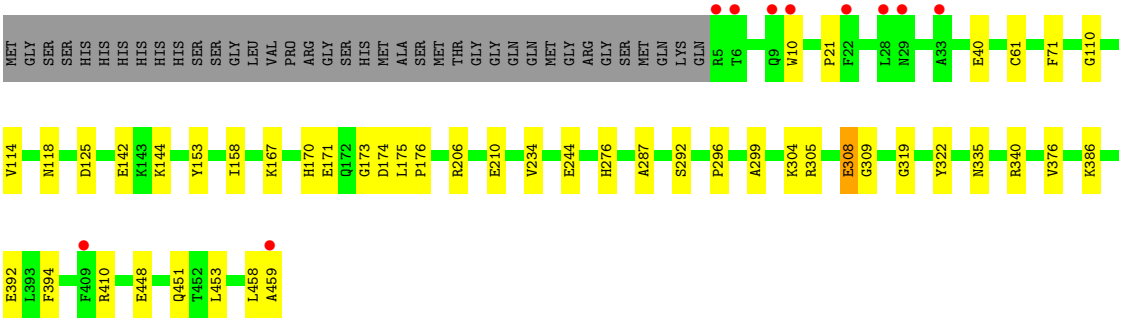
• Molecule 1: Probable aminotransferase

Chain CCC:



• Molecule 1: Probable aminotransferase

Chain DDD:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER MET GLN LYS GLN R5 T6 Q9 W10 P21 F22 L28 N29 A33 E40 C61 F71 G110
V114 N118 D125 E142 K143 K144 Y153 I158 K167 H170 E171 Q172 G173 D174 L175 P176 R206 E210 V234 E244 H276 A287 S292 P296 A299 K304 R305 E308 G309 G319 Y322 N335 R340 V376 K386
E392 L393 F394 F409 R410 E448 Q451 T452 L453 L458 A459

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.33Å 61.38Å 116.48Å 103.56° 89.38° 105.42°	Depositor
Resolution (Å)	39.43 – 1.60 57.44 – 1.60	Depositor EDS
% Data completeness (in resolution range)	76.1 (39.43-1.60) 76.1 (57.44-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.261 0.227 , 0.261	Depositor DCC
R_{free} test set	7878 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17188	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9432e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, NA, AN7, PO4, EDO, PLP

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	0.64	0/3901	0.74	0/5271
1	BBB	0.65	0/3973	0.75	0/5367
1	CCC	0.64	0/3913	0.74	0/5286
1	DDD	0.64	0/3871	0.73	0/5235
All	All	0.64	0/15658	0.74	0/21159

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	3728	0	3697	34	0
1	BBB	3771	0	3768	48	0
1	CCC	3734	0	3728	32	0
1	DDD	3711	0	3659	50	0
2	AAA	21	0	8	8	0
2	BBB	21	0	8	0	0
2	CCC	21	0	8	4	0
2	DDD	21	0	8	4	0
3	AAA	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	4	0	6	0	0
3	CCC	4	0	6	0	0
3	DDD	4	0	6	0	0
4	AAA	13	0	0	0	0
4	BBB	26	0	0	0	0
4	CCC	17	0	0	1	0
4	DDD	21	0	0	0	0
5	BBB	15	0	6	6	0
6	BBB	5	0	0	0	0
6	DDD	5	0	0	0	0
7	CCC	7	0	10	0	0
8	AAA	526	0	0	9	0
8	BBB	567	0	0	18	0
8	CCC	453	0	0	8	0
8	DDD	485	0	0	17	0
All	All	17188	0	14930	146	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.

The worst 5 of 146 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:BBB:304[A]:LYS:HE2	8:BBB:602:HOH:O	1.14	1.23
1:BBB:206[A]:ARG:HG3	8:BBB:608:HOH:O	1.01	1.16
1:BBB:288[B]:LYS:NZ	5:BBB:503[B]:PLP:C4A	2.11	1.13
1:AAA:308[B]:GLU:HG3	8:AAA:639:HOH:O	1.45	1.12
1:DDD:206[A]:ARG:HG3	8:DDD:619:HOH:O	0.95	1.12

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	480/493 (97%)	461 (96%)	18 (4%)	1 (0%)	47	26
1	BBB	488/493 (99%)	471 (96%)	16 (3%)	1 (0%)	47	26
1	CCC	482/493 (98%)	465 (96%)	16 (3%)	1 (0%)	47	26
1	DDD	476/493 (97%)	460 (97%)	15 (3%)	1 (0%)	47	26
All	All	1926/1972 (98%)	1857 (96%)	65 (3%)	4 (0%)	47	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	287	ALA
1	DDD	287	ALA
1	AAA	287	ALA
1	CCC	287	ALA

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	391/394 (99%)	391 (100%)	0	100	100
1	BBB	399/394 (101%)	395 (99%)	4 (1%)	76	61
1	CCC	393/394 (100%)	391 (100%)	2 (0%)	88	80
1	DDD	387/394 (98%)	385 (100%)	2 (0%)	88	80
All	All	1570/1576 (100%)	1562 (100%)	8 (0%)	91	80

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	308	GLU
1	DDD	142	GLU
1	CCC	409[A]	PHE
1	BBB	451	GLN
1	CCC	409[B]	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 90 ligands modelled in this entry, 77 are monoatomic - leaving 13 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	CCC	501	4	21,21,21	2.20	2 (9%)	28,30,30	1.17	2 (7%)
3	EDO	CCC	503	-	3,3,3	0.07	0	2,2,2	0.40	0
7	PEG	CCC	502	-	6,6,6	0.21	0	5,5,5	0.21	0
3	EDO	DDD	502	-	3,3,3	0.10	0	2,2,2	0.18	0
6	PO4	DDD	503	-	4,4,4	0.74	0	6,6,6	0.43	0
2	AN7	DDD	501	4	21,21,21	2.62	2 (9%)	28,30,30	1.07	1 (3%)
3	EDO	AAA	502	-	3,3,3	0.17	0	2,2,2	0.28	0
6	PO4	BBB	504	-	4,4,4	0.73	0	6,6,6	0.47	0
3	EDO	BBB	502	-	3,3,3	0.08	0	2,2,2	0.41	0
5	PLP	BBB	503[B]	-	15,15,16	0.64	0	20,22,23	1.57	4 (20%)
3	EDO	AAA	503	-	3,3,3	0.07	0	2,2,2	0.21	0
2	AN7	AAA	501	4	21,21,21	2.62	1 (4%)	28,30,30	1.09	2 (7%)
2	AN7	BBB	501[A]	4	21,21,21	2.63	2 (9%)	28,30,30	0.90	1 (3%)

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	CCC	501	4	-	1/15/15/15	0/1/1/1
3	EDO	CCC	503	-	-	1/1/1/1	-
7	PEG	CCC	502	-	-	2/4/4/4	-
3	EDO	DDD	502	-	-	0/1/1/1	-
2	AN7	DDD	501	4	-	6/15/15/15	0/1/1/1
3	EDO	AAA	502	-	-	1/1/1/1	-
3	EDO	BBB	502	-	-	1/1/1/1	-
5	PLP	BBB	503[B]	-	-	0/6/6/8	0/1/1/1
3	EDO	AAA	503	-	-	1/1/1/1	-
2	AN7	AAA	501	4	-	5/15/15/15	0/1/1/1
2	AN7	BBB	501[A]	4	-	6/15/15/15	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	AN7	CAO-CAP	-11.55	1.39	1.54
2	DDD	501	AN7	CAO-CAP	-11.53	1.40	1.54
2	BBB	501[A]	AN7	CAO-CAP	-11.38	1.40	1.54
2	CCC	501	AN7	CAO-CAP	-9.25	1.42	1.54
2	BBB	501[A]	AN7	OAE-CAO	-3.31	1.20	1.30

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BBB	503[B]	PLP	C4A-C4-C5	4.19	125.25	120.94
2	CCC	501	AN7	CAJ-CAI-CAP	3.87	127.19	121.48
2	DDD	501	AN7	CAJ-CAI-CAP	3.51	126.66	121.48
5	BBB	503[B]	PLP	C3-C4-C5	-3.31	115.16	118.74
2	AAA	501	AN7	CAJ-CAI-CAP	2.89	125.74	121.48

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	AN7	CAJ-CAI-CAP-CAO
2	AAA	501	AN7	OAB-CAO-CAP-CAI
2	AAA	501	AN7	OAE-CAO-CAP-CAI

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Mol	Chain	Res	Type	Atoms
2	BBB	501[A]	AN7	CAJ-CAI-CAP-CAO
2	BBB	501[A]	AN7	OAB-CAO-CAP-CAI

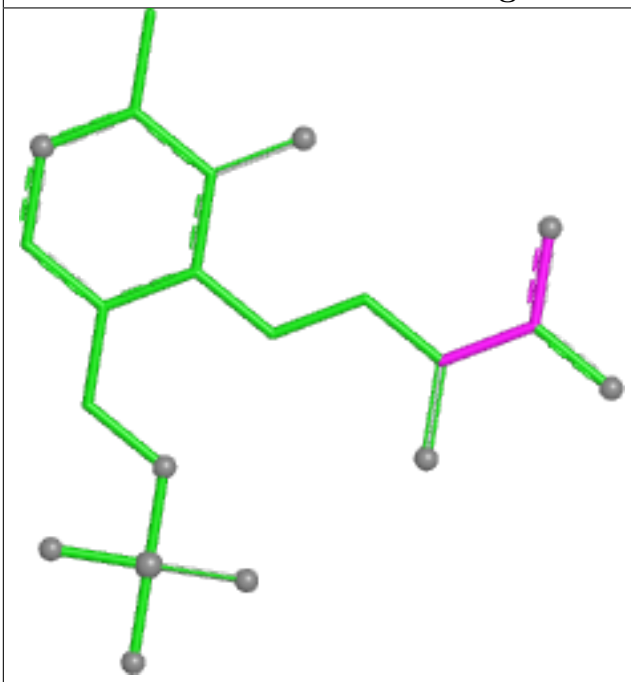
There are no ring outliers.

4 monomers are involved in 22 short contacts:

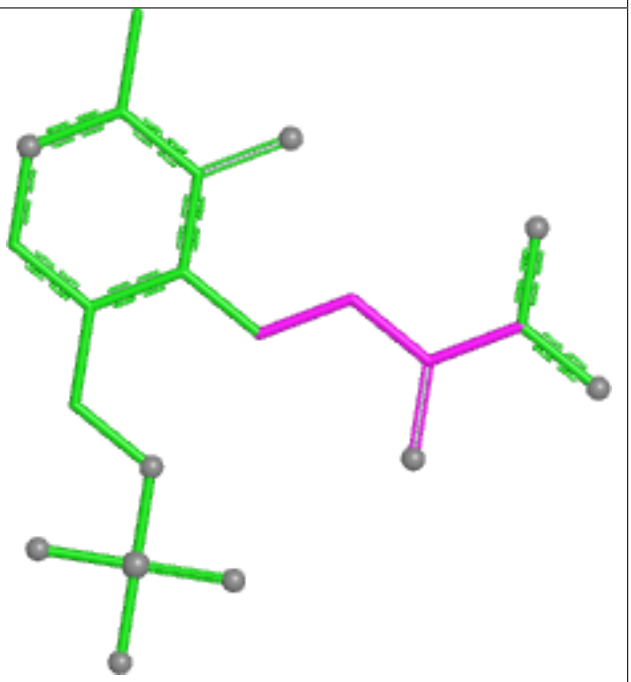
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	501	AN7	4	0
2	DDD	501	AN7	4	0
5	BBB	503[B]	PLP	6	0
2	AAA	501	AN7	8	0

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 then 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.

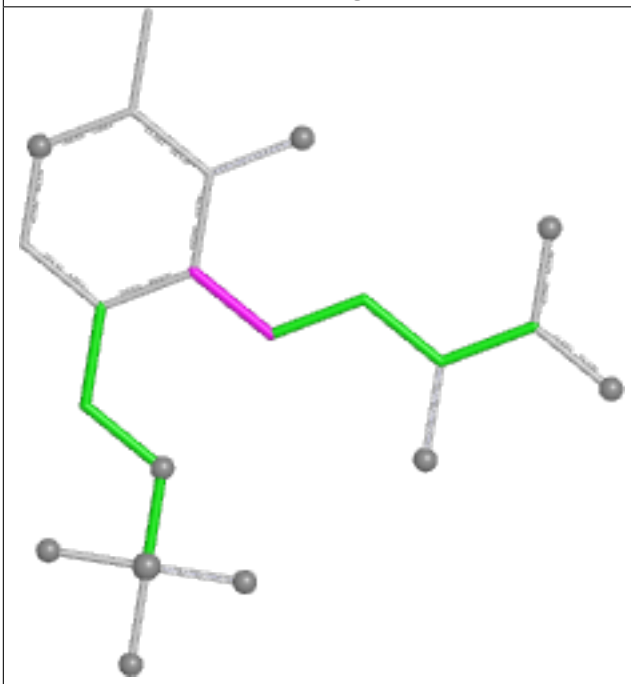
Ligand AN7 CCC 501



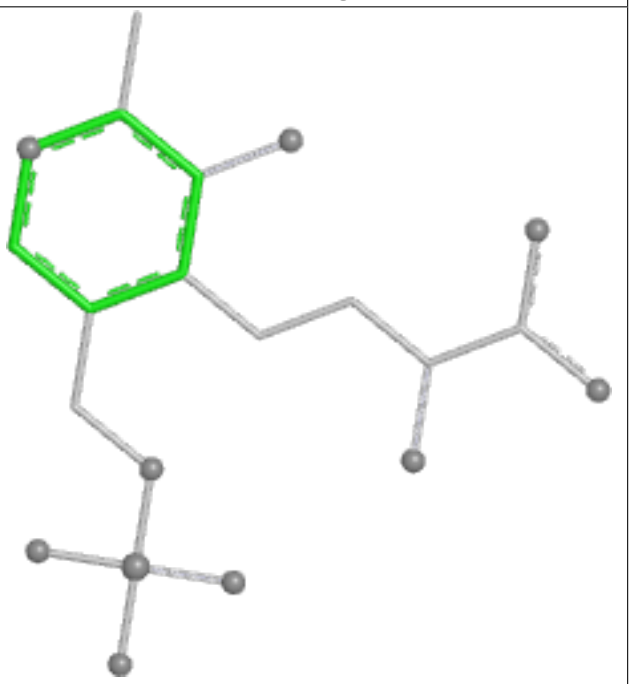
Bond lengths



Bond angles

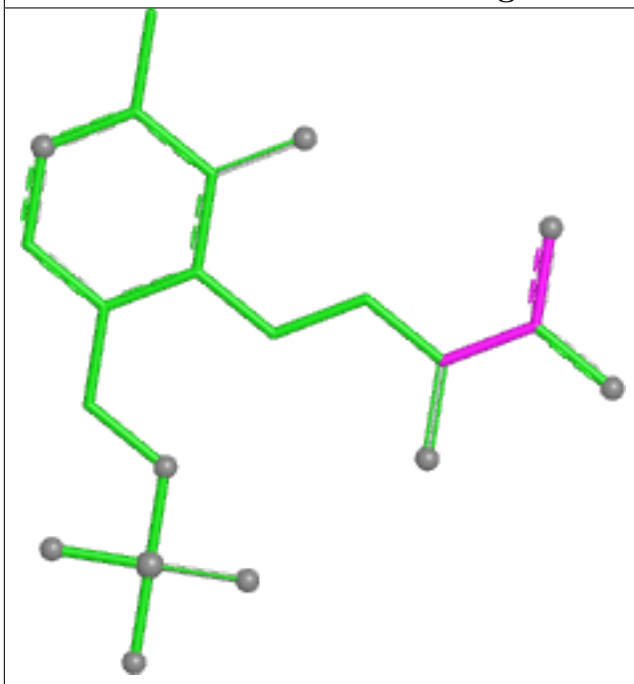


Torsions



Rings

Ligand AN7 DDD 501



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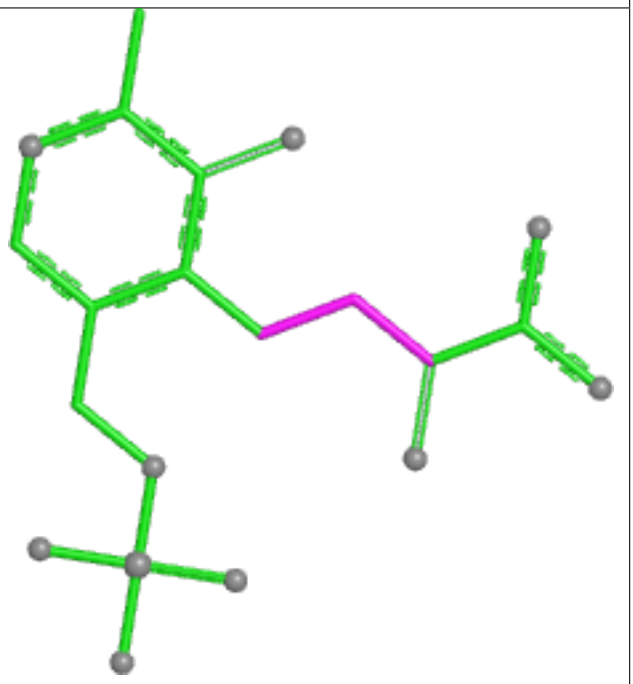
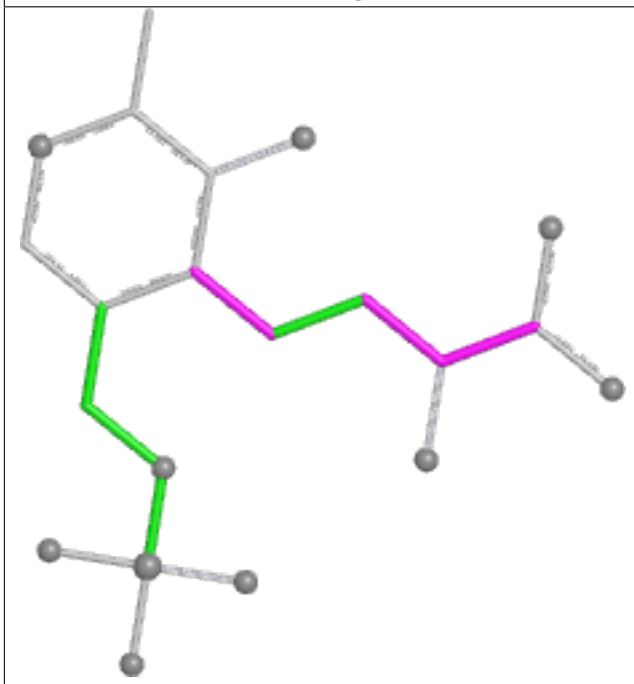
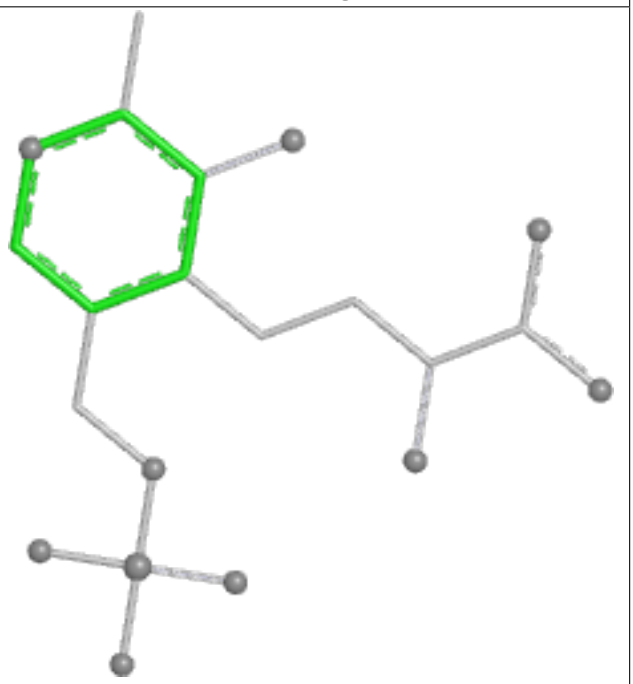


Bond angles

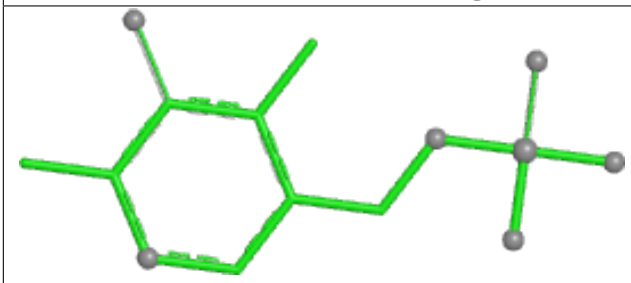


Torsions

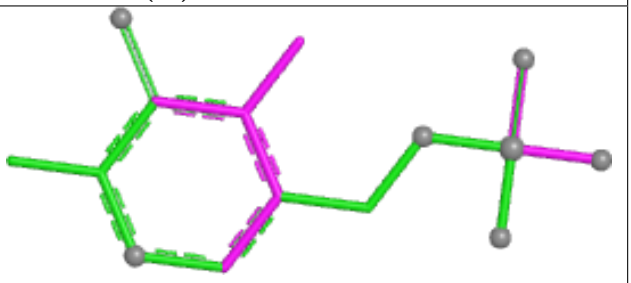


Rings

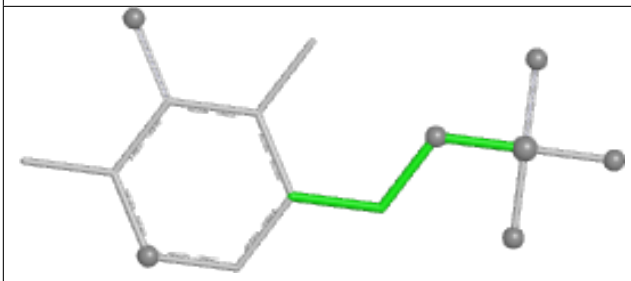
Ligand PLP BBB 503 (B)



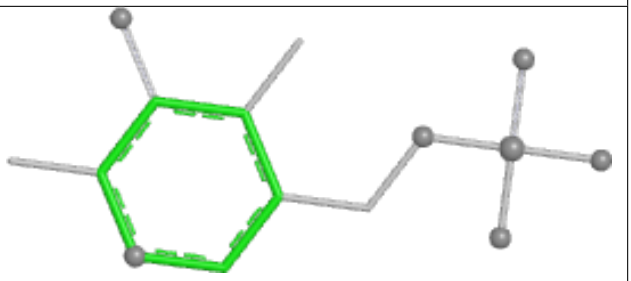
Bond lengths



Bond angles

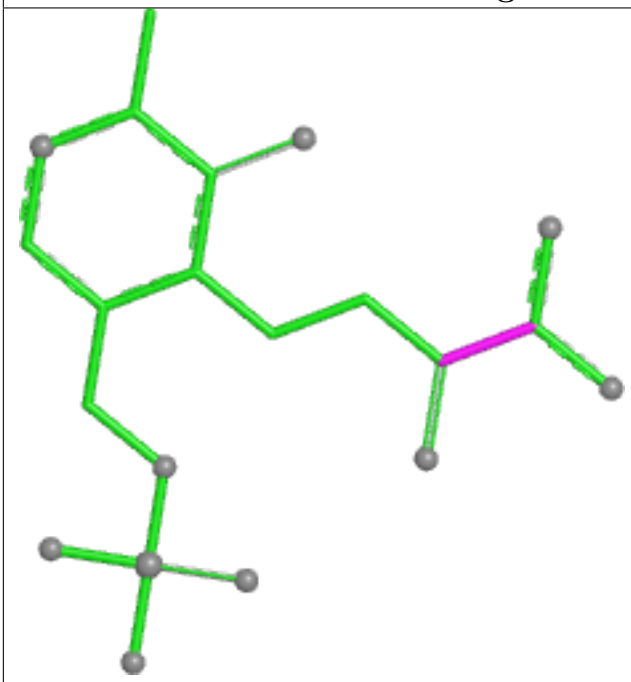


Torsions

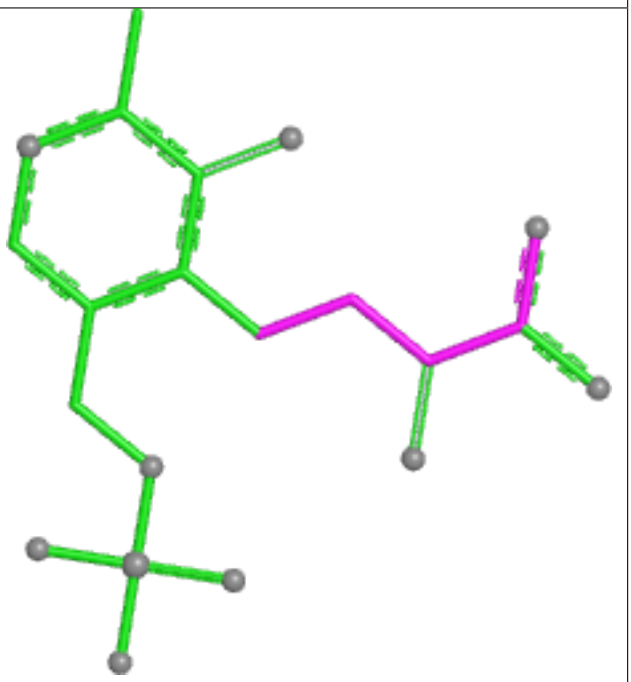


Rings

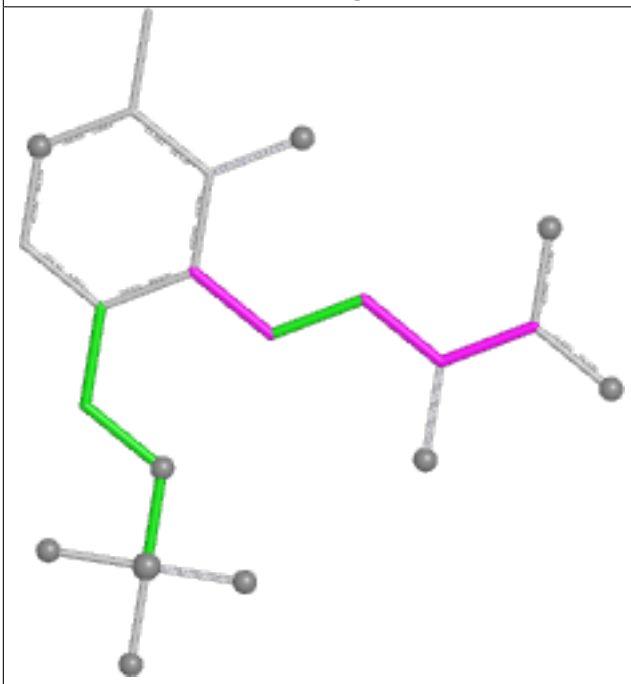
Ligand AN7 AAA 501



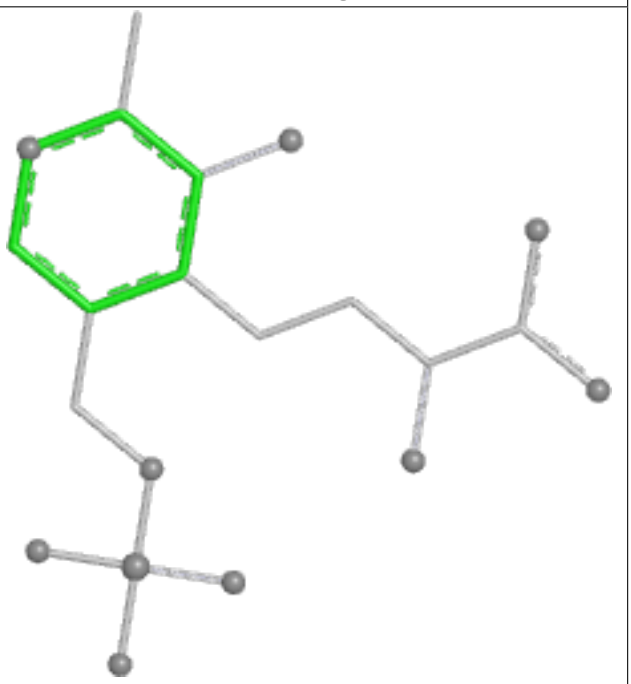
Bond lengths



Bond angles

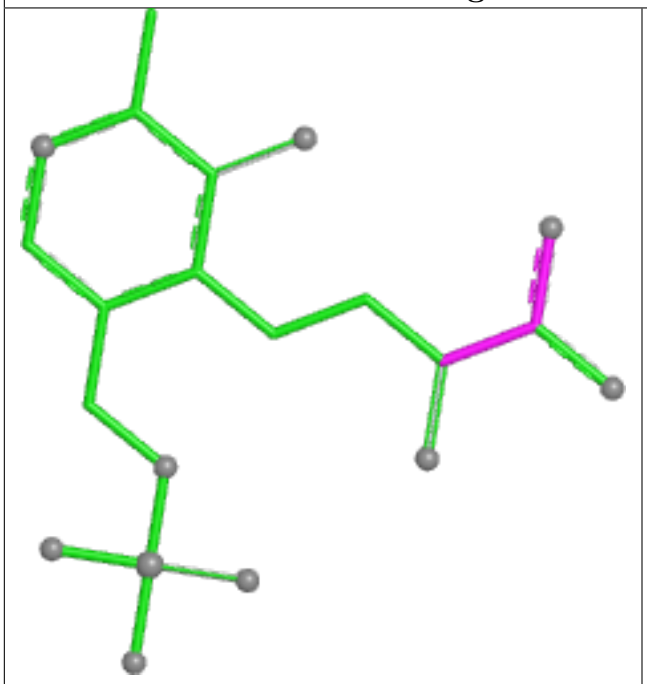


Torsions

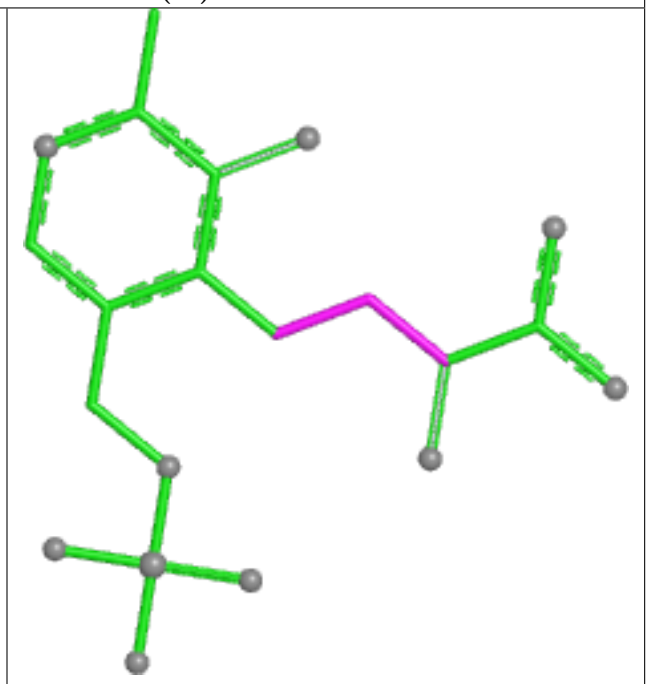


Rings

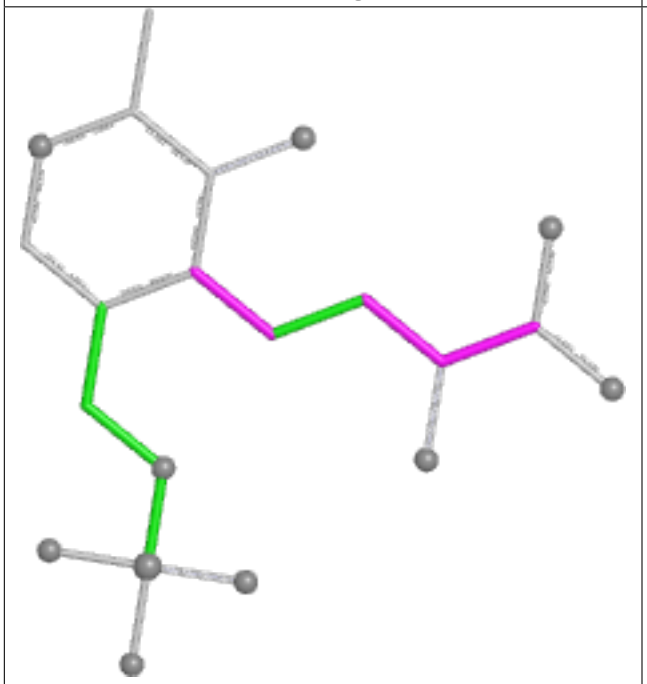
Ligand AN7 BBB 501 (A)



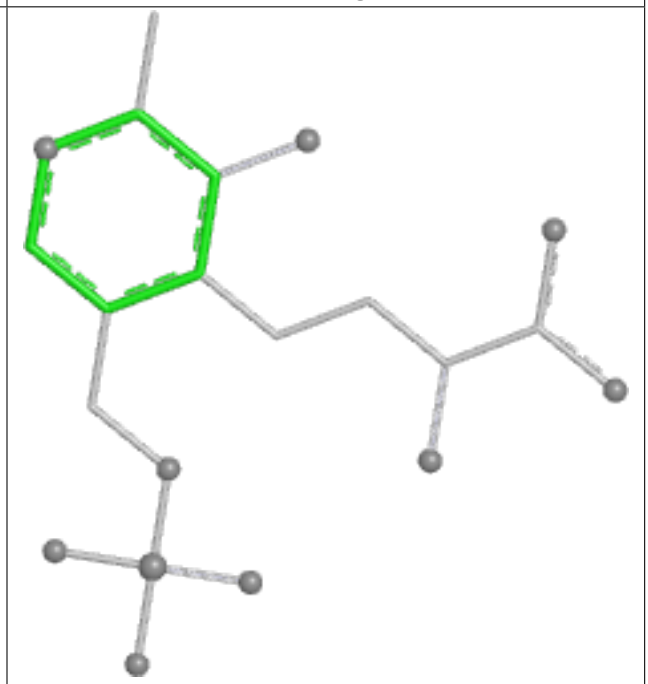
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	455/493 (92%)	-0.28	4 (0%)	84	84	5, 12, 23, 58	0
1	BBB	455/493 (92%)	-0.24	7 (1%)	73	73	4, 12, 24, 40	0
1	CCC	455/493 (92%)	-0.17	11 (2%)	59	56	5, 14, 34, 77	0
1	DDD	455/493 (92%)	-0.08	10 (2%)	62	60	5, 16, 45, 111	0
All	All	1820/1972 (92%)	-0.19	32 (1%)	68	67	4, 13, 32, 111	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	459	ALA	4.9
1	DDD	28	LEU	4.8
1	DDD	5	ARG	4.3
1	BBB	6	THR	3.8
1	DDD	409[A]	PHE	3.7

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 monosaccharides 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, 95^{th} 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
4	NA	DDD	505	1/1	0.19	0.81	60,60,60,60	0
4	NA	DDD	510	1/1	0.21	0.35	51,51,51,51	0
4	NA	BBB	527	1/1	0.38	0.35	54,54,54,54	0
4	NA	DDD	514	1/1	0.48	0.57	70,70,70,70	0
4	NA	BBB	525	1/1	0.51	0.14	55,55,55,55	0
4	NA	BBB	530	1/1	0.52	0.30	47,47,47,47	0
4	NA	DDD	516	1/1	0.58	0.21	49,49,49,49	0
4	NA	CCC	519	1/1	0.62	0.15	26,26,26,26	1
4	NA	BBB	529	1/1	0.66	0.35	48,48,48,48	0
4	NA	CCC	516	1/1	0.67	0.26	42,42,42,42	0
4	NA	CCC	509	1/1	0.67	0.31	44,44,44,44	0
4	NA	DDD	517	1/1	0.68	0.22	39,39,39,39	0
4	NA	BBB	509	1/1	0.69	0.16	41,41,41,41	0
4	NA	DDD	512	1/1	0.70	0.17	46,46,46,46	0
4	NA	BBB	514	1/1	0.71	0.22	36,36,36,36	0
4	NA	BBB	524	1/1	0.72	0.24	33,33,33,33	0
3	EDO	BBB	502	4/4	0.72	0.29	41,41,42,44	0
4	NA	BBB	519	1/1	0.73	0.17	47,47,47,47	0
3	EDO	AAA	502	4/4	0.75	0.32	34,35,35,36	0
4	NA	CCC	504	1/1	0.76	0.17	42,42,42,42	0
4	NA	BBB	508	1/1	0.77	0.30	39,39,39,39	0
4	NA	BBB	522	1/1	0.78	0.12	37,37,37,37	0
4	NA	DDD	513	1/1	0.79	0.13	41,41,41,41	0
4	NA	CCC	511	1/1	0.79	0.21	43,43,43,43	0
3	EDO	AAA	503	4/4	0.80	0.41	34,35,36,36	0
4	NA	AAA	516	1/1	0.80	0.40	48,48,48,48	0
4	NA	BBB	528	1/1	0.81	0.25	47,47,47,47	0
4	NA	CCC	510	1/1	0.82	0.23	39,39,39,39	0
4	NA	DDD	508	1/1	0.82	0.65	57,57,57,57	0
7	PEG	CCC	502	7/7	0.82	0.23	27,33,37,37	0
4	NA	DDD	520	1/1	0.83	0.17	62,62,62,62	0
4	NA	BBB	505	1/1	0.84	0.08	47,47,47,47	0
4	NA	AAA	508	1/1	0.84	0.12	39,39,39,39	0
4	NA	CCC	520	1/1	0.84	0.31	44,44,44,44	0
4	NA	DDD	515	1/1	0.84	0.17	49,49,49,49	0
4	NA	BBB	526	1/1	0.85	0.13	37,37,37,37	0
4	NA	AAA	512	1/1	0.85	0.21	42,42,42,42	0
4	NA	DDD	509	1/1	0.85	0.09	37,37,37,37	0
4	NA	DDD	523	1/1	0.85	0.14	41,41,41,41	0
4	NA	CCC	506	1/1	0.85	0.38	45,45,45,45	0
4	NA	BBB	515	1/1	0.87	0.21	39,39,39,39	0
4	NA	DDD	504	1/1	0.88	0.11	25,25,25,25	0
3	EDO	DDD	502	4/4	0.88	0.24	32,32,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	DDD	518	1/1	0.88	0.14	31,31,31,31	0
4	NA	DDD	506	1/1	0.88	0.38	36,36,36,36	0
4	NA	DDD	522	1/1	0.88	0.12	32,32,32,32	0
4	NA	BBB	513	1/1	0.88	0.20	40,40,40,40	0
4	NA	DDD	524	1/1	0.88	0.15	39,39,39,39	0
4	NA	BBB	523	1/1	0.88	0.16	44,44,44,44	0
4	NA	BBB	517	1/1	0.89	0.16	42,42,42,42	0
4	NA	DDD	521	1/1	0.90	0.27	47,47,47,47	0
4	NA	AAA	513	1/1	0.90	0.15	43,43,43,43	0
4	NA	AAA	514	1/1	0.90	0.28	47,47,47,47	0
3	EDO	CCC	503	4/4	0.90	0.18	27,28,28,29	0
4	NA	BBB	510	1/1	0.90	0.28	37,37,37,37	0
4	NA	BBB	506	1/1	0.91	0.32	30,30,30,30	0
4	NA	BBB	521	1/1	0.91	0.10	37,37,37,37	0
4	NA	AAA	505	1/1	0.92	0.26	31,31,31,31	0
4	NA	AAA	509	1/1	0.92	0.21	46,46,46,46	0
4	NA	CCC	507	1/1	0.92	0.28	27,27,27,27	0
4	NA	DDD	519	1/1	0.92	0.07	24,24,24,24	0
4	NA	CCC	508	1/1	0.92	0.09	35,35,35,35	0
4	NA	BBB	511	1/1	0.93	0.20	36,36,36,36	0
4	NA	BBB	516	1/1	0.93	0.36	41,41,41,41	0
4	NA	AAA	511	1/1	0.93	0.10	43,43,43,43	0
4	NA	AAA	515	1/1	0.93	0.13	41,41,41,41	0
4	NA	BBB	520	1/1	0.93	0.17	37,37,37,37	0
4	NA	BBB	507	1/1	0.94	0.07	37,37,37,37	0
4	NA	CCC	515	1/1	0.94	0.19	37,37,37,37	0
4	NA	BBB	518	1/1	0.94	0.12	36,36,36,36	0
4	NA	BBB	512	1/1	0.94	0.07	33,33,33,33	0
2	AN7	DDD	501	21/21	0.94	0.13	14,20,35,35	0
4	NA	CCC	513	1/1	0.95	0.18	35,35,35,35	0
4	NA	CCC	514	1/1	0.95	0.12	42,42,42,42	0
2	AN7	CCC	501	21/21	0.95	0.11	12,18,33,36	0
4	NA	DDD	507	1/1	0.95	0.19	31,31,31,31	0
2	AN7	AAA	501	21/21	0.95	0.12	9,14,26,28	0
4	NA	AAA	507	1/1	0.95	0.20	39,39,39,39	0
2	AN7	BBB	501[A]	21/21	0.95	0.10	8,13,16,17	21
4	NA	AAA	504	1/1	0.96	0.14	33,33,33,33	0
4	NA	AAA	510	1/1	0.96	0.12	38,38,38,38	0
4	NA	CCC	512	1/1	0.96	0.05	40,40,40,40	0
4	NA	DDD	511	1/1	0.96	0.19	39,39,39,39	0
4	NA	CCC	517	1/1	0.96	0.14	33,33,33,33	0
5	PLP	BBB	503[B]	15/16	0.96	0.09	4,8,9,11	15

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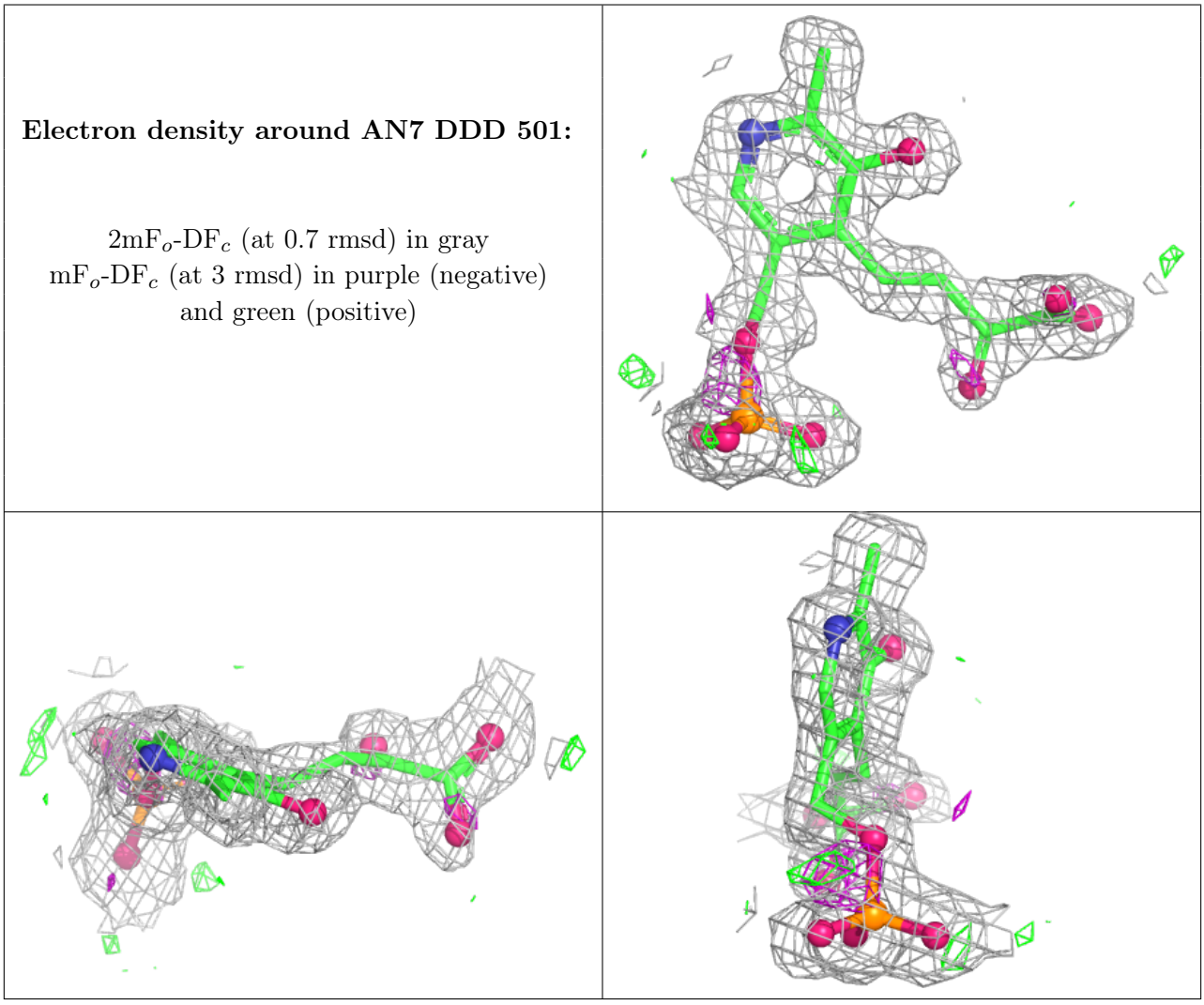
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	AAA	506	1/1	0.96	0.30	32,32,32,32	0
6	PO4	BBB	504	5/5	0.97	0.10	26,26,30,30	0
4	NA	CCC	518	1/1	0.97	0.07	24,24,24,24	0
6	PO4	DDD	503	5/5	0.98	0.13	32,37,38,38	0
4	NA	CCC	505	1/1	0.98	0.23	26,26,26,26	0

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.

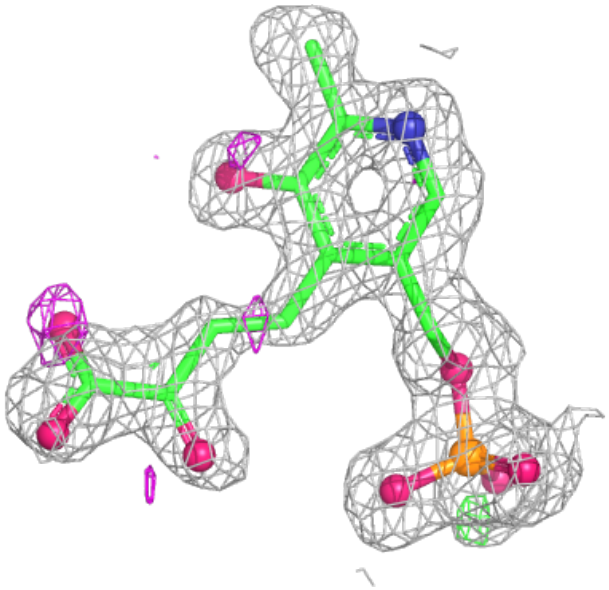
Electron density around AN7 DDD 501:

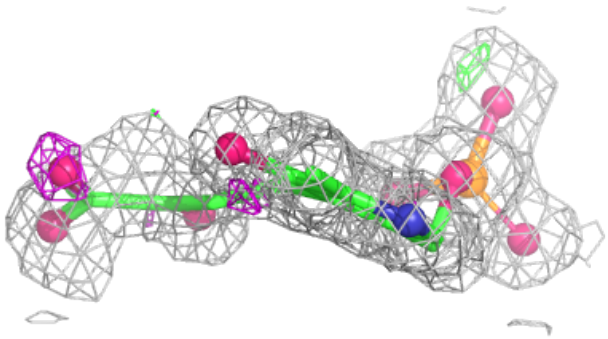
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

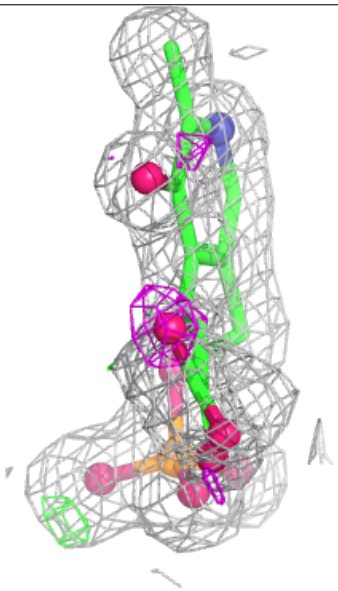


Electron density around AN7 CCC 501:

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

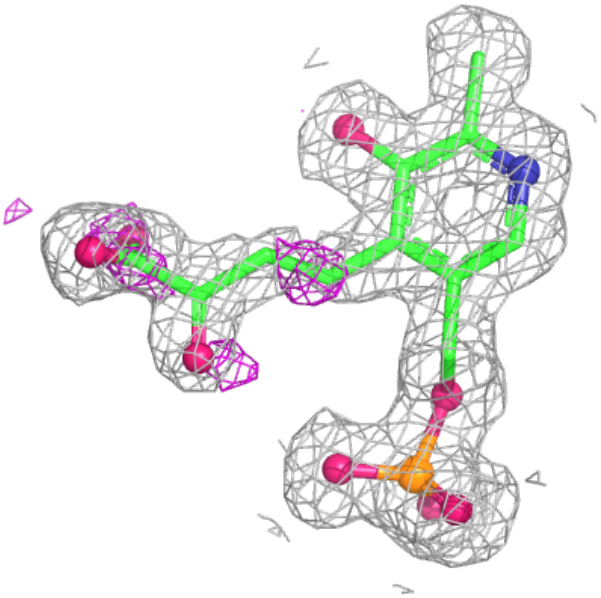


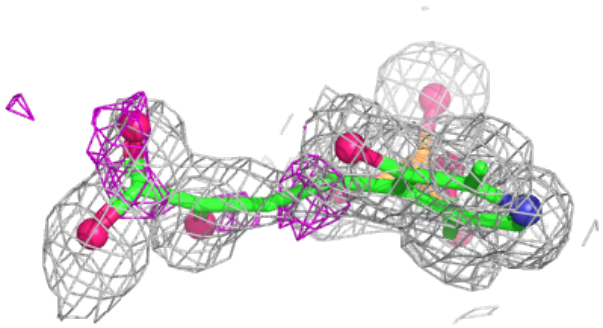


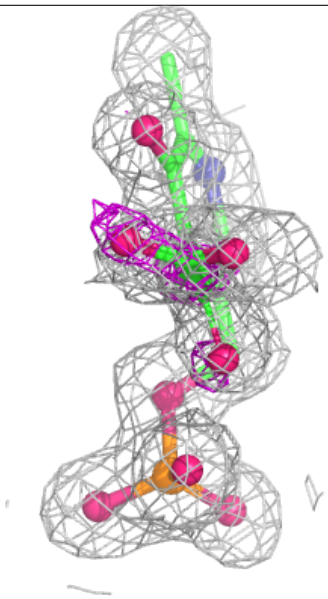


Electron density around AN7 AAA 501:

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

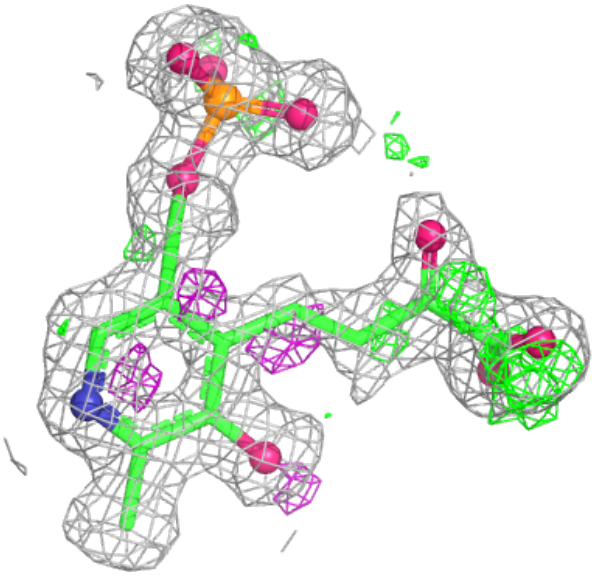


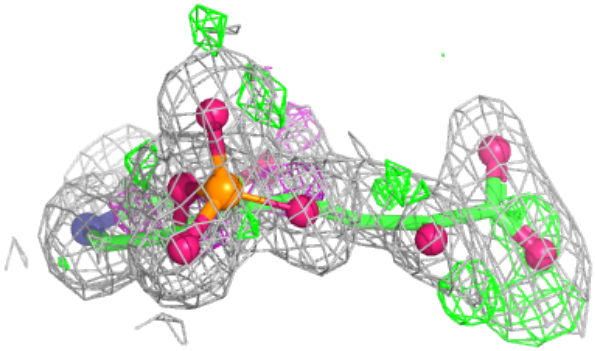




Electron density around AN7 BBB 501 (A):

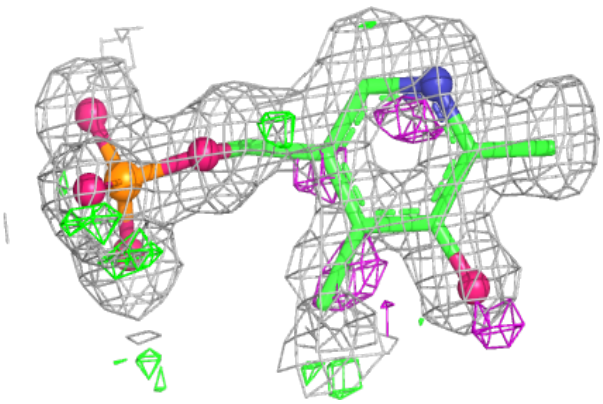
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

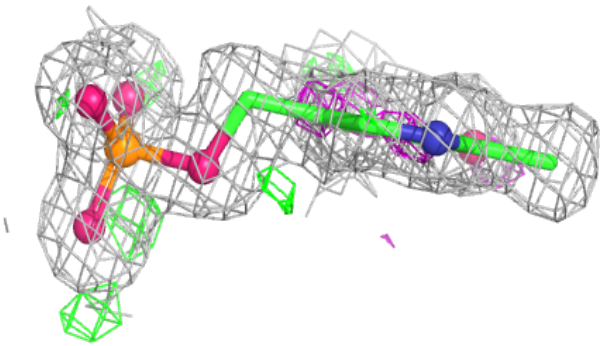


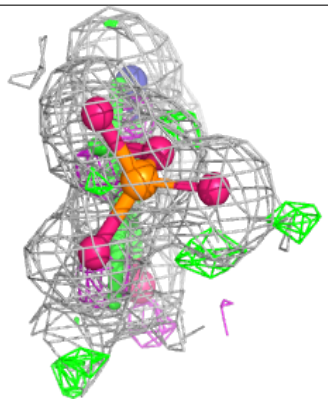


Electron density around PLP BBB 503 (B):

$2mF_o$-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

There are no such residues in this entry.