



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 12:31 AM UTC

PDB ID : 4M6V / pdb_00004m6v
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with pyruvate and biocytin
Authors : Lietzan, A.D.; St.Maurice, M.
Deposited on : 2013-08-11
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

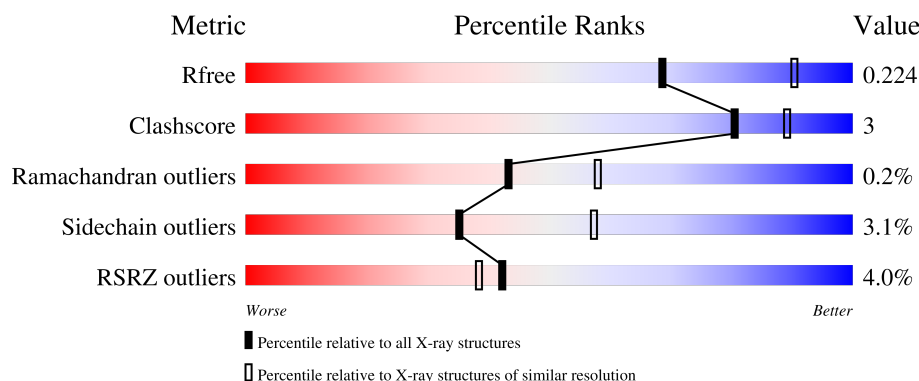
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	632	% 87% 6% • 6%
1	B	632	4% 88% 5% 6%
1	C	632	3% 88% 5% 6%
1	D	632	6% 87% 6% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18461 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 PYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	2	0
			4564	2901	769	871	23			
1	B	593	Total	C	N	O	S	0	2	0
			4435	2822	742	848	23			
1	C	596	Total	C	N	O	S	0	3	0
			4491	2859	750	859	23			
1	D	593	Total	C	N	O	S	0	2	0
			4404	2801	739	841	23			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q2K340
A	437	GLY	-	expression tag	UNP Q2K340
A	438	SER	-	expression tag	UNP Q2K340
A	439	SER	-	expression tag	UNP Q2K340
A	440	HIS	-	expression tag	UNP Q2K340
A	441	HIS	-	expression tag	UNP Q2K340
A	442	HIS	-	expression tag	UNP Q2K340
A	443	HIS	-	expression tag	UNP Q2K340
A	444	HIS	-	expression tag	UNP Q2K340
A	445	HIS	-	expression tag	UNP Q2K340
A	446	HIS	-	expression tag	UNP Q2K340
A	447	HIS	-	expression tag	UNP Q2K340
A	448	ASP	-	expression tag	UNP Q2K340
A	449	TYR	-	expression tag	UNP Q2K340
A	450	ASP	-	expression tag	UNP Q2K340
A	451	ILE	-	expression tag	UNP Q2K340
A	452	PRO	-	expression tag	UNP Q2K340
A	453	THR	-	expression tag	UNP Q2K340
A	454	SER	-	expression tag	UNP Q2K340
A	455	GLU	-	expression tag	UNP Q2K340
A	456	ASN	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	expression tag	UNP Q2K340
A	458	TYR	-	expression tag	UNP Q2K340
A	459	PHE	-	expression tag	UNP Q2K340
A	460	GLN	-	expression tag	UNP Q2K340
A	461	GLY	-	expression tag	UNP Q2K340
A	462	LEU	-	expression tag	UNP Q2K340
A	463	LEU	-	expression tag	UNP Q2K340
A	464	HIS	-	expression tag	UNP Q2K340
B	436	MET	-	expression tag	UNP Q2K340
B	437	GLY	-	expression tag	UNP Q2K340
B	438	SER	-	expression tag	UNP Q2K340
B	439	SER	-	expression tag	UNP Q2K340
B	440	HIS	-	expression tag	UNP Q2K340
B	441	HIS	-	expression tag	UNP Q2K340
B	442	HIS	-	expression tag	UNP Q2K340
B	443	HIS	-	expression tag	UNP Q2K340
B	444	HIS	-	expression tag	UNP Q2K340
B	445	HIS	-	expression tag	UNP Q2K340
B	446	HIS	-	expression tag	UNP Q2K340
B	447	HIS	-	expression tag	UNP Q2K340
B	448	ASP	-	expression tag	UNP Q2K340
B	449	TYR	-	expression tag	UNP Q2K340
B	450	ASP	-	expression tag	UNP Q2K340
B	451	ILE	-	expression tag	UNP Q2K340
B	452	PRO	-	expression tag	UNP Q2K340
B	453	THR	-	expression tag	UNP Q2K340
B	454	SER	-	expression tag	UNP Q2K340
B	455	GLU	-	expression tag	UNP Q2K340
B	456	ASN	-	expression tag	UNP Q2K340
B	457	LEU	-	expression tag	UNP Q2K340
B	458	TYR	-	expression tag	UNP Q2K340
B	459	PHE	-	expression tag	UNP Q2K340
B	460	GLN	-	expression tag	UNP Q2K340
B	461	GLY	-	expression tag	UNP Q2K340
B	462	LEU	-	expression tag	UNP Q2K340
B	463	LEU	-	expression tag	UNP Q2K340
B	464	HIS	-	expression tag	UNP Q2K340
C	436	MET	-	expression tag	UNP Q2K340
C	437	GLY	-	expression tag	UNP Q2K340
C	438	SER	-	expression tag	UNP Q2K340
C	439	SER	-	expression tag	UNP Q2K340
C	440	HIS	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	expression tag	UNP Q2K340
C	442	HIS	-	expression tag	UNP Q2K340
C	443	HIS	-	expression tag	UNP Q2K340
C	444	HIS	-	expression tag	UNP Q2K340
C	445	HIS	-	expression tag	UNP Q2K340
C	446	HIS	-	expression tag	UNP Q2K340
C	447	HIS	-	expression tag	UNP Q2K340
C	448	ASP	-	expression tag	UNP Q2K340
C	449	TYR	-	expression tag	UNP Q2K340
C	450	ASP	-	expression tag	UNP Q2K340
C	451	ILE	-	expression tag	UNP Q2K340
C	452	PRO	-	expression tag	UNP Q2K340
C	453	THR	-	expression tag	UNP Q2K340
C	454	SER	-	expression tag	UNP Q2K340
C	455	GLU	-	expression tag	UNP Q2K340
C	456	ASN	-	expression tag	UNP Q2K340
C	457	LEU	-	expression tag	UNP Q2K340
C	458	TYR	-	expression tag	UNP Q2K340
C	459	PHE	-	expression tag	UNP Q2K340
C	460	GLN	-	expression tag	UNP Q2K340
C	461	GLY	-	expression tag	UNP Q2K340
C	462	LEU	-	expression tag	UNP Q2K340
C	463	LEU	-	expression tag	UNP Q2K340
C	464	HIS	-	expression tag	UNP Q2K340
D	436	MET	-	expression tag	UNP Q2K340
D	437	GLY	-	expression tag	UNP Q2K340
D	438	SER	-	expression tag	UNP Q2K340
D	439	SER	-	expression tag	UNP Q2K340
D	440	HIS	-	expression tag	UNP Q2K340
D	441	HIS	-	expression tag	UNP Q2K340
D	442	HIS	-	expression tag	UNP Q2K340
D	443	HIS	-	expression tag	UNP Q2K340
D	444	HIS	-	expression tag	UNP Q2K340
D	445	HIS	-	expression tag	UNP Q2K340
D	446	HIS	-	expression tag	UNP Q2K340
D	447	HIS	-	expression tag	UNP Q2K340
D	448	ASP	-	expression tag	UNP Q2K340
D	449	TYR	-	expression tag	UNP Q2K340
D	450	ASP	-	expression tag	UNP Q2K340
D	451	ILE	-	expression tag	UNP Q2K340
D	452	PRO	-	expression tag	UNP Q2K340
D	453	THR	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	expression tag	UNP Q2K340
D	455	GLU	-	expression tag	UNP Q2K340
D	456	ASN	-	expression tag	UNP Q2K340
D	457	LEU	-	expression tag	UNP Q2K340
D	458	TYR	-	expression tag	UNP Q2K340
D	459	PHE	-	expression tag	UNP Q2K340
D	460	GLN	-	expression tag	UNP Q2K340
D	461	GLY	-	expression tag	UNP Q2K340
D	462	LEU	-	expression tag	UNP Q2K340
D	463	LEU	-	expression tag	UNP Q2K340
D	464	HIS	-	expression tag	UNP Q2K340

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

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

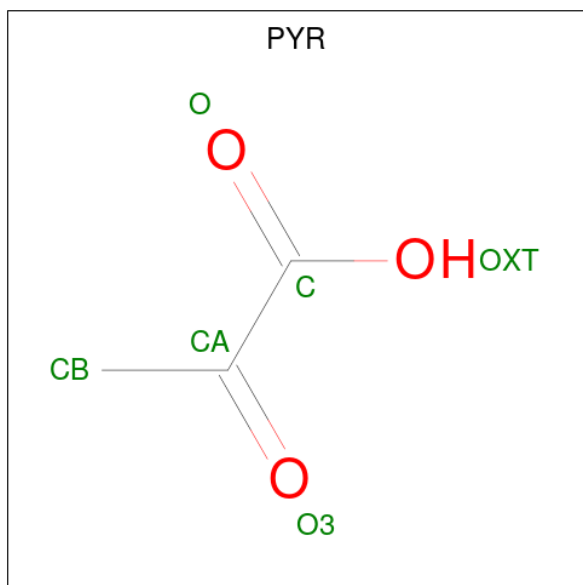
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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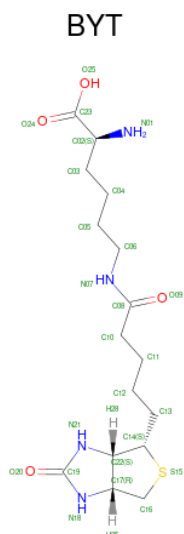
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



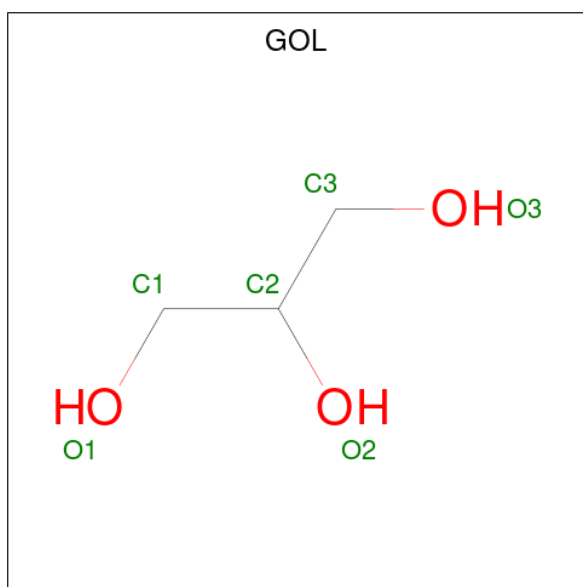
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is Biocytin (CCD ID: BYT) (formula: $C_{16}H_{28}N_4O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 25	C 16	N 4	O 4	S 1	0	0
6	A	1	Total 18	C 12	N 3	O 2	S 1	0	0
6	B	1	Total 25	C 16	N 4	O 4	S 1	0	0
6	B	1	Total 14	C 10	N 2	O 1	S 1	0	0
6	C	1	Total 25	C 16	N 4	O 4	S 1	0	0
6	C	1	Total 16	C 10	N 3	O 2	S 1	0	0
6	D	1	Total 25	C 16	N 4	O 4	S 1	0	0
6	D	1	Total 10	C 6	N 2	O 1	S 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

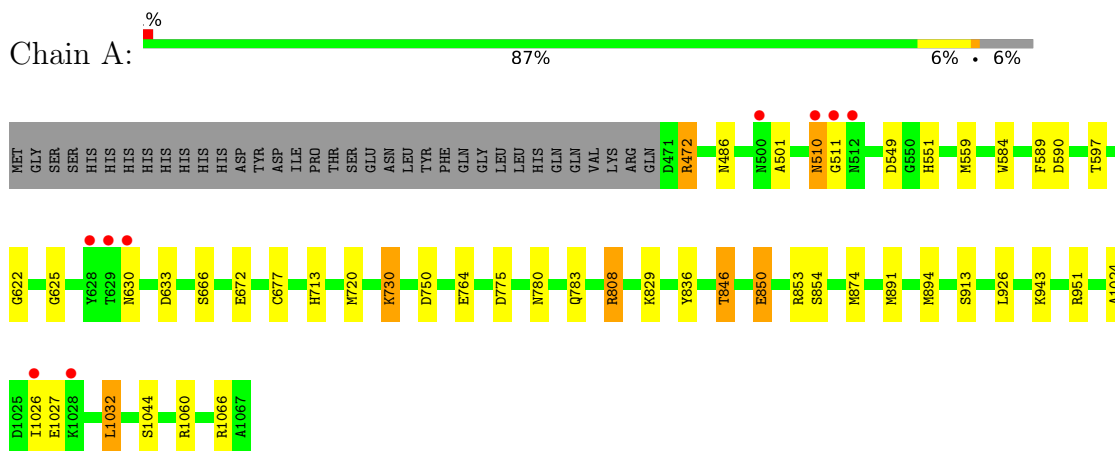
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	0
			143	143		
8	B	85	Total	O	0	0
			85	85		
8	C	77	Total	O	0	0
			77	77		
8	D	56	Total	O	0	0
			56	56		

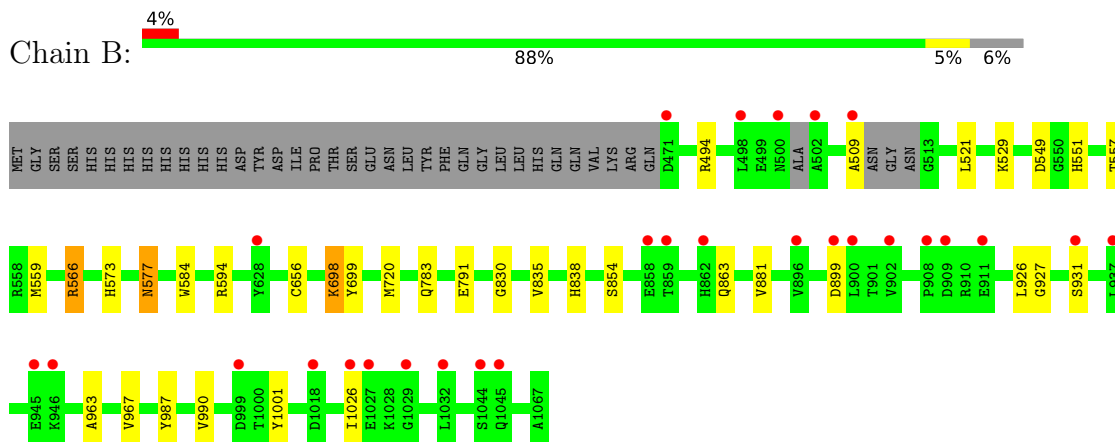
3 Residue-property plots [i](#)

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.

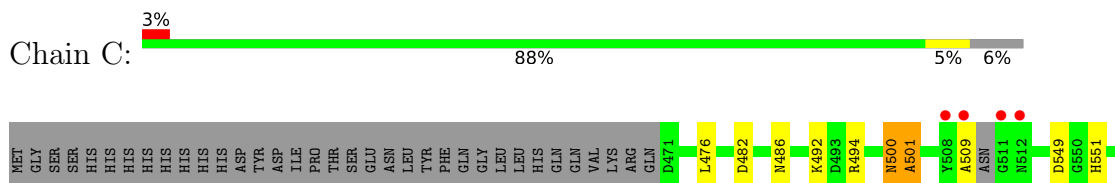
• Molecule 1: PYRUVATE CARBOXYLASE

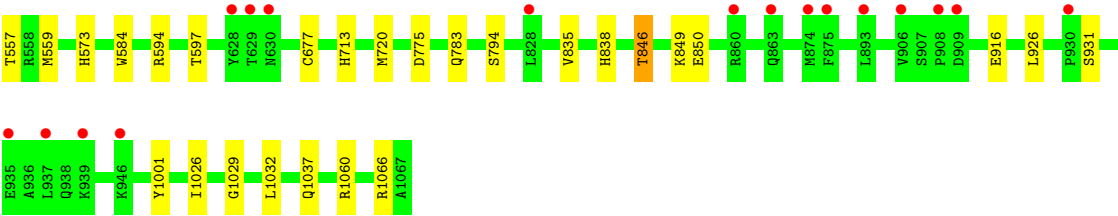


• Molecule 1: PYRUVATE CARBOXYLASE

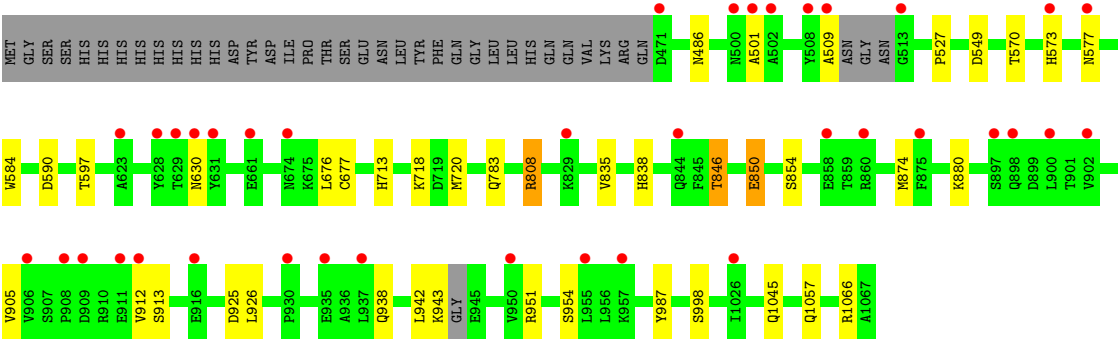
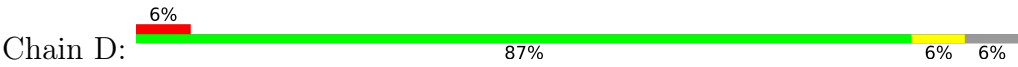


• Molecule 1: PYRUVATE CARBOXYLASE





• Molecule 1: PYRUVATE CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.64Å 157.83Å 244.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.40 49.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.66-2.40) 99.6 (49.66-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.223 0.189 , 0.224	Depositor DCC
R_{free} test set	6448 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	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	0.96	EDS
Total number of atoms	18461	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 2.39% 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: MG, BYT, ZN, CL, KCX, GOL, PYR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	0/4655	0.94	4/6330 (0.1%)
1	B	0.77	1/4524 (0.0%)	0.89	2/6166 (0.0%)
1	C	0.73	0/4585	0.90	1/6246 (0.0%)
1	D	0.65	0/4493	0.83	0/6134
All	All	0.77	1/18257 (0.0%)	0.89	7/24876 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	927	GLY	C-O	7.99	1.29	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	PHE	CA-C-N	7.36	130.37	120.65
1	A	589	PHE	C-N-CA	7.36	130.37	120.65
1	A	590	ASP	N-CA-CB	-6.86	99.90	109.91
1	B	830	GLY	CA-C-N	5.67	125.68	119.89
1	B	830	GLY	C-N-CA	5.67	125.68	119.89
1	A	472	ARG	N-CA-C	-5.41	105.55	111.82
1	C	492	LYS	CB-CA-C	-5.01	103.02	110.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1029	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4564	0	4461	32	0
1	B	4435	0	4224	17	0
1	C	4491	0	4302	23	0
1	D	4404	0	4180	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
6	A	43	0	45	3	0
6	B	39	0	42	2	0
6	C	41	0	42	7	0
6	D	35	0	34	2	0
7	B	6	0	8	3	0
7	C	6	0	8	1	0
8	A	143	0	0	7	0
8	B	85	0	0	3	0
8	C	77	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	56	0	0	2	0
All	All	18461	0	17346	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (92) 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:C:850:GLU:HG3	6:C:1107:BYT:H28	1.56	0.87
1:A:472:ARG:HB3	1:A:1026:ILE:HD11	1.57	0.86
1:A:850:GLU:HG3	6:A:1106:BYT:H28	1.59	0.85
1:A:1060:ARG:NH1	1:C:1037:GLN:OE1	2.10	0.84
1:C:1001:TYR:CE2	6:C:1106:BYT:H18	2.16	0.81
1:B:577:ASN:HB2	8:B:1229:HOH:O	1.81	0.79
1:C:500:ASN:HD22	1:C:501:ALA:H	1.29	0.79
1:C:850:GLU:CG	6:C:1107:BYT:H28	2.17	0.75
1:A:850:GLU:HG2	8:A:1322:HOH:O	1.87	0.74
1:A:853:ARG:NE	8:A:1321:HOH:O	2.19	0.74
1:A:472:ARG:CB	1:A:1026:ILE:HD11	2.20	0.72
1:C:500:ASN:ND2	1:C:501:ALA:H	1.88	0.70
1:A:780:ASN:H	7:B:1101:GOL:H11	1.58	0.68
1:A:677:CYS:H	1:A:713:HIS:HD2	1.42	0.67
1:A:633:ASP:OD1	1:A:951:ARG:NH1	2.28	0.66
1:A:1026:ILE:HB	1:A:1032:LEU:HD11	1.76	0.66
1:C:677:CYS:H	1:C:713:HIS:HD2	1.44	0.64
1:A:808:ARG:HD3	8:A:1336:HOH:O	1.99	0.63
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.64	0.62
1:D:942:LEU:O	1:D:943:LYS:CB	2.49	0.59
1:B:509:ALA:HA	1:B:573[B]:HIS:CE1	2.37	0.59
1:C:500:ASN:HD22	1:C:501:ALA:N	2.00	0.59
1:A:1024:ALA:O	1:A:1032:LEU:HD12	2.04	0.58
1:C:846:THR:HG22	6:C:1107:BYT:O20	2.02	0.58
1:A:730:LYS:HG3	8:A:1333:HOH:O	2.04	0.57
1:D:720:MET:HE3	1:D:880:LYS:O	2.04	0.57
1:A:829:LYS:NZ	8:B:1201:HOH:O	2.34	0.56
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.69	0.56
1:D:808:ARG:HD3	8:D:1213:HOH:O	2.04	0.56
8:A:1316:HOH:O	7:B:1101:GOL:H11	2.06	0.55
1:D:527:PRO:HB2	1:D:713:HIS:CD2	2.41	0.55
1:C:486:ASN:ND2	1:C:1066:ARG:H	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:ASN:HD21	1:C:1066:ARG:H	1.56	0.53
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.74	0.53
1:D:509:ALA:HA	1:D:573[B]:HIS:CE1	2.44	0.53
1:B:698:LYS:HE2	1:B:699:TYR:N	2.24	0.52
1:A:943:LYS:NZ	8:A:1340:HOH:O	2.42	0.52
1:C:850:GLU:HG3	6:C:1107:BYT:C22	2.36	0.52
1:D:912:VAL:HG12	1:D:913:SER:N	2.26	0.51
1:C:551:HIS:CE1	1:C:559:MET:HB3	2.46	0.50
1:C:500:ASN:ND2	1:C:500:ASN:H	2.09	0.50
1:B:1001:TYR:CE2	6:B:1106:BYT:H19	2.47	0.50
1:D:846:THR:HG21	8:D:1239:HOH:O	2.11	0.50
1:C:1001:TYR:HE2	6:C:1106:BYT:H18	1.75	0.49
1:A:846:THR:CG2	6:A:1106:BYT:O20	2.60	0.49
1:A:486:ASN:HD21	1:A:1066:ARG:H	1.59	0.49
1:A:677:CYS:H	1:A:713:HIS:CD2	2.25	0.49
1:D:874:MET:HE1	1:D:905:VAL:HG11	1.94	0.49
1:C:500:ASN:HD22	1:C:500:ASN:N	2.10	0.49
1:A:486:ASN:ND2	1:A:1066:ARG:H	2.11	0.49
1:A:750:ASP:OD2	7:B:1101:GOL:O1	2.24	0.48
1:B:566:ARG:CG	1:B:566:ARG:HH11	2.26	0.48
1:D:677:CYS:H	1:D:713:HIS:CD2	2.31	0.48
1:D:630:ASN:OD1	1:D:925:ASP:O	2.32	0.48
1:B:551:HIS:CE1	1:B:559:MET:HB3	2.49	0.48
1:B:987:TYR:HB3	1:B:990:VAL:HB	1.96	0.47
1:C:500:ASN:ND2	1:C:500:ASN:N	2.60	0.47
1:D:570:THR:HA	1:D:573[B]:HIS:CD2	2.50	0.47
1:A:510:ASN:HD22	1:A:511:GLY:H	1.63	0.46
1:B:529:LYS:NZ	8:B:1219:HOH:O	2.48	0.46
1:A:850:GLU:OE2	1:A:853:ARG:NE	2.49	0.46
1:D:676:LEU:HA	1:D:713:HIS:HD2	1.79	0.46
1:C:509:ALA:HA	1:C:573[B]:HIS:CE1	2.51	0.45
1:B:494:ARG:HD2	6:B:1107:BYT:H16	1.98	0.45
1:A:551:HIS:CE1	1:A:559:MET:HB3	2.52	0.44
1:A:677:CYS:N	1:A:713:HIS:HD2	2.14	0.44
1:A:622:GLY:O	1:A:666:SER:OG	2.33	0.44
1:A:630:ASN:ND2	8:A:1270:HOH:O	2.50	0.43
1:B:509:ALA:HA	1:B:573[B]:HIS:NE2	2.33	0.43
7:C:1102:GOL:O3	7:C:1102:GOL:O1	2.29	0.43
1:B:656:CYS:HA	1:B:881:VAL:CG1	2.48	0.43
1:A:846:THR:HG22	6:A:1106:BYT:O20	2.19	0.43
1:D:835:VAL:HA	1:D:838:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:MET:HE1	1:A:891[B]:MET:HE3	2.00	0.42
1:B:566:ARG:CG	1:B:566:ARG:NH1	2.82	0.42
1:B:557:THR:HG22	1:B:557:THR:O	2.19	0.42
1:A:633:ASP:CG	1:A:951:ARG:HH12	2.27	0.42
1:C:677:CYS:H	1:C:713:HIS:CD2	2.30	0.42
1:D:850:GLU:HG3	6:D:1106:BYT:H28	2.01	0.42
1:C:482:ASP:HB3	6:C:1106:BYT:H25	2.01	0.42
1:D:486:ASN:ND2	1:D:1066:ARG:H	2.16	0.42
1:A:836:TYR:CD2	1:B:791:GLU:HG2	2.55	0.42
1:A:894:MET:HE1	1:A:913:SER:O	2.20	0.42
1:B:963:ALA:O	1:B:967:VAL:HG23	2.20	0.42
1:D:938:GLN:HG2	1:D:942:LEU:HD12	2.01	0.42
1:B:835:VAL:HA	1:B:838:HIS:CE1	2.56	0.41
1:C:1026:ILE:HD12	1:C:1032:LEU:HD11	2.03	0.41
1:D:590:ASP:HB3	1:D:987:TYR:CZ	2.56	0.41
1:D:846:THR:HG23	6:D:1106:BYT:O20	2.21	0.41
1:D:951:ARG:O	1:D:954:SER:OG	2.36	0.41
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.85	0.40
1:C:835:VAL:HA	1:C:838:HIS:CE1	2.57	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	A	596/632 (94%)	583 (98%)	11 (2%)	2 (0%)	36	50
1	B	588/632 (93%)	574 (98%)	14 (2%)	0	100	100
1	C	594/632 (94%)	579 (98%)	14 (2%)	1 (0%)	43	58
1	D	588/632 (93%)	570 (97%)	17 (3%)	1 (0%)	43	58
All	All	2366/2528 (94%)	2306 (98%)	56 (2%)	4 (0%)	43	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	A	625	GLY
1	C	501	ALA
1	D	501	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/519 (90%)	452 (97%)	16 (3%)	32	54
1	B	438/519 (84%)	425 (97%)	13 (3%)	36	58
1	C	448/519 (86%)	432 (96%)	16 (4%)	31	52
1	D	435/519 (84%)	424 (98%)	11 (2%)	42	64
All	All	1789/2076 (86%)	1733 (97%)	56 (3%)	35	57

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	584	TRP
1	A	597	THR
1	A	672	GLU
1	A	720	MET
1	A	730	LYS
1	A	764	GLU
1	A	775	ASP
1	A	808	ARG
1	A	846	THR
1	A	850	GLU
1	A	854	SER
1	A	926	LEU
1	A	1027	GLU
1	A	1032	LEU
1	A	1044	SER

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Mol	Chain	Res	Type
1	B	521	LEU
1	B	566	ARG
1	B	577	ASN
1	B	584	TRP
1	B	594	ARG
1	B	698	LYS
1	B	720	MET
1	B	854	SER
1	B	863	GLN
1	B	899	ASP
1	B	926	LEU
1	B	931	SER
1	B	1026	ILE
1	C	476	LEU
1	C	494	ARG
1	C	500	ASN
1	C	557	THR
1	C	584	TRP
1	C	594	ARG
1	C	597	THR
1	C	720	MET
1	C	775	ASP
1	C	794	SER
1	C	846	THR
1	C	849	LYS
1	C	916	GLU
1	C	926	LEU
1	C	931	SER
1	C	1060	ARG
1	D	577	ASN
1	D	584	TRP
1	D	597	THR
1	D	808	ARG
1	D	846	THR
1	D	850	GLU
1	D	854	SER
1	D	926	LEU
1	D	998	SER
1	D	1045	GLN
1	D	1057	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	510	ASN
1	A	577	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	A	847	ASN
1	B	577	ASN
1	B	624	ASN
1	B	630	ASN
1	B	642	GLN
1	B	662	ASN
1	B	783	GLN
1	B	866	GLN
1	B	873	GLN
1	C	486	ASN
1	C	500	ASN
1	C	577	ASN
1	C	624	ASN
1	C	713	HIS
1	C	783	GLN
1	C	820	GLN
1	C	938	GLN
1	D	486	ASN
1	D	674	ASN
1	D	713	HIS
1	D	783	GLN
1	D	1037	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	A	718	2,1	10,11,12	0.70	0	6,12,14	1.23	0
1	KCX	B	718	2,1	10,11,12	0.71	0	6,12,14	0.74	0
1	KCX	D	718	2,1	10,11,12	0.80	0	6,12,14	2.63	2 (33%)
1	KCX	C	718	2,1	10,11,12	0.65	0	6,12,14	0.86	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
1	KCX	A	718	2,1	-	2/9/10/12	-
1	KCX	B	718	2,1	-	1/9/10/12	-
1	KCX	D	718	2,1	-	2/9/10/12	-
1	KCX	C	718	2,1	-	2/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	718	KCX	OQ1-CX-NZ	-5.53	116.51	124.92
1	D	718	KCX	CE-NZ-CX	3.12	127.27	121.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	C	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	C	718	KCX	CG-CD-CE-NZ
1	D	718	KCX	CG-CD-CE-NZ
1	B	718	KCX	CG-CD-CE-NZ
1	A	718	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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
5	PYR	A	1104	-	5,5,5	1.33	1 (20%)	3,6,6	1.81	1 (33%)
6	BYT	B	1107	-	15,15,26	3.52	6 (40%)	20,20,34	6.34	11 (55%)
6	BYT	D	1105	-	25,26,26	2.67	8 (32%)	31,34,34	4.76	12 (38%)
5	PYR	C	1105	-	5,5,5	1.59	2 (40%)	3,6,6	1.59	1 (33%)
7	GOL	B	1101	-	5,5,5	0.41	0	5,5,5	1.11	0
5	PYR	D	1104	-	5,5,5	1.39	0	3,6,6	1.72	1 (33%)
7	GOL	C	1102	-	5,5,5	0.21	0	5,5,5	0.32	0
6	BYT	A	1105	-	25,26,26	2.56	8 (32%)	31,34,34	4.18	11 (35%)
6	BYT	A	1106	-	19,19,26	3.33	8 (42%)	25,25,34	5.15	12 (48%)
6	BYT	C	1106	-	25,26,26	3.09	9 (36%)	31,34,34	5.47	12 (38%)
6	BYT	B	1106	-	25,26,26	2.64	8 (32%)	31,34,34	5.22	11 (35%)
5	PYR	B	1105	-	5,5,5	1.33	1 (20%)	3,6,6	1.06	0
6	BYT	D	1106	-	10,11,26	3.09	5 (50%)	15,16,34	6.84	10 (66%)
6	BYT	C	1107	-	17,17,26	3.25	7 (41%)	23,23,34	5.77	9 (39%)

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
5	PYR	A	1104	-	-	1/4/4/4	-
6	BYT	B	1107	-	-	2/5/26/40	0/2/2/2
6	BYT	D	1105	-	-	5/19/40/40	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	C	1105	-	-	1/4/4/4	-
5	PYR	D	1104	-	-	2/4/4/4	-
7	GOL	C	1102	-	-	4/4/4/4	-
6	BYT	A	1105	-	-	1/19/40/40	0/2/2/2
6	BYT	A	1106	-	-	5/10/31/40	0/2/2/2
6	BYT	C	1106	-	-	7/19/40/40	0/2/2/2
6	BYT	D	1106	-	-	-	0/2/2/2
6	BYT	B	1106	-	-	7/19/40/40	0/2/2/2
5	PYR	B	1105	-	-	1/4/4/4	-
7	GOL	B	1101	-	-	2/4/4/4	-
6	BYT	C	1107	-	-	3/7/28/40	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1106	BYT	C14-S15	-11.70	1.64	1.82
6	B	1107	BYT	C14-S15	-9.00	1.68	1.82
6	A	1105	BYT	C14-S15	-8.65	1.68	1.82
6	C	1107	BYT	C14-S15	-8.16	1.69	1.82
6	A	1106	BYT	C14-S15	-8.11	1.69	1.82
6	B	1106	BYT	C14-S15	-8.03	1.69	1.82
6	D	1105	BYT	C14-S15	-7.93	1.70	1.82
6	C	1106	BYT	C16-S15	-6.07	1.64	1.81
6	A	1106	BYT	C19-N18	5.51	1.45	1.35
6	A	1106	BYT	C16-S15	-5.51	1.65	1.81
6	A	1106	BYT	C08-N07	5.21	1.45	1.33
6	C	1107	BYT	C19-N18	5.18	1.44	1.35
6	B	1107	BYT	C16-S15	-5.01	1.67	1.81
6	D	1106	BYT	C19-N21	4.89	1.44	1.35
6	A	1105	BYT	C08-N07	4.87	1.44	1.33
6	C	1107	BYT	C16-S15	-4.77	1.67	1.81
6	B	1107	BYT	C19-N18	4.76	1.44	1.35
6	B	1106	BYT	C16-S15	-4.75	1.68	1.81
6	D	1105	BYT	C08-N07	4.70	1.44	1.33
6	D	1105	BYT	C19-N21	4.69	1.43	1.35
6	D	1106	BYT	C16-S15	-4.69	1.68	1.81
6	B	1107	BYT	C19-N21	4.58	1.43	1.35
6	A	1105	BYT	C16-S15	-4.56	1.68	1.81
6	B	1106	BYT	C08-N07	4.48	1.44	1.33
6	D	1106	BYT	C19-N18	4.47	1.43	1.35
6	A	1106	BYT	C17-C22	4.38	1.68	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1105	BYT	C16-S15	-4.32	1.69	1.81
6	D	1106	BYT	C17-C22	4.24	1.67	1.55
6	C	1107	BYT	C19-N21	4.19	1.42	1.35
6	B	1107	BYT	C17-C22	4.14	1.67	1.55
6	D	1105	BYT	C19-N18	3.97	1.42	1.35
6	B	1106	BYT	C19-N18	3.96	1.42	1.35
6	C	1107	BYT	C17-C22	3.80	1.66	1.55
6	C	1106	BYT	C08-N07	3.68	1.42	1.33
6	B	1106	BYT	C17-C22	3.64	1.66	1.55
6	C	1107	BYT	C08-N07	3.60	1.44	1.32
6	A	1106	BYT	C19-N21	3.52	1.41	1.35
6	D	1105	BYT	C17-C22	3.47	1.65	1.55
6	B	1106	BYT	C19-N21	3.34	1.41	1.35
6	B	1107	BYT	C16-C17	3.11	1.59	1.53
6	A	1105	BYT	C17-C22	3.10	1.64	1.55
6	D	1105	BYT	C16-C17	3.00	1.59	1.53
6	D	1106	BYT	C16-C17	2.97	1.59	1.53
6	C	1107	BYT	C16-C17	2.96	1.59	1.53
6	A	1105	BYT	C19-N21	2.94	1.40	1.35
6	C	1106	BYT	C17-C22	2.92	1.64	1.55
6	A	1106	BYT	C16-C17	2.92	1.59	1.53
6	C	1106	BYT	C19-N18	2.78	1.40	1.35
6	B	1106	BYT	O24-C23	2.75	1.30	1.22
6	B	1106	BYT	C16-C17	2.72	1.58	1.53
6	C	1106	BYT	C19-N21	2.62	1.40	1.35
6	A	1106	BYT	C17-N18	2.51	1.49	1.46
6	C	1106	BYT	O09-C08	-2.43	1.18	1.23
6	A	1105	BYT	C19-N18	2.38	1.39	1.35
6	A	1105	BYT	C16-C17	2.36	1.58	1.53
5	C	1105	PYR	CA-C	-2.29	1.46	1.54
6	D	1105	BYT	O24-C23	2.15	1.28	1.22
6	A	1105	BYT	O24-C23	2.12	1.28	1.22
5	A	1104	PYR	CA-C	-2.10	1.47	1.54
6	C	1106	BYT	O25-C23	-2.08	1.24	1.30
5	C	1105	PYR	OXT-C	-2.08	1.24	1.30
5	B	1105	PYR	CA-C	-2.06	1.47	1.54
6	C	1106	BYT	O20-C19	-2.04	1.19	1.23

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1106	BYT	C16-C17-N18	-25.79	79.96	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1106	BYT	C16-C17-N18	-25.07	80.89	113.18
6	B	1107	BYT	C16-C17-N18	-24.23	81.97	113.18
6	C	1107	BYT	C16-C17-N18	-23.35	83.10	113.18
6	D	1105	BYT	C16-C17-N18	-22.54	84.14	113.18
6	D	1106	BYT	C16-C17-N18	-21.96	84.89	113.18
6	A	1105	BYT	C16-C17-N18	-18.93	88.79	113.18
6	A	1106	BYT	C16-C17-N18	-18.29	89.62	113.18
6	A	1106	BYT	N21-C19-N18	8.50	118.67	108.85
6	D	1106	BYT	N21-C19-N18	7.79	117.85	108.85
6	A	1106	BYT	O20-C19-N21	-7.75	114.74	125.89
6	C	1107	BYT	C16-S15-C14	7.69	105.97	89.98
6	B	1107	BYT	N21-C19-N18	7.64	117.67	108.85
6	C	1106	BYT	N21-C19-N18	7.50	117.52	108.85
6	D	1106	BYT	C16-S15-C14	7.37	105.36	90.01
6	A	1105	BYT	N21-C19-N18	7.32	117.31	108.85
6	B	1106	BYT	N21-C19-N18	7.32	117.30	108.85
6	C	1106	BYT	C16-S15-C14	7.04	104.63	89.98
6	B	1106	BYT	C16-S15-C14	6.69	103.89	89.98
6	D	1105	BYT	N21-C19-N18	6.55	116.42	108.85
6	C	1106	BYT	C14-C22-C17	-6.34	101.14	108.89
6	C	1107	BYT	N21-C19-N18	6.30	116.14	108.85
6	A	1106	BYT	C22-N21-C19	-6.17	104.89	112.56
6	B	1107	BYT	C16-S15-C14	6.04	102.55	89.98
6	A	1106	BYT	C16-S15-C14	5.92	102.30	89.98
6	D	1105	BYT	C16-S15-C14	5.83	102.11	89.98
6	D	1106	BYT	C22-N21-C19	-5.73	105.45	112.56
6	C	1107	BYT	C22-N21-C19	-5.67	105.52	112.56
6	B	1107	BYT	C22-N21-C19	-5.63	105.57	112.56
6	C	1106	BYT	C22-N21-C19	-5.39	105.87	112.56
6	A	1106	BYT	C14-C22-N21	-5.15	107.89	113.34
6	A	1105	BYT	C14-C22-C17	-5.11	102.64	108.89
6	D	1105	BYT	C22-N21-C19	-5.11	106.21	112.56
6	D	1105	BYT	C14-C22-C17	-4.97	102.82	108.89
6	C	1107	BYT	C14-C22-N21	-4.85	108.20	113.34
6	A	1106	BYT	C17-N18-C19	-4.83	105.29	112.38
6	C	1107	BYT	O20-C19-N21	-4.81	118.98	125.89
6	B	1106	BYT	C22-N21-C19	-4.80	106.60	112.56
6	A	1105	BYT	C22-N21-C19	-4.76	106.65	112.56
6	D	1106	BYT	C17-N18-C19	-4.62	105.59	112.38
6	B	1106	BYT	O20-C19-N21	-4.61	119.26	125.89
6	B	1107	BYT	C17-N18-C19	-4.58	105.65	112.38
6	B	1106	BYT	C17-N18-C19	-4.49	105.79	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1107	BYT	C17-C22-N21	4.41	107.66	102.68
6	B	1107	BYT	O20-C19-N21	-4.40	119.56	125.89
6	C	1106	BYT	C17-N18-C19	-4.34	106.00	112.38
6	A	1106	BYT	C17-C22-N21	4.21	107.43	102.68
6	D	1105	BYT	C17-N18-C19	-4.02	106.47	112.38
6	B	1107	BYT	C14-C22-C17	-4.02	103.97	108.89
6	A	1105	BYT	C17-N18-C19	-4.01	106.50	112.38
6	A	1106	BYT	C10-C08-N07	3.84	123.34	116.34
6	A	1106	BYT	C14-C22-C17	-3.84	104.20	108.89
6	D	1106	BYT	O20-C19-N21	-3.64	120.66	125.89
6	D	1106	BYT	C14-C22-C17	-3.50	104.61	108.89
6	C	1106	BYT	O20-C19-N21	-3.33	121.11	125.89
6	C	1107	BYT	C17-N18-C19	-3.27	107.57	112.38
6	A	1105	BYT	O20-C19-N18	-3.22	121.25	125.89
6	D	1105	BYT	O20-C19-N18	-3.17	121.33	125.89
6	C	1106	BYT	O20-C19-N18	-3.17	121.33	125.89
6	B	1107	BYT	C17-C22-N21	3.13	106.21	102.68
6	A	1105	BYT	O20-C19-N21	-3.10	121.43	125.89
6	A	1105	BYT	C16-S15-C14	3.10	96.43	89.98
6	D	1106	BYT	O20-C19-N18	-3.09	121.45	125.89
6	D	1106	BYT	C17-C22-N21	3.03	106.10	102.68
6	C	1106	BYT	C17-C22-N21	2.97	106.03	102.68
6	B	1106	BYT	C14-C22-C17	-2.95	105.29	108.89
6	B	1107	BYT	C14-C22-N21	-2.85	110.32	113.34
6	A	1106	BYT	C22-C14-S15	2.82	108.23	105.03
6	D	1105	BYT	C17-C22-N21	2.78	105.81	102.68
6	B	1106	BYT	C14-C22-N21	-2.75	110.43	113.34
6	A	1106	BYT	O09-C08-N07	-2.73	117.68	123.03
6	D	1105	BYT	C12-C13-C14	-2.69	107.85	114.04
6	C	1106	BYT	C10-C08-N07	2.67	121.21	116.34
5	A	1104	PYR	OXT-C-CA	2.61	120.84	113.59
6	D	1105	BYT	C14-C22-N21	2.60	116.09	113.34
6	D	1105	BYT	O20-C19-N21	-2.55	122.22	125.89
6	B	1106	BYT	C17-C22-N21	2.48	105.47	102.68
6	A	1105	BYT	C17-C22-N21	2.37	105.35	102.68
6	C	1107	BYT	C14-C22-C17	-2.37	106.00	108.89
6	C	1106	BYT	C06-N07-C08	-2.35	118.44	122.82
6	D	1105	BYT	C22-C17-N18	2.33	105.01	102.43
5	C	1105	PYR	OXT-C-CA	2.32	120.03	113.59
5	D	1104	PYR	OXT-C-CA	2.30	119.96	113.59
6	B	1107	BYT	O20-C19-N18	-2.19	122.75	125.89
6	D	1106	BYT	C22-C17-N18	2.18	104.84	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1107	BYT	C22-C17-N18	2.17	104.83	102.43
6	B	1106	BYT	C22-C17-N18	2.14	104.81	102.43
6	A	1105	BYT	C16-C17-C22	-2.14	105.67	109.06
6	A	1105	BYT	C13-C14-C22	-2.13	108.48	114.51
6	C	1106	BYT	O09-C08-C10	-2.05	118.31	122.02
6	B	1106	BYT	C11-C10-C08	-2.02	107.58	113.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1105	PYR	OXT-C-CA-CB
5	D	1104	PYR	OXT-C-CA-CB
6	A	1106	BYT	C12-C13-C14-S15
6	A	1106	BYT	C12-C13-C14-C22
6	B	1106	BYT	C12-C13-C14-S15
6	B	1106	BYT	C12-C13-C14-C22
6	B	1107	BYT	C12-C13-C14-S15
6	B	1107	BYT	C12-C13-C14-C22
6	C	1106	BYT	C12-C13-C14-S15
6	C	1106	BYT	C12-C13-C14-C22
6	C	1107	BYT	C12-C13-C14-S15
6	C	1107	BYT	C12-C13-C14-C22
7	B	1101	GOL	C1-C2-C3-O3
7	C	1102	GOL	C1-C2-C3-O3
7	C	1102	GOL	O2-C2-C3-O3
6	A	1106	BYT	C10-C08-N07-C06
6	C	1107	BYT	C08-C10-C11-C12
6	B	1106	BYT	C08-C10-C11-C12
6	A	1106	BYT	O09-C08-N07-C06
6	C	1106	BYT	C10-C11-C12-C13
6	B	1106	BYT	C11-C12-C13-C14
7	C	1102	GOL	O1-C1-C2-C3
6	C	1106	BYT	C04-C05-C06-N07
6	C	1106	BYT	C08-C10-C11-C12
6	B	1106	BYT	C04-C05-C06-N07
6	B	1106	BYT	C03-C04-C05-C06
6	D	1105	BYT	C02-C03-C04-C05
6	D	1105	BYT	C04-C05-C06-N07
7	B	1101	GOL	O2-C2-C3-O3
6	D	1105	BYT	C23-C02-C03-C04
6	B	1106	BYT	C02-C03-C04-C05

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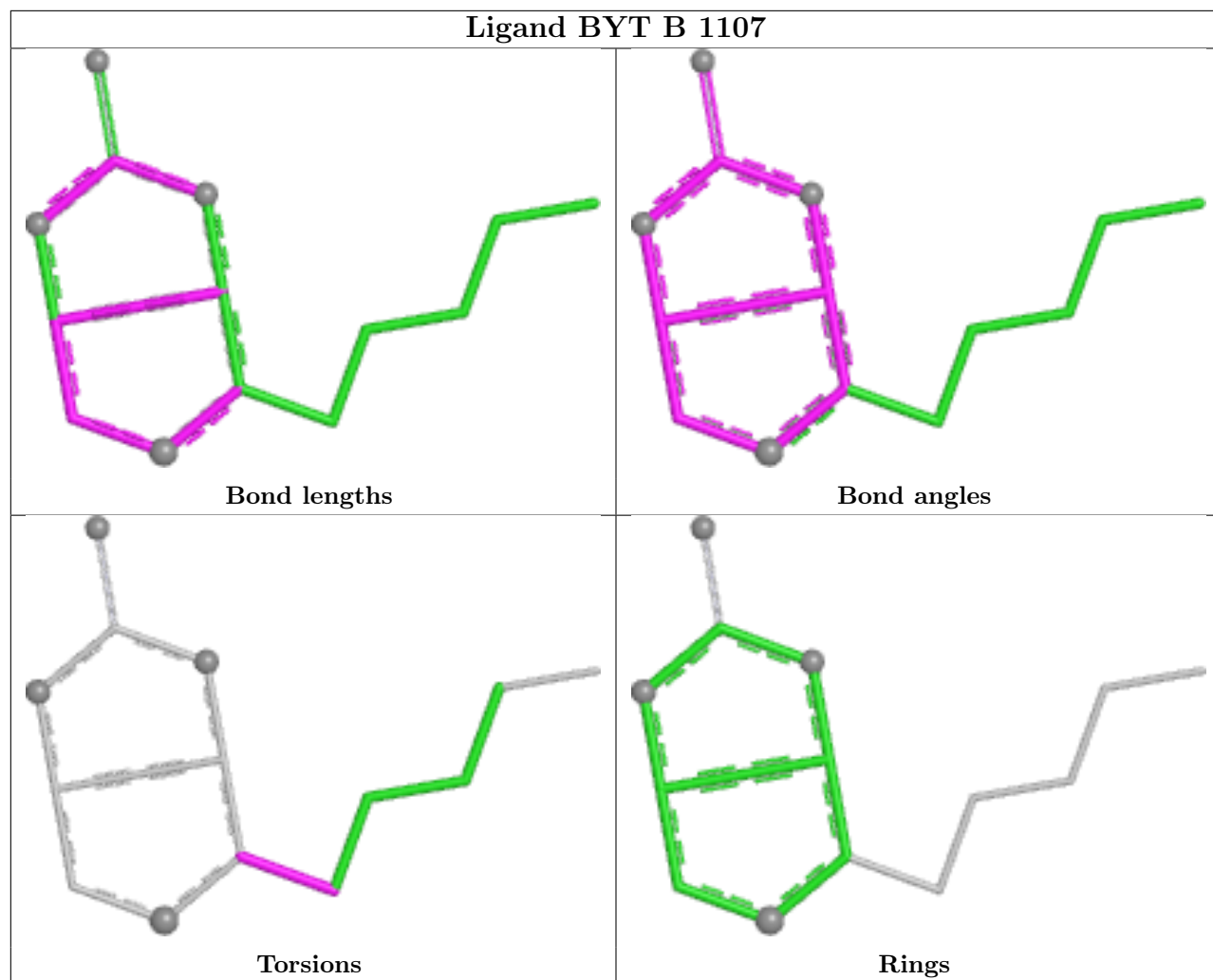
Mol	Chain	Res	Type	Atoms
5	A	1104	PYR	OXT-C-CA-O3
5	B	1105	PYR	OXT-C-CA-O3
6	D	1105	BYT	C03-C04-C05-C06
6	D	1105	BYT	C08-C10-C11-C12
6	A	1105	BYT	N01-C02-C23-O25
6	C	1106	BYT	C03-C04-C05-C06
6	A	1106	BYT	C11-C12-C13-C14
5	D	1104	PYR	O-C-CA-O3
6	C	1106	BYT	C02-C03-C04-C05
7	C	1102	GOL	O1-C1-C2-O2

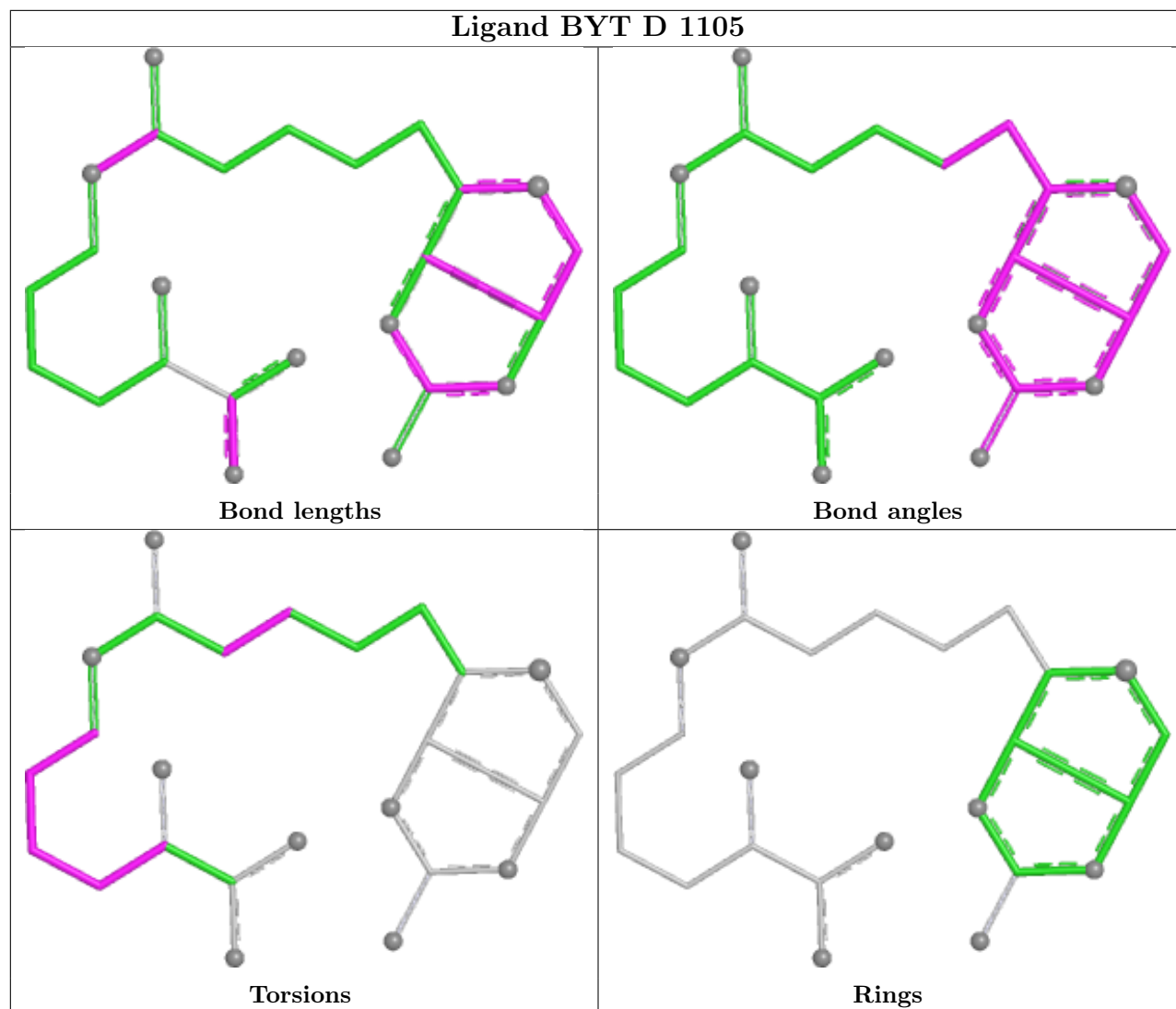
There are no ring outliers.

8 monomers are involved in 18 short contacts:

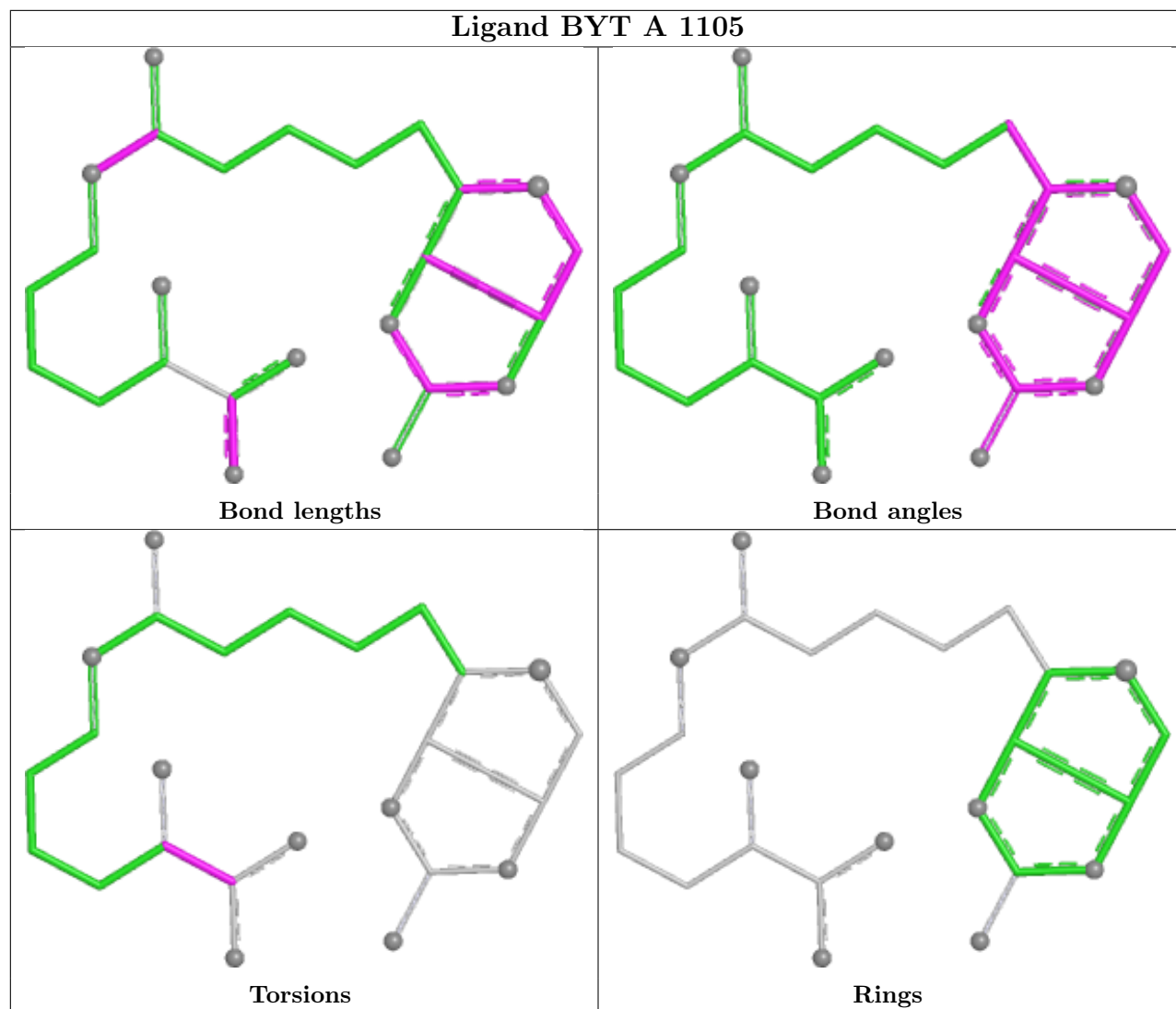
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1107	BYT	1	0
7	B	1101	GOL	3	0
7	C	1102	GOL	1	0
6	A	1106	BYT	3	0
6	C	1106	BYT	3	0
6	B	1106	BYT	1	0
6	D	1106	BYT	2	0
6	C	1107	BYT	4	0

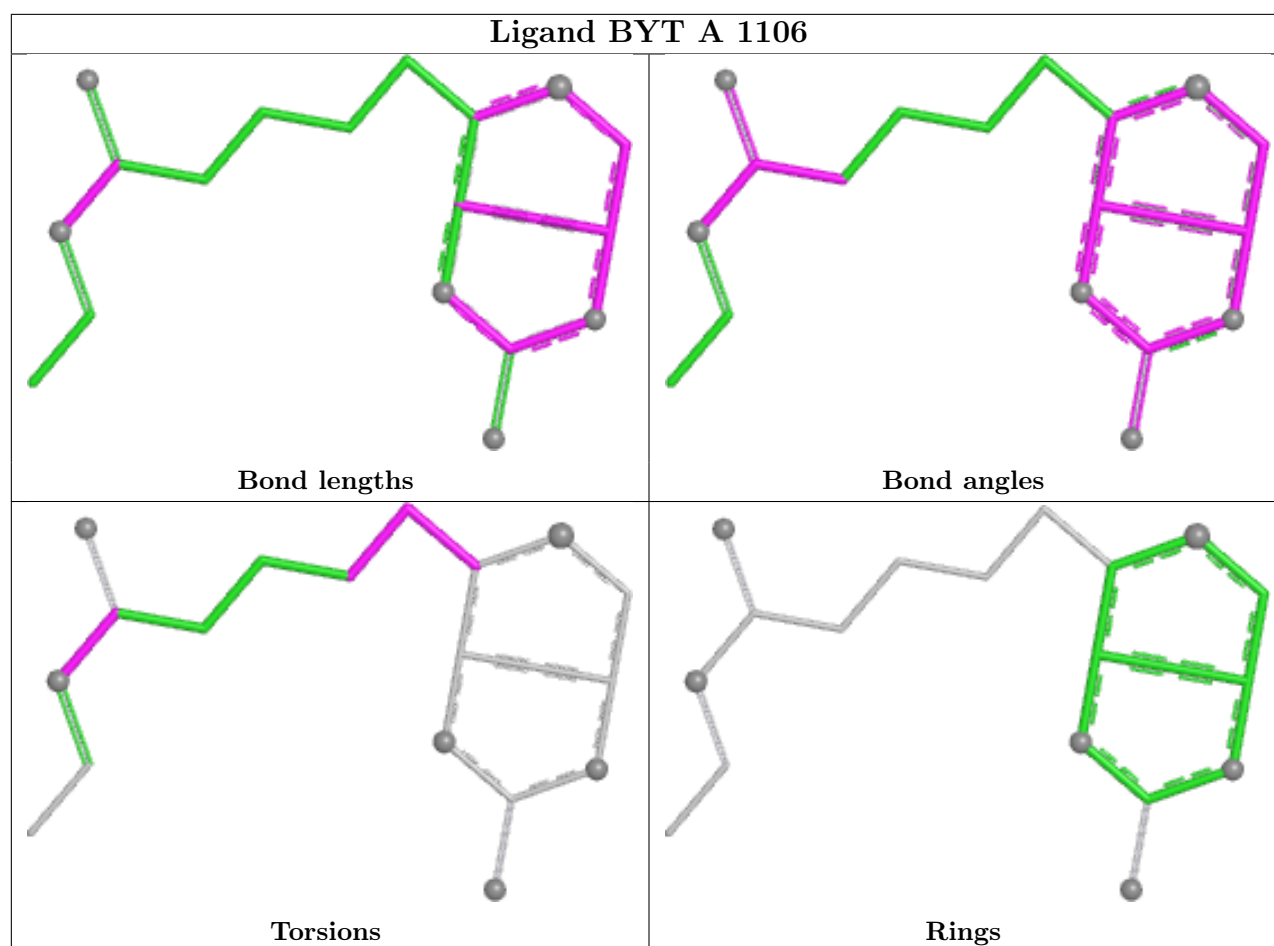
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

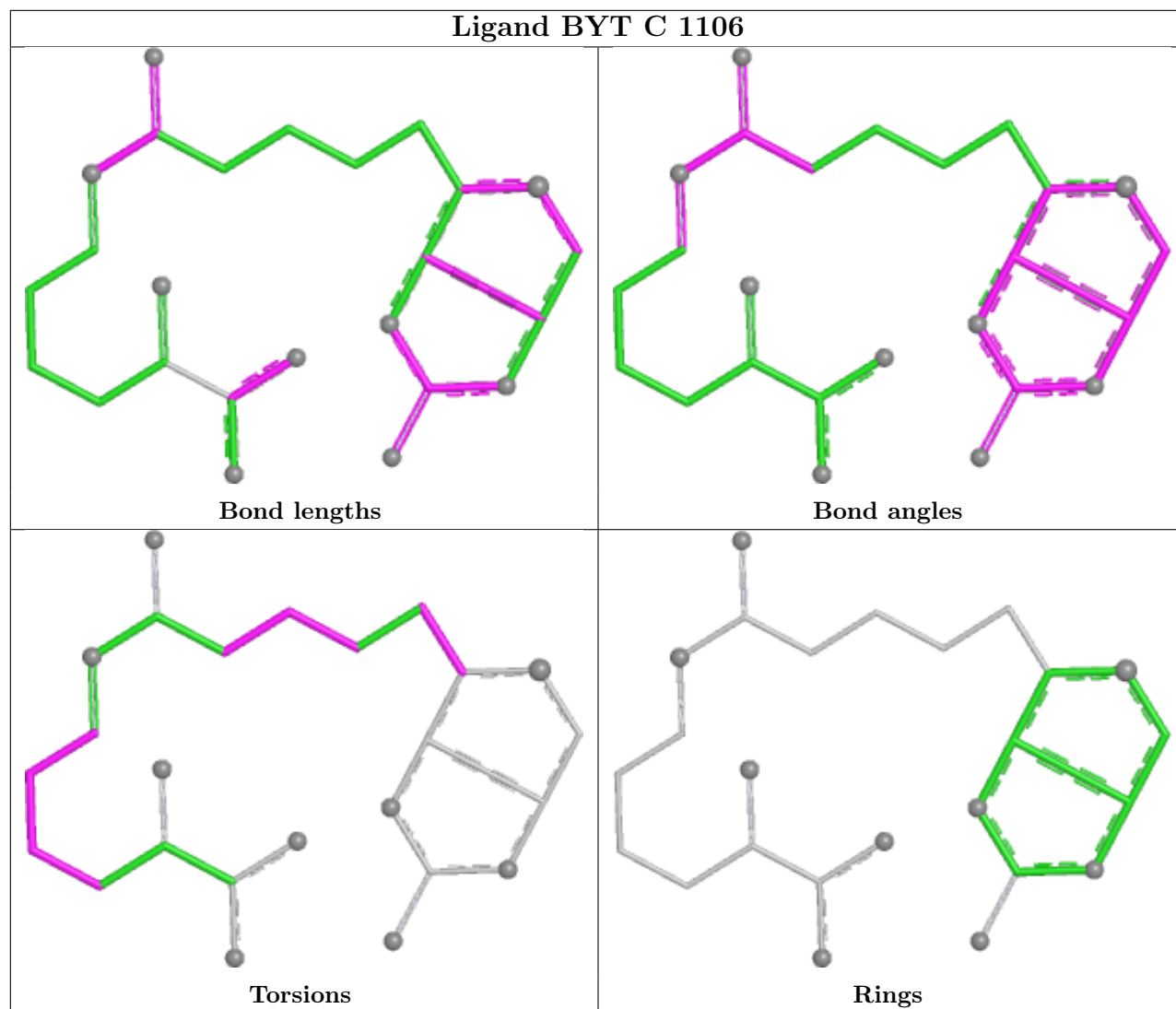




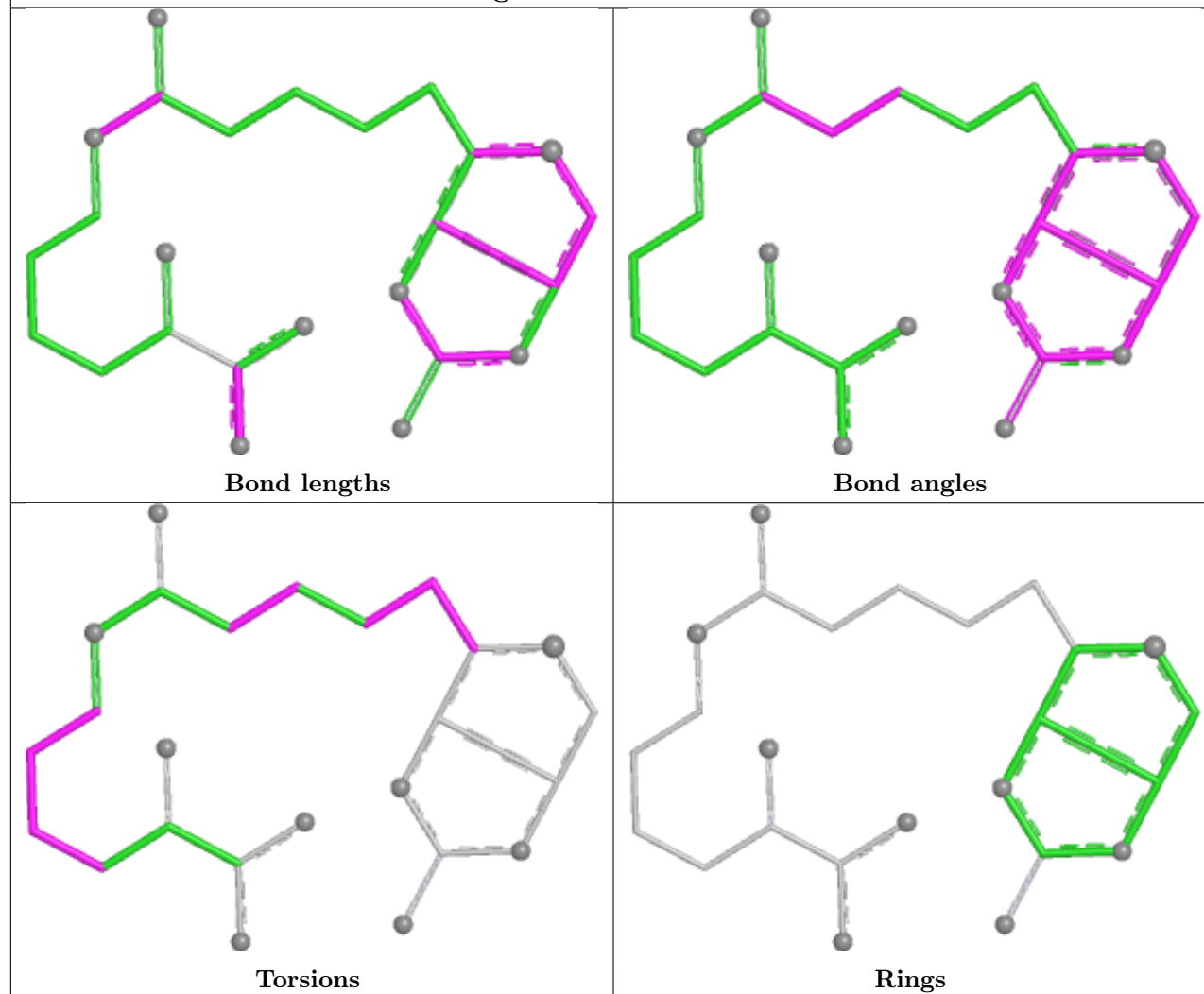
Ligand BYT A 1105



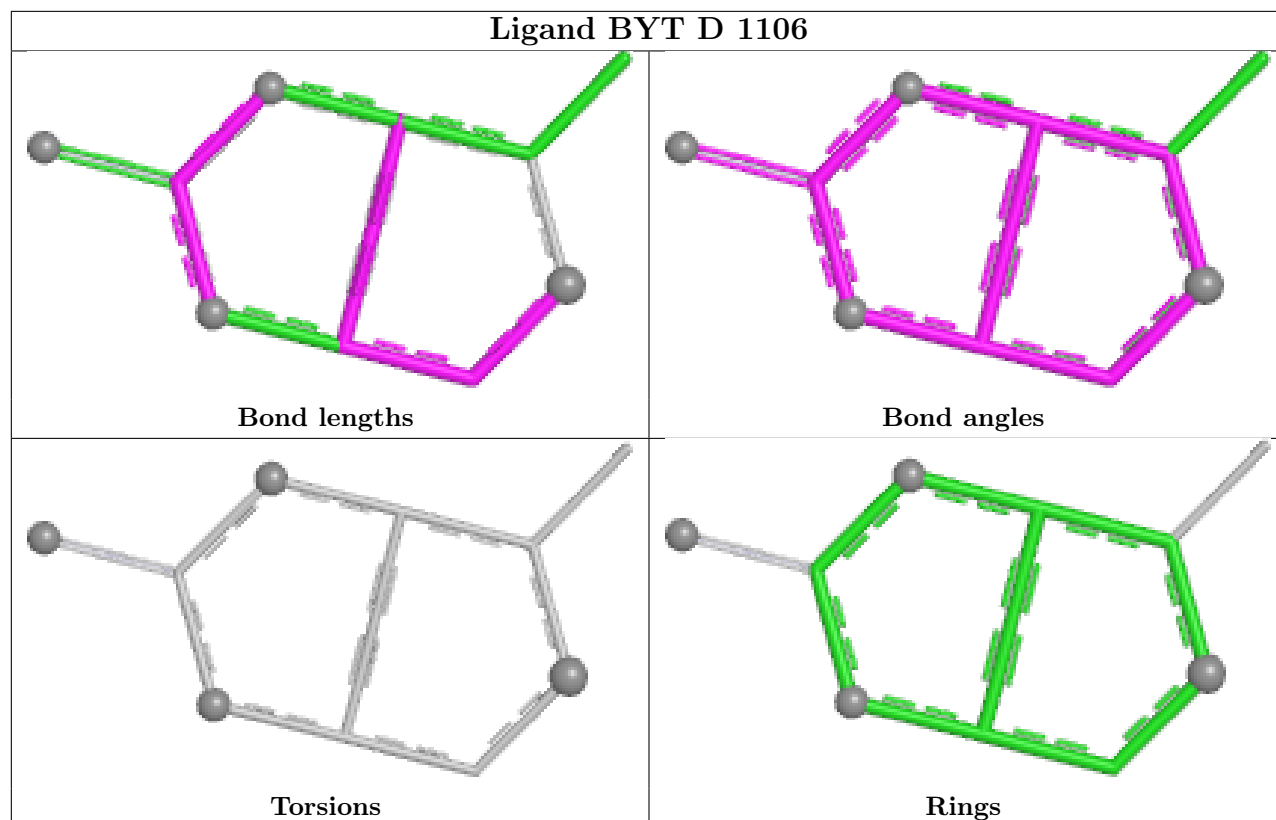




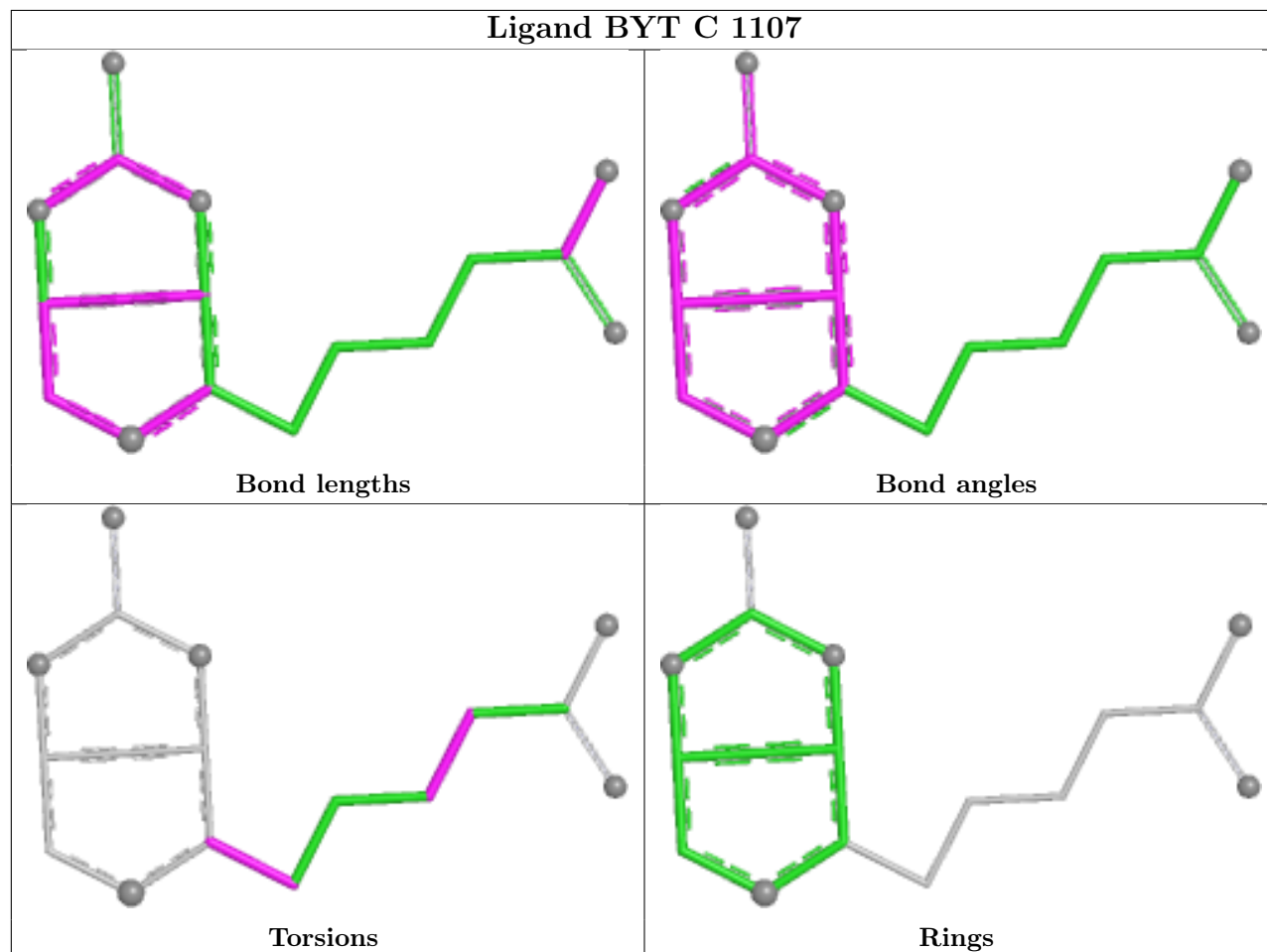
Ligand BYT B 1106



Ligand BYT D 1106



Ligand BYT C 1107



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/632 (94%)	-0.40	9 (1%) 72 68	23, 45, 68, 130	21 (3%)
1	B	592/632 (93%)	0.15	28 (4%) 36 32	26, 65, 121, 168	15 (2%)
1	C	595/632 (94%)	0.06	21 (3%) 47 43	27, 59, 115, 170	18 (3%)
1	D	592/632 (93%)	0.43	38 (6%) 25 22	38, 76, 115, 158	16 (2%)
All	All	2375/2528 (93%)	0.06	96 (4%) 42 38	23, 60, 113, 170	70 (2%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	628	TYR	11.3
1	A	512	ASN	5.5
1	B	509	ALA	5.0
1	C	509	ALA	5.0
1	B	500	ASN	5.0
1	D	500	ASN	4.8
1	D	937	LEU	4.7
1	D	630	ASN	4.5
1	C	512	ASN	4.3
1	C	511	GLY	4.2
1	B	909	ASP	4.2
1	C	630	ASN	3.9
1	D	509	ALA	3.8
1	D	501	ALA	3.7
1	D	513	GLY	3.5
1	D	950	VAL	3.4
1	D	909	ASP	3.4
1	B	1027	GLU	3.3
1	D	508	TYR	3.2
1	C	937	LEU	3.2
1	D	623	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	858	GLU	3.2
1	C	628	TYR	3.1
1	B	999	ASP	3.1
1	C	906	VAL	3.1
1	D	902	VAL	3.0
1	C	909	ASP	3.0
1	D	629	THR	3.0
1	B	862	HIS	3.0
1	A	500	ASN	2.9
1	B	859	THR	2.9
1	B	628	TYR	2.9
1	A	511	GLY	2.9
1	A	1026	ILE	2.9
1	D	908	PRO	2.9
1	B	1045	GLN	2.9
1	B	937	LEU	2.7
1	D	661	GLU	2.7
1	D	502	ALA	2.7
1	B	1018	ASP	2.7
1	D	875	PHE	2.7
1	A	630	ASN	2.7
1	A	628	TYR	2.7
1	D	912	VAL	2.6
1	B	1026	ILE	2.6
1	D	957	LYS	2.6
1	B	858	GLU	2.5
1	C	935	GLU	2.5
1	B	911	GLU	2.5
1	D	1026	ILE	2.5
1	A	1028	LYS	2.5
1	D	916	GLU	2.5
1	D	860	ARG	2.5
1	A	629	THR	2.5
1	B	908	PRO	2.4
1	B	1029	GLY	2.4
1	D	911	GLU	2.4
1	D	573[A]	HIS	2.4
1	C	629	THR	2.4
1	B	1044	SER	2.4
1	D	674	ASN	2.4
1	C	939	LYS	2.4
1	B	902	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	935	GLU	2.4
1	D	471	ASP	2.4
1	D	955	LEU	2.3
1	B	896	VAL	2.3
1	C	946	LYS	2.3
1	C	860	ARG	2.3
1	D	844	GLN	2.3
1	A	510	ASN	2.3
1	B	502	ALA	2.3
1	C	908	PRO	2.3
1	D	898	GLN	2.3
1	B	899	ASP	2.3
1	B	945	GLU	2.3
1	D	930	PRO	2.3
1	C	893	LEU	2.2
1	C	508	TYR	2.2
1	D	631	TYR	2.2
1	D	906	VAL	2.2
1	B	498	LEU	2.2
1	D	900	LEU	2.2
1	B	931	SER	2.1
1	C	875	PHE	2.1
1	B	900	LEU	2.1
1	C	828	LEU	2.1
1	C	874	MET	2.1
1	D	577	ASN	2.1
1	D	829	LYS	2.1
1	C	930	PRO	2.1
1	C	863	GLN	2.0
1	B	1032	LEU	2.0
1	B	946	LYS	2.0
1	B	471	ASP	2.0
1	D	897	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	D	718	12/13	0.95	0.09	56,62,65,66	0
1	KCX	B	718	12/13	0.96	0.07	45,48,50,51	0
1	KCX	C	718	12/13	0.98	0.05	49,52,53,55	0
1	KCX	A	718	12/13	0.98	0.06	34,37,39,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

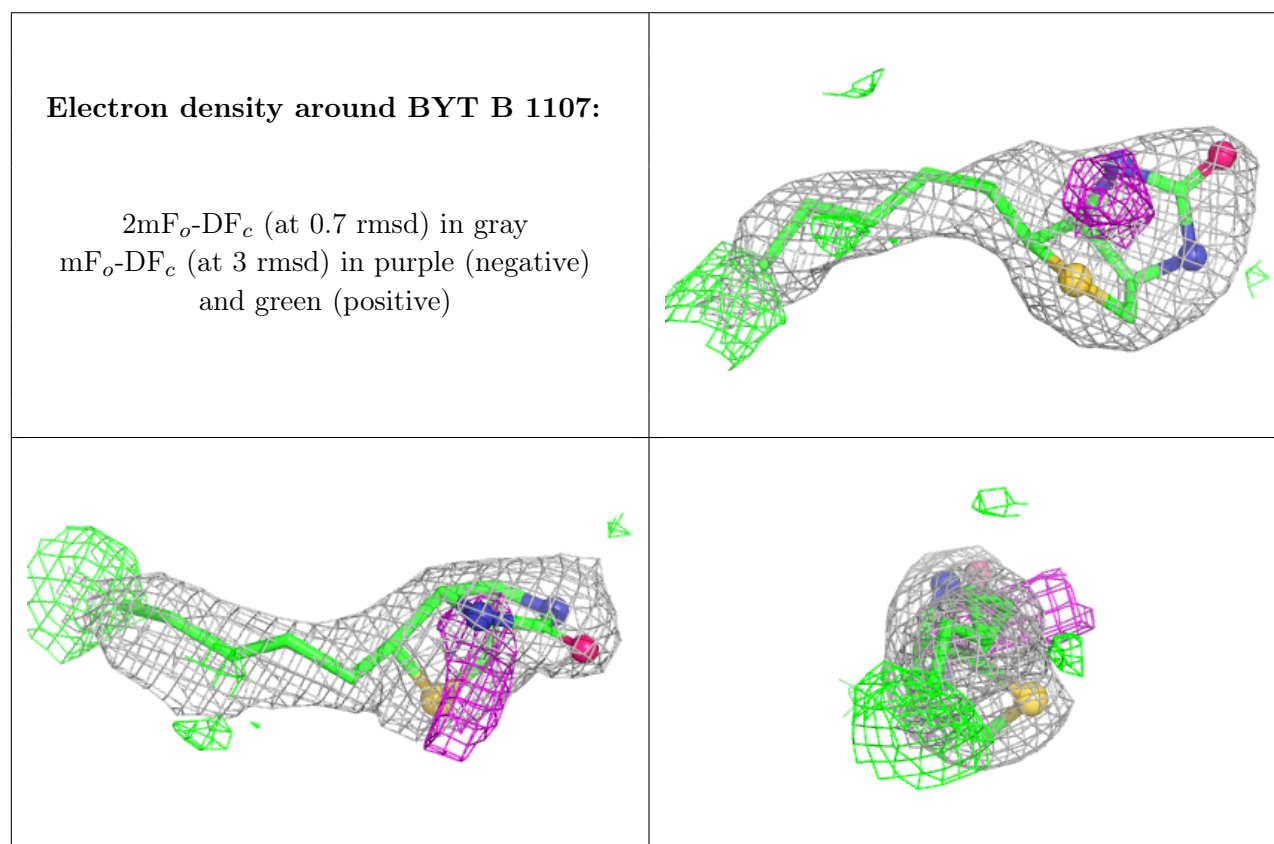
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BYT	B	1107	14/25	0.78	0.21	63,75,85,85	1
6	BYT	D	1106	10/25	0.81	0.19	78,81,83,84	0
6	BYT	C	1107	16/25	0.89	0.15	72,78,83,84	0
3	MG	A	1102	1/1	0.89	0.09	60,60,60,60	0
5	PYR	D	1104	6/6	0.90	0.15	70,77,77,78	0
6	BYT	A	1106	18/25	0.91	0.14	37,46,82,83	1
7	GOL	B	1101	6/6	0.92	0.11	48,48,50,53	0
6	BYT	B	1106	25/25	0.93	0.10	71,77,83,84	0
5	PYR	B	1105	6/6	0.94	0.15	63,64,66,67	0
7	GOL	C	1102	6/6	0.94	0.17	60,63,69,72	0
6	BYT	D	1105	25/25	0.95	0.10	67,70,76,76	0
4	CL	B	1104	1/1	0.95	0.08	86,86,86,86	0
4	CL	C	1104	1/1	0.95	0.11	70,70,70,70	0
4	CL	D	1103	1/1	0.95	0.07	83,83,83,83	0
6	BYT	C	1106	25/25	0.96	0.08	51,55,61,61	0
5	PYR	A	1104	6/6	0.96	0.12	41,44,47,47	0
5	PYR	C	1105	6/6	0.96	0.12	56,62,65,65	0
6	BYT	A	1105	25/25	0.97	0.06	40,45,47,48	0
4	CL	A	1103	1/1	0.98	0.08	47,47,47,47	0
3	MG	B	1103	1/1	0.98	0.08	43,43,43,43	0
3	MG	C	1103	1/1	0.99	0.04	56,56,56,56	0
3	MG	D	1102	1/1	0.99	0.04	82,82,82,82	0
2	ZN	C	1101	1/1	1.00	0.01	49,49,49,49	0
2	ZN	D	1101	1/1	1.00	0.02	57,57,57,57	0
2	ZN	A	1101	1/1	1.00	0.01	37,37,37,37	0

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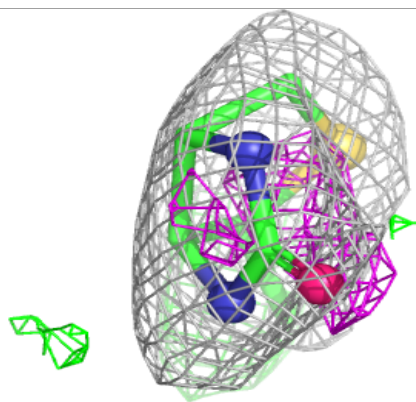
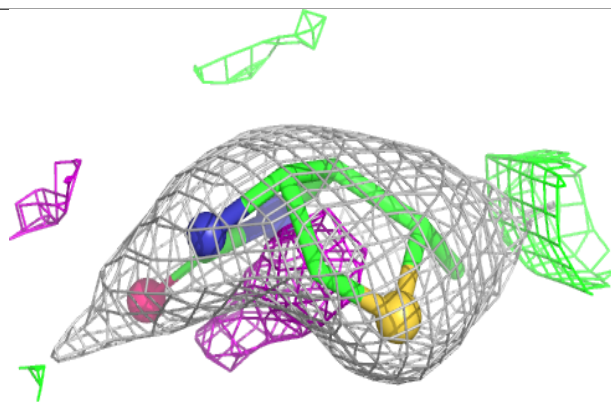
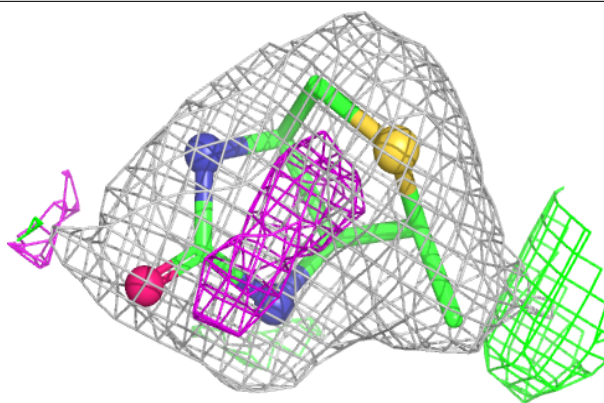
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	1102	1/1	1.00	0.01	46,46,46,46	0

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.

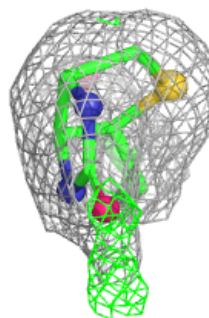
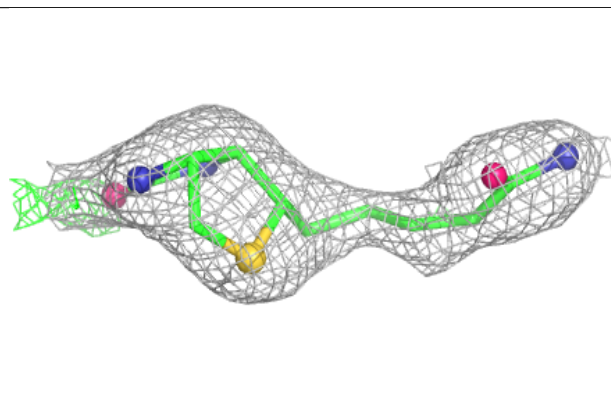
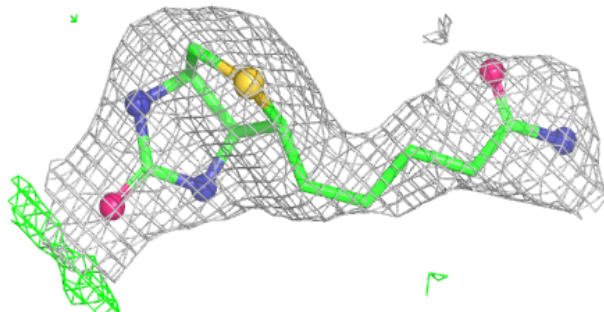


Electron density around BYT D 1106:

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

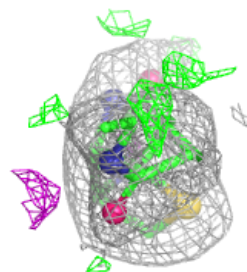
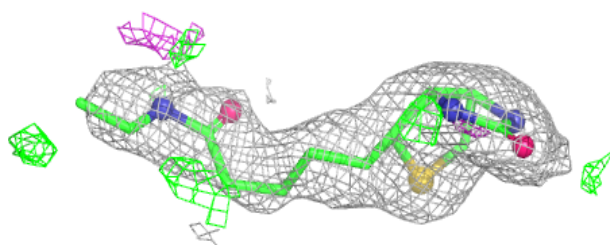
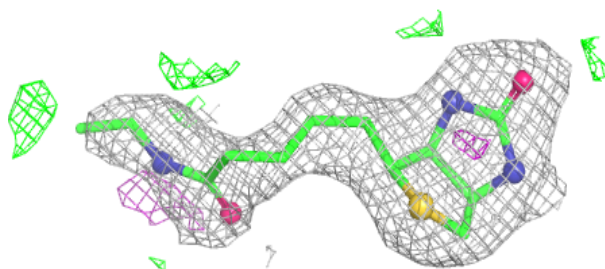
**Electron density around BYT C 1107:**

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

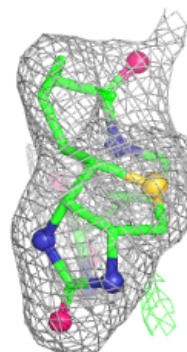
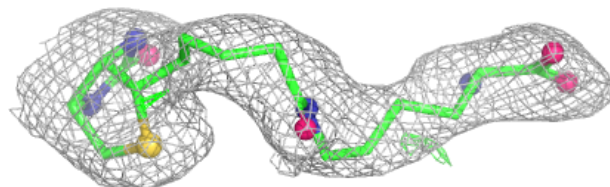
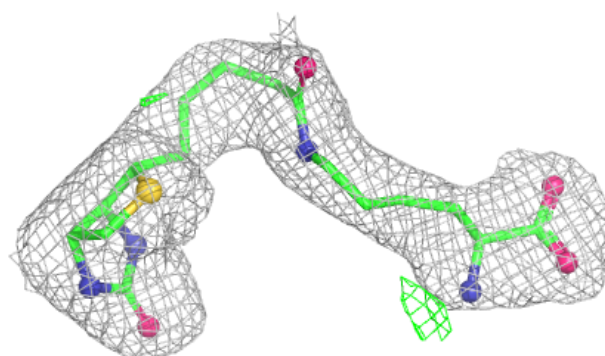


Electron density around BYT A 1106:

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

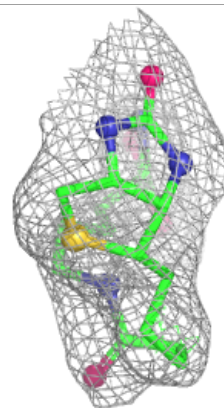
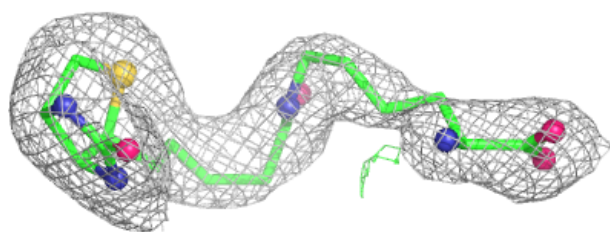
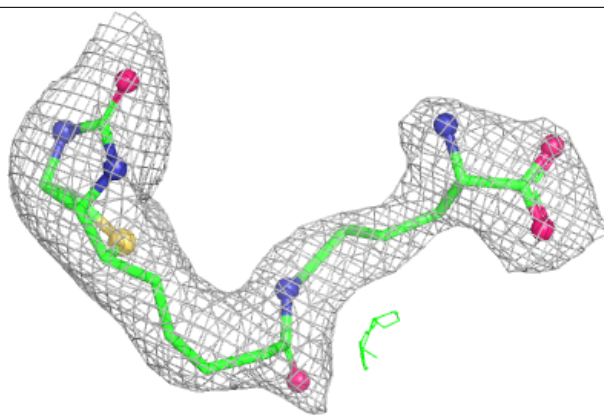
**Electron density around BYT B 1106:**

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

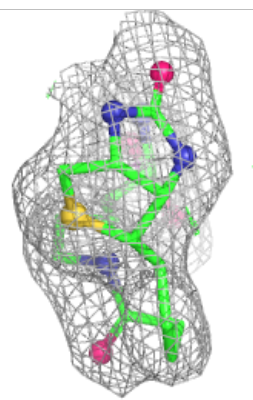
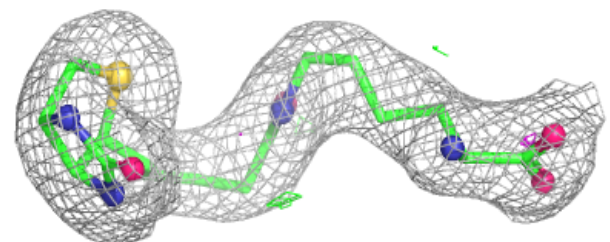
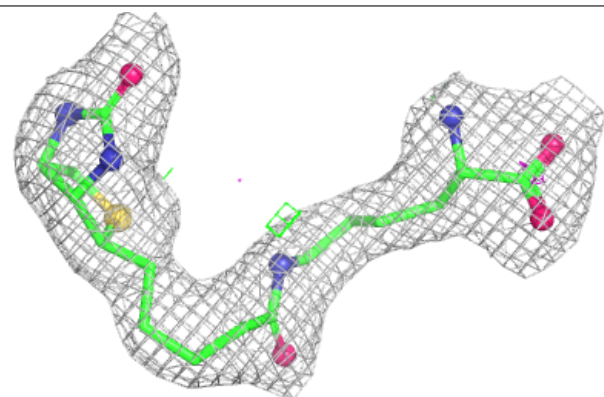


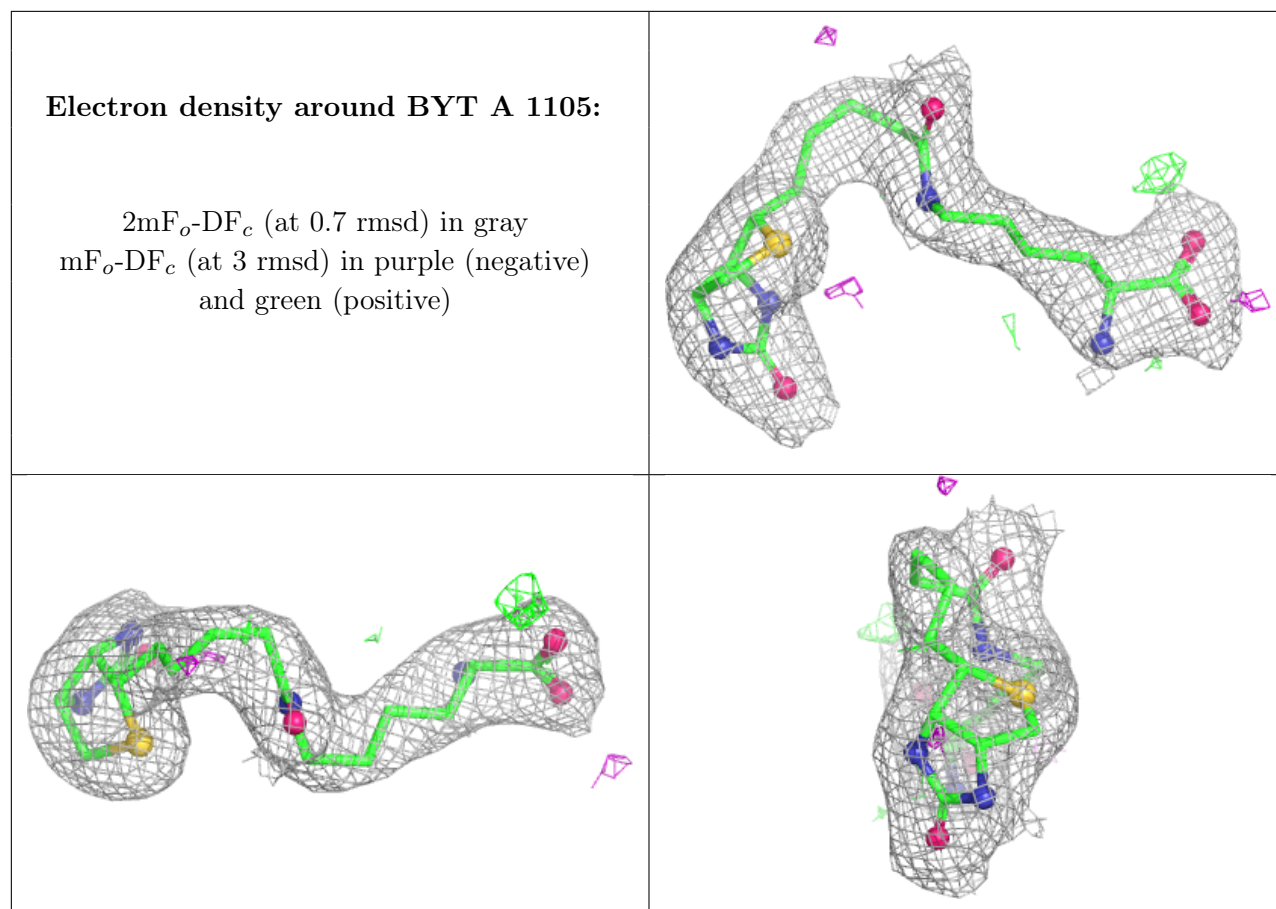
Electron density around BYT D 1105:

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

**Electron density around BYT C 1106:**

$2mF_o-DF_c$ (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.