Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:51 AM EST

PDB ID	:	4M6V
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:

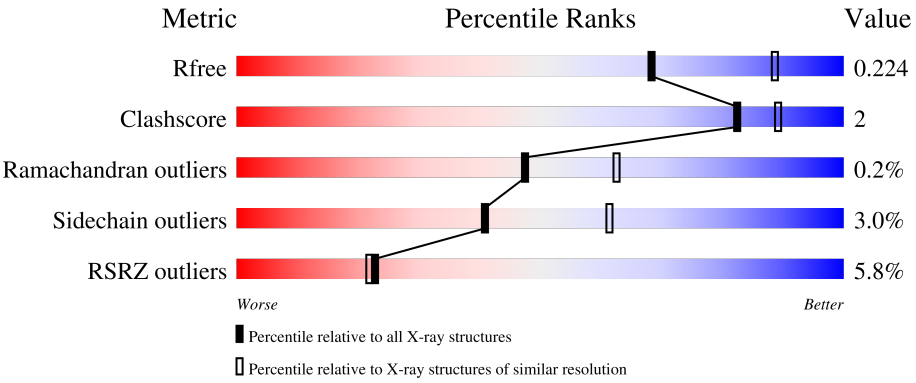
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	2% 87% 6% • 6%
1	B	632	7% 88% 5% • 6%
1	C	632	5% 89% 5% • 6%
1	D	632	9% 88% 6% 6%

2 Entry composition (i)

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

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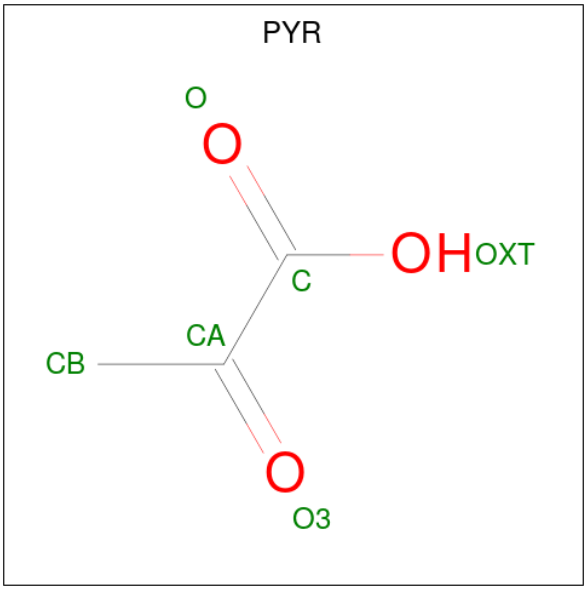
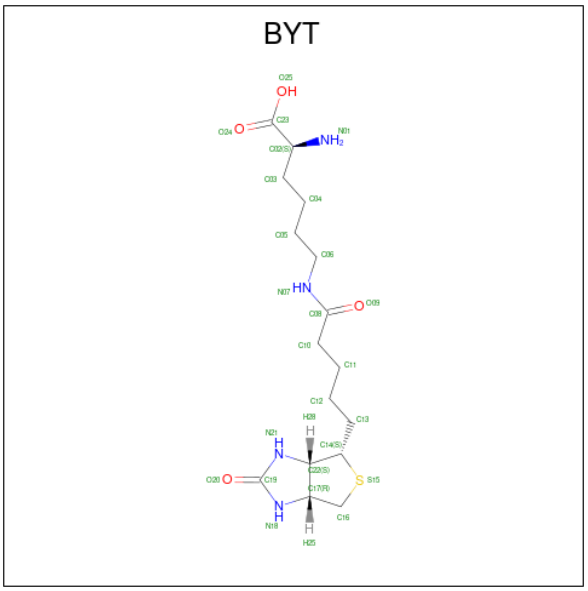
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



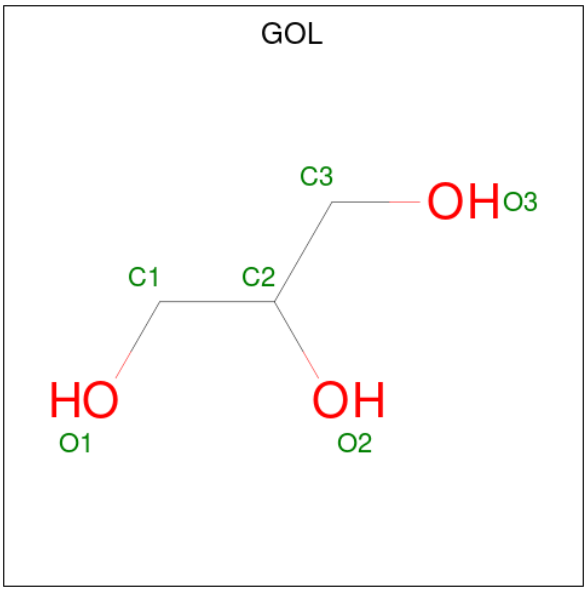
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is Biocytin (three-letter code: BYT) (formula: $C_{16}H_{28}N_4O_4S$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

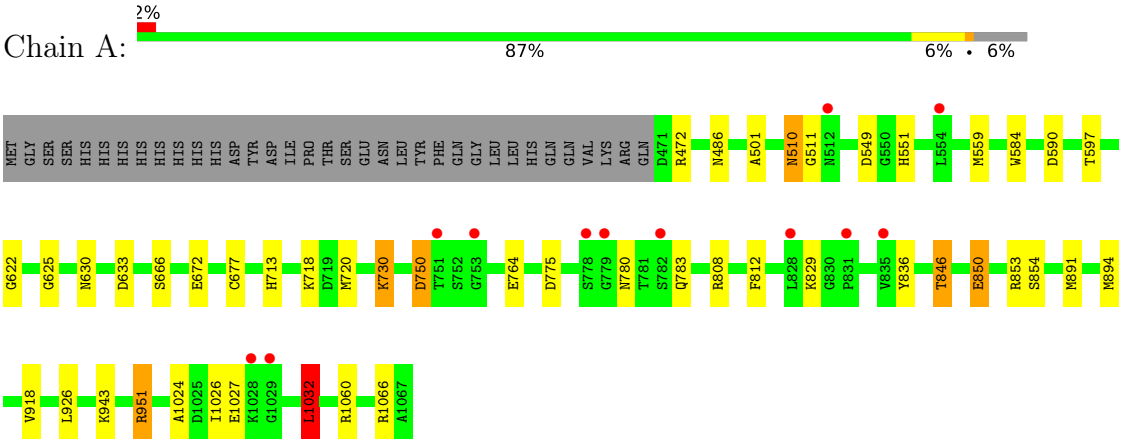
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	143	Total O 143 143	0	0
8	B	85	Total O 85 85	0	0
8	C	77	Total O 77 77	0	0
8	D	56	Total O 56 56	0	0

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.

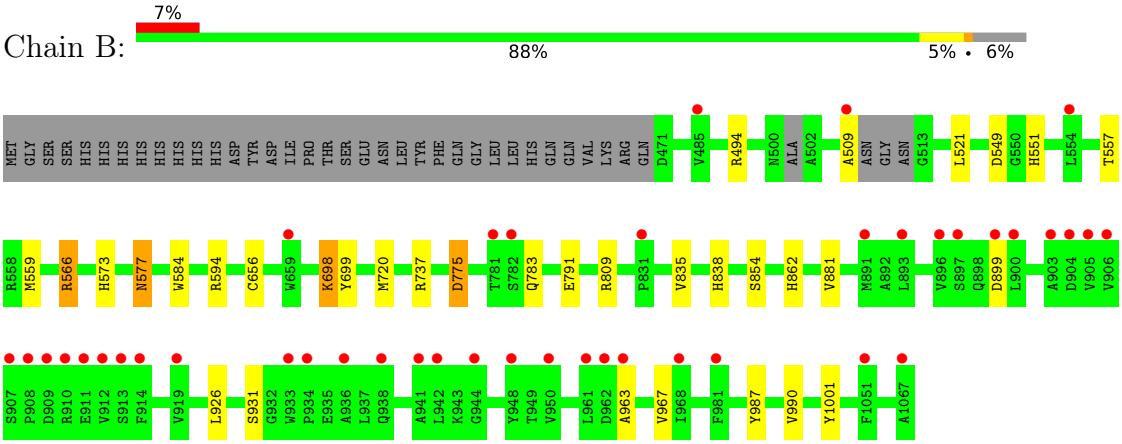
• Molecule 1: PYRUVATE CARBOXYLASE

Chain A:



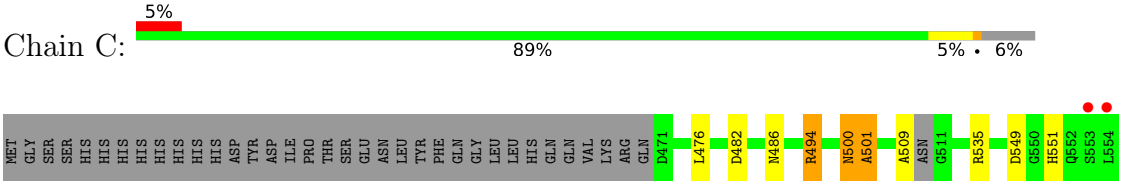
• Molecule 1: PYRUVATE CARBOXYLASE

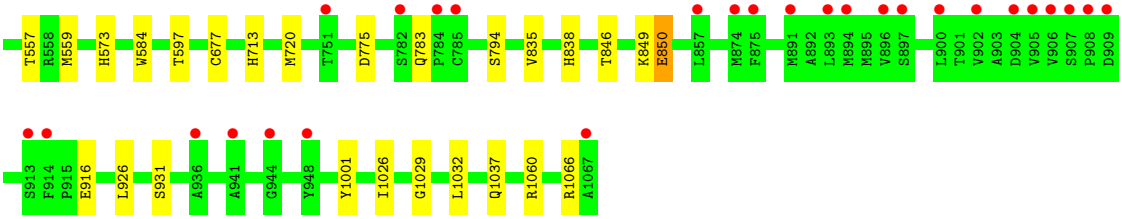
Chain B:



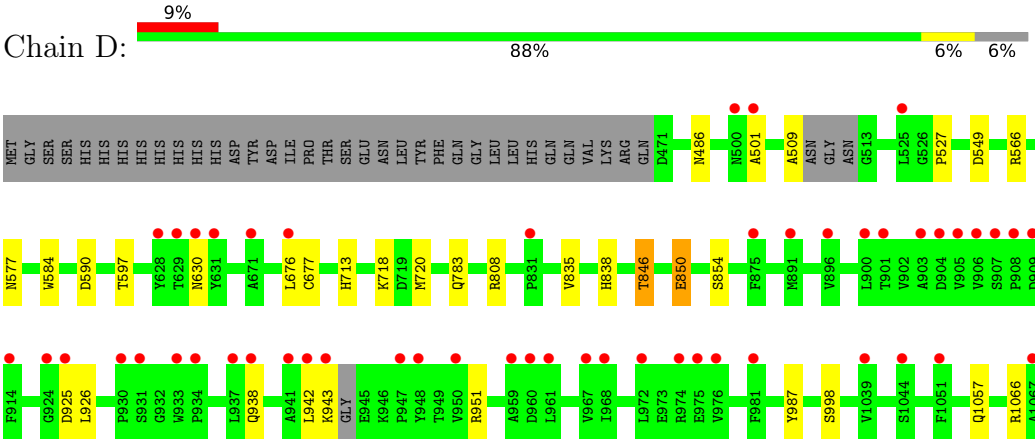
• Molecule 1: PYRUVATE CARBOXYLASE

Chain C:





• Molecule 1: PYRUVATE CARBOXYLASE



4 Data and refinement statistics (i)

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 49.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.66-2.40) 99.6 (49.61-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.31 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, KCX, CL, PYR, GOL, MG, BYT

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	0.64	0/4655	0.75	5/6330 (0.1%)
1	B	0.55	0/4524	0.69	4/6166 (0.1%)
1	C	0.52	0/4585	0.68	2/6246 (0.0%)
1	D	0.45	0/4493	0.61	0/6134
All	All	0.54	0/18257	0.69	11/24876 (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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	775	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	737	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	B	809	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	951	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	A	750	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	494	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	590	ASP	N-CA-CB	-5.95	99.90	110.60
1	A	1032	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	951	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	C	535	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	737	ARG	NE-CZ-NH2	5.07	122.83	120.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4564	0	4461	33	0
1	B	4435	0	4224	18	0
1	C	4491	0	4302	23	0
1	D	4404	0	4180	17	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	0	0
8	A	143	0	0	7	0
8	B	85	0	0	2	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	88	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 2.

All (88) 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:891[B]:MET:HE2	1:A:918:VAL:HG11	1.79	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:A:829:LYS:NZ	8:B:1201:HOH:O	2.34	0.61
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:A:812:PHE:HE1	1:B:862:HIS:CD2	2.23	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
1:A:812:PHE:CE1	1:B:862:HIS:CD2	2.93	0.56
8:A:1316:HOH:O	7:B:1101:GOL:H11	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:943:LYS:NZ	8:A:1340:HOH:O	2.42	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:500:ASN:ND2	1:C:500:ASN:N	2.60	0.49
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: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: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: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: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
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:A:894:MET:HB2	1:A:894:MET:HE3	1.92	0.43
1:D:835:VAL:HA	1:D:838:HIS:CE1	2.53	0.43
1:A:622:GLY:O	1:A:666:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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 (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	A	596/632 (94%)	583 (98%)	11 (2%)	2 (0%)	41	55
1	B	588/632 (93%)	574 (98%)	14 (2%)	0	100	100
1	C	594/632 (94%)	579 (98%)	14 (2%)	1 (0%)	47	62
1	D	588/632 (93%)	570 (97%)	17 (3%)	1 (0%)	47	62
All	All	2366/2528 (94%)	2306 (98%)	56 (2%)	4 (0%)	47	62

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 (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	A	468/519 (90%)	454 (97%)	14 (3%)	41	61
1	B	438/519 (84%)	426 (97%)	12 (3%)	44	65
1	C	448/519 (86%)	433 (97%)	15 (3%)	38	57
1	D	435/519 (84%)	423 (97%)	12 (3%)	43	63
All	All	1789/2076 (86%)	1736 (97%)	53 (3%)	41	61

All (53) 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	846	THR
1	A	850	GLU
1	A	854	SER
1	A	926	LEU
1	A	1027	GLU
1	A	1032	LEU
1	B	521	LEU
1	B	566	ARG
1	B	577	ASN
1	B	584	TRP

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Mol	Chain	Res	Type
1	B	594	ARG
1	B	698	LYS
1	B	720	MET
1	B	775	ASP
1	B	854	SER
1	B	899	ASP
1	B	926	LEU
1	B	931	SER
1	C	476	LEU
1	C	494	ARG
1	C	500	ASN
1	C	557	THR
1	C	584	TRP
1	C	597	THR
1	C	720	MET
1	C	775	ASP
1	C	794	SER
1	C	849	LYS
1	C	850	GLU
1	C	916	GLU
1	C	926	LEU
1	C	931	SER
1	C	1060	ARG
1	D	566	ARG
1	D	577	ASN
1	D	584	TRP
1	D	597	THR
1	D	720	MET
1	D	846	THR
1	D	850	GLU
1	D	854	SER
1	D	926	LEU
1	D	951	ARG
1	D	998	SER
1	D	1057	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	510	ASN
1	A	577	ASN

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Mol	Chain	Res	Type
1	A	624	ASN
1	A	630	ASN
1	A	713	HIS
1	A	783	GLN
1	B	486	ASN
1	B	624	ASN
1	B	783	GLN
1	B	928	GLN
1	C	486	ASN
1	C	500	ASN
1	C	577	ASN
1	C	713	HIS
1	C	783	GLN
1	C	938	GLN
1	D	486	ASN
1	D	713	HIS
1	D	783	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	B	718	1,2	9,11,12	0.74	0	5,12,14	0.85	0
1	KCX	A	718	1,2	9,11,12	0.73	0	5,12,14	1.34	1 (20%)
1	KCX	D	718	1,2	9,11,12	0.83	0	5,12,14	2.89	2 (40%)
1	KCX	C	718	1,2	9,11,12	0.66	0	5,12,14	1.00	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	B	718	1,2	-	1/9/10/12	-
1	KCX	A	718	1,2	-	2/9/10/12	-
1	KCX	D	718	1,2	-	2/9/10/12	-
1	KCX	C	718	1,2	-	2/9/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	718	KCX	OQ1-CX-NZ	-5.45	116.51	124.96
1	D	718	KCX	CE-NZ-CX	3.35	127.27	121.89
1	A	718	KCX	CE-NZ-CX	2.03	125.15	121.89

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 monosaccharides 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	$\#\|Z\| > 2$
6	BYT	B	1106	-	25,26,26	2.70	8 (32%)	33,34,34	5.28	11 (33%)
6	BYT	D	1106	-	10,11,26	3.27	5 (50%)	15,16,34	7.23	10 (66%)
5	PYR	C	1105	-	5,5,5	1.48	1 (20%)	3,6,6	1.52	1 (33%)
6	BYT	A	1105	-	25,26,26	2.59	8 (32%)	33,34,34	4.34	12 (36%)
6	BYT	B	1107	-	15,15,26	3.63	7 (46%)	20,20,34	6.67	12 (60%)
6	BYT	C	1106	-	25,26,26	3.08	9 (36%)	33,34,34	5.55	13 (39%)
6	BYT	A	1106	-	19,19,26	3.43	8 (42%)	24,25,34	5.64	12 (50%)
7	GOL	B	1101	-	5,5,5	0.38	0	5,5,5	1.03	0
7	GOL	C	1102	-	5,5,5	0.20	0	5,5,5	0.30	0
6	BYT	C	1107	-	17,17,26	3.36	8 (47%)	23,23,34	6.04	9 (39%)
5	PYR	A	1104	-	5,5,5	1.22	0	3,6,6	1.75	1 (33%)
6	BYT	D	1105	-	25,26,26	2.75	8 (32%)	33,34,34	4.85	12 (36%)
5	PYR	D	1104	-	5,5,5	1.28	0	3,6,6	1.65	1 (33%)
5	PYR	B	1105	-	5,5,5	1.22	0	3,6,6	0.98	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
6	BYT	B	1106	-	-	7/19/40/40	0/2/2/2
6	BYT	D	1106	-	-	-	0/2/2/2
5	PYR	C	1105	-	-	2/4/4/4	-
6	BYT	A	1105	-	-	1/19/40/40	0/2/2/2
6	BYT	B	1107	-	-	3/5/26/40	0/2/2/2
6	BYT	C	1106	-	-	7/19/40/40	0/2/2/2
6	BYT	A	1106	-	-	5/10/31/40	0/2/2/2
7	GOL	B	1101	-	-	2/4/4/4	-
7	GOL	C	1102	-	-	3/4/4/4	-
6	BYT	C	1107	-	-	3/7/28/40	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	A	1104	-	-	1/4/4/4	-
6	BYT	D	1105	-	-	5/19/40/40	0/2/2/2
5	PYR	D	1104	-	-	2/4/4/4	-
5	PYR	B	1105	-	-	1/4/4/4	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1106	BYT	C14-S15	-11.57	1.64	1.82
6	B	1107	BYT	C14-S15	-8.90	1.68	1.82
6	A	1105	BYT	C14-S15	-8.54	1.68	1.82
6	C	1107	BYT	C14-S15	-8.06	1.69	1.82
6	A	1106	BYT	C14-S15	-8.01	1.69	1.82
6	B	1106	BYT	C14-S15	-7.93	1.69	1.82
6	D	1105	BYT	C14-S15	-7.83	1.70	1.82
6	A	1106	BYT	C19-N18	6.06	1.45	1.35
6	C	1106	BYT	C16-S15	-5.77	1.64	1.81
6	C	1107	BYT	C19-N18	5.70	1.44	1.35
6	A	1106	BYT	C08-N07	5.43	1.45	1.33
6	D	1106	BYT	C19-N21	5.38	1.44	1.35
6	B	1107	BYT	C19-N18	5.23	1.44	1.35
6	A	1106	BYT	C16-S15	-5.23	1.65	1.81
6	D	1105	BYT	C19-N21	5.16	1.43	1.35
6	A	1105	BYT	C08-N07	5.07	1.44	1.33
6	B	1107	BYT	C19-N21	5.03	1.43	1.35
6	D	1106	BYT	C19-N18	4.91	1.43	1.35
6	D	1105	BYT	C08-N07	4.90	1.44	1.33
6	B	1107	BYT	C16-S15	-4.75	1.67	1.81
6	B	1106	BYT	C08-N07	4.67	1.44	1.33
6	C	1107	BYT	C19-N21	4.60	1.42	1.35
6	A	1106	BYT	C17-C22	4.58	1.68	1.55
6	C	1107	BYT	C16-S15	-4.52	1.67	1.81
6	B	1106	BYT	C16-S15	-4.50	1.68	1.81
6	D	1106	BYT	C16-S15	-4.45	1.68	1.81
6	D	1106	BYT	C17-C22	4.43	1.67	1.55
6	D	1105	BYT	C19-N18	4.36	1.42	1.35
6	B	1106	BYT	C19-N18	4.35	1.42	1.35
6	A	1105	BYT	C16-S15	-4.33	1.68	1.81
6	B	1107	BYT	C17-C22	4.32	1.67	1.55
6	D	1105	BYT	C16-S15	-4.10	1.69	1.81
6	C	1107	BYT	C17-C22	3.97	1.66	1.55
6	A	1106	BYT	C19-N21	3.87	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1106	BYT	C08-N07	3.83	1.42	1.33
6	B	1106	BYT	C17-C22	3.80	1.66	1.55
6	B	1106	BYT	C19-N21	3.66	1.41	1.35
6	D	1105	BYT	C17-C22	3.63	1.65	1.55
6	C	1107	BYT	C08-N07	3.59	1.44	1.32
6	B	1107	BYT	C16-C17	3.59	1.59	1.53
6	D	1105	BYT	C16-C17	3.46	1.59	1.53
6	D	1106	BYT	C16-C17	3.42	1.59	1.53
6	C	1107	BYT	C16-C17	3.41	1.59	1.53
6	A	1106	BYT	C16-C17	3.37	1.59	1.53
6	A	1105	BYT	C17-C22	3.24	1.64	1.55
6	A	1105	BYT	C19-N21	3.22	1.40	1.35
6	B	1106	BYT	C16-C17	3.13	1.58	1.53
6	C	1106	BYT	C17-C22	3.05	1.64	1.55
6	C	1106	BYT	C19-N18	3.05	1.40	1.35
6	C	1106	BYT	C19-N21	2.87	1.40	1.35
6	A	1105	BYT	C16-C17	2.71	1.58	1.53
6	B	1106	BYT	O24-C23	2.66	1.30	1.22
6	A	1105	BYT	C19-N18	2.60	1.39	1.35
6	A	1106	BYT	C17-N18	2.49	1.49	1.46
6	C	1106	BYT	O09-C08	-2.38	1.18	1.23
6	B	1107	BYT	C14-C22	2.25	1.58	1.53
6	C	1107	BYT	C13-C14	2.18	1.57	1.52
6	C	1106	BYT	C16-C17	2.12	1.57	1.53
6	D	1105	BYT	O24-C23	2.08	1.28	1.22
6	C	1106	BYT	O20-C19	-2.08	1.19	1.23
5	C	1105	PYR	CA-C	-2.07	1.46	1.54
6	A	1105	BYT	O24-C23	2.05	1.28	1.22

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1106	BYT	C16-C17-N18	-26.02	79.96	113.03
6	B	1106	BYT	C16-C17-N18	-25.29	80.89	113.03
6	B	1107	BYT	C16-C17-N18	-24.43	81.97	113.03
6	C	1107	BYT	C16-C17-N18	-23.55	83.10	113.03
6	D	1105	BYT	C16-C17-N18	-22.73	84.14	113.03
6	D	1106	BYT	C16-C17-N18	-22.14	84.89	113.03
6	A	1105	BYT	C16-C17-N18	-19.07	88.79	113.03
6	A	1106	BYT	C16-C17-N18	-18.42	89.62	113.03
6	A	1106	BYT	N21-C19-N18	10.56	118.67	108.76
6	D	1106	BYT	N21-C19-N18	9.69	117.85	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1107	BYT	N21-C19-N18	9.50	117.67	108.76
6	C	1106	BYT	N21-C19-N18	9.34	117.52	108.76
6	A	1105	BYT	N21-C19-N18	9.11	117.31	108.76
6	B	1106	BYT	N21-C19-N18	9.10	117.30	108.76
6	A	1106	BYT	C22-N21-C19	-8.29	104.89	112.62
6	D	1105	BYT	N21-C19-N18	8.16	116.42	108.76
6	C	1107	BYT	N21-C19-N18	7.86	116.14	108.76
6	C	1107	BYT	C16-S15-C14	7.83	105.97	89.89
6	A	1106	BYT	O20-C19-N21	-7.80	114.74	125.94
6	D	1106	BYT	C22-N21-C19	-7.70	105.45	112.62
6	C	1107	BYT	C22-N21-C19	-7.62	105.52	112.62
6	B	1107	BYT	C22-N21-C19	-7.56	105.57	112.62
6	D	1106	BYT	C16-S15-C14	7.50	105.36	89.92
6	C	1106	BYT	C22-N21-C19	-7.24	105.87	112.62
6	C	1106	BYT	C16-S15-C14	7.17	104.63	89.89
6	D	1105	BYT	C22-N21-C19	-6.87	106.21	112.62
6	B	1106	BYT	C16-S15-C14	6.81	103.89	89.89
6	C	1106	BYT	C14-C22-C17	-6.72	101.14	108.94
6	B	1106	BYT	C22-N21-C19	-6.46	106.60	112.62
6	A	1105	BYT	C22-N21-C19	-6.40	106.65	112.62
6	B	1107	BYT	C16-S15-C14	6.16	102.55	89.89
6	A	1106	BYT	C16-S15-C14	6.04	102.30	89.89
6	D	1105	BYT	C16-S15-C14	5.95	102.11	89.89
6	A	1106	BYT	C14-C22-N21	-5.84	107.89	113.13
6	A	1106	BYT	C17-N18-C19	-5.51	105.29	112.46
6	C	1107	BYT	C14-C22-N21	-5.50	108.20	113.13
6	A	1105	BYT	C14-C22-C17	-5.43	102.64	108.94
6	D	1106	BYT	C17-N18-C19	-5.28	105.59	112.46
6	D	1105	BYT	C14-C22-C17	-5.27	102.82	108.94
6	B	1107	BYT	C17-N18-C19	-5.23	105.65	112.46
6	B	1106	BYT	C17-N18-C19	-5.12	105.79	112.46
6	C	1106	BYT	C17-N18-C19	-4.95	106.00	112.46
6	C	1107	BYT	O20-C19-N21	-4.85	118.98	125.94
6	B	1106	BYT	O20-C19-N21	-4.65	119.26	125.94
6	C	1107	BYT	C17-C22-N21	4.64	107.66	102.67
6	D	1105	BYT	C17-N18-C19	-4.60	106.47	112.46
6	A	1105	BYT	C17-N18-C19	-4.58	106.50	112.46
6	B	1107	BYT	O20-C19-N21	-4.44	119.56	125.94
6	A	1106	BYT	C17-C22-N21	4.43	107.43	102.67
6	B	1107	BYT	C14-C22-C17	-4.28	103.97	108.94
6	A	1106	BYT	C10-C08-N07	4.11	123.34	116.42
6	A	1106	BYT	C14-C22-C17	-4.09	104.20	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1107	BYT	C17-N18-C19	-3.75	107.57	112.46
6	D	1106	BYT	C14-C22-C17	-3.73	104.61	108.94
6	D	1106	BYT	O20-C19-N21	-3.68	120.66	125.94
6	A	1105	BYT	C16-C17-C22	-3.44	105.67	108.66
6	C	1106	BYT	O20-C19-N21	-3.36	121.11	125.94
6	D	1105	BYT	C14-C22-N21	3.31	116.09	113.13
6	B	1107	BYT	C17-C22-N21	3.29	106.21	102.67
6	A	1105	BYT	O20-C19-N18	-3.26	121.25	125.94
6	D	1105	BYT	O20-C19-N18	-3.21	121.33	125.94
6	C	1106	BYT	O20-C19-N18	-3.21	121.33	125.94
6	D	1106	BYT	C17-C22-N21	3.19	106.10	102.67
6	A	1105	BYT	C16-S15-C14	3.19	96.43	89.89
6	A	1106	BYT	C22-C14-S15	3.18	108.23	105.20
6	B	1106	BYT	C14-C22-C17	-3.14	105.29	108.94
6	A	1105	BYT	O20-C19-N21	-3.14	121.43	125.94
6	B	1107	BYT	C14-C22-N21	-3.13	110.32	113.13
6	D	1106	BYT	O20-C19-N18	-3.13	121.45	125.94
6	C	1106	BYT	C17-C22-N21	3.12	106.03	102.67
6	B	1106	BYT	C14-C22-N21	-3.00	110.43	113.13
6	D	1105	BYT	C12-C13-C14	-2.96	107.85	113.86
6	D	1105	BYT	C17-C22-N21	2.93	105.81	102.67
6	C	1106	BYT	C10-C08-N07	2.84	121.21	116.42
6	A	1106	BYT	O09-C08-N07	-2.83	117.68	123.01
6	B	1106	BYT	C17-C22-N21	2.61	105.47	102.67
6	D	1105	BYT	O20-C19-N21	-2.59	122.22	125.94
6	C	1107	BYT	C14-C22-C17	-2.53	106.00	108.94
6	B	1107	BYT	C16-C17-C22	-2.52	106.48	108.66
5	A	1104	PYR	OXT-C-CA	2.51	120.84	113.97
6	A	1105	BYT	C17-C22-N21	2.49	105.35	102.67
6	D	1105	BYT	C22-C17-N18	2.43	105.01	102.43
6	A	1105	BYT	C14-C22-N21	2.39	115.27	113.13
6	C	1106	BYT	C06-N07-C08	-2.37	118.44	122.84
6	D	1106	BYT	C22-C17-N18	2.27	104.84	102.43
6	B	1107	BYT	C22-C17-N18	2.26	104.83	102.43
6	B	1106	BYT	C22-C17-N18	2.24	104.81	102.43
6	B	1107	BYT	O20-C19-N18	-2.22	122.75	125.94
5	C	1105	PYR	OXT-C-CA	2.21	120.03	113.97
5	D	1104	PYR	OXT-C-CA	2.19	119.96	113.97
6	A	1105	BYT	C13-C14-C22	-2.15	108.48	114.73
6	C	1106	BYT	C17-C16-S15	-2.13	104.48	106.31
6	C	1106	BYT	O09-C08-C10	-2.03	118.31	122.02
6	B	1106	BYT	C11-C10-C08	-2.02	107.58	113.26

There are no chirality outliers.

All (42) 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	C	1106	BYT	C10-C11-C12-C13
6	A	1106	BYT	O09-C08-N07-C06
6	B	1106	BYT	C08-C10-C11-C12
6	B	1106	BYT	C11-C12-C13-C14
7	C	1102	GOL	O1-C1-C2-C3
6	C	1106	BYT	C08-C10-C11-C12
6	C	1106	BYT	C04-C05-C06-N07
6	D	1105	BYT	C02-C03-C04-C05
6	B	1106	BYT	C03-C04-C05-C06
6	B	1106	BYT	C04-C05-C06-N07
6	B	1106	BYT	C02-C03-C04-C05
6	D	1105	BYT	C04-C05-C06-N07
5	C	1105	PYR	O-C-CA-CB
5	D	1104	PYR	O-C-CA-CB
6	D	1105	BYT	C23-C02-C03-C04
7	B	1101	GOL	O2-C2-C3-O3
6	D	1105	BYT	C03-C04-C05-C06
6	A	1106	BYT	C11-C12-C13-C14
5	A	1104	PYR	OXT-C-CA-O3
5	B	1105	PYR	OXT-C-CA-O3
6	D	1105	BYT	C08-C10-C11-C12
6	C	1106	BYT	C02-C03-C04-C05
6	A	1105	BYT	N01-C02-C23-O25

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Mol	Chain	Res	Type	Atoms
6	C	1106	BYT	C03-C04-C05-C06
6	B	1107	BYT	C11-C12-C13-C14

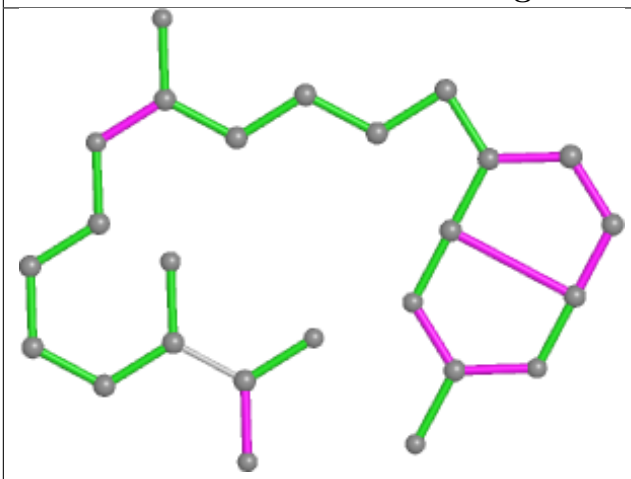
There are no ring outliers.

7 monomers are involved in 17 short contacts:

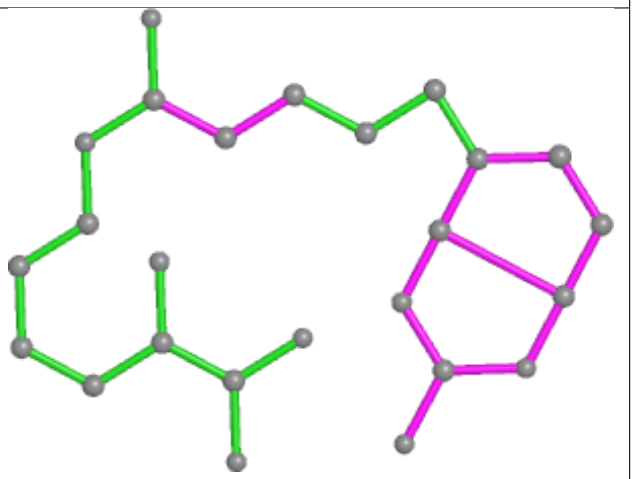
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1106	BYT	1	0
6	D	1106	BYT	2	0
6	B	1107	BYT	1	0
6	C	1106	BYT	3	0
6	A	1106	BYT	3	0
7	B	1101	GOL	3	0
6	C	1107	BYT	4	0

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 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.

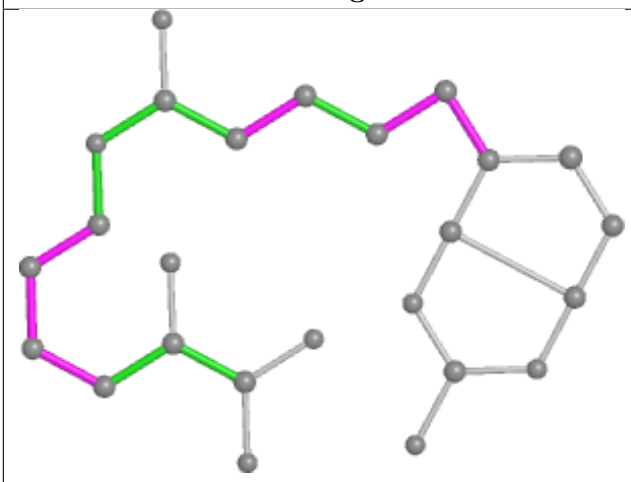
Ligand BYT B 1106



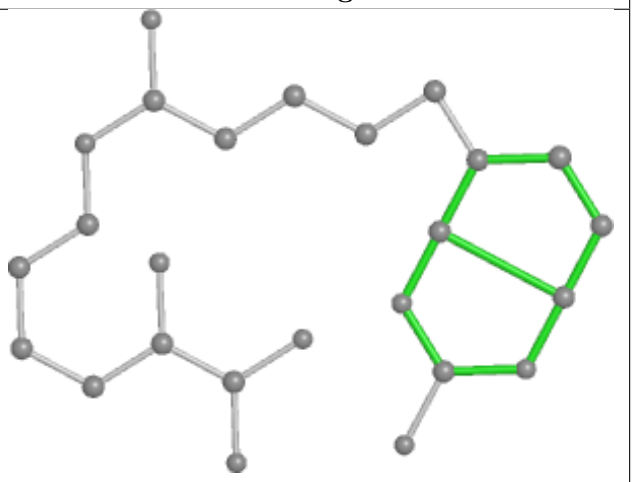
Bond lengths



Bond angles

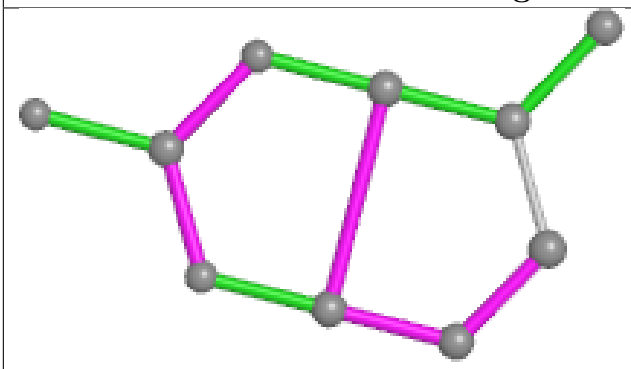


Torsions

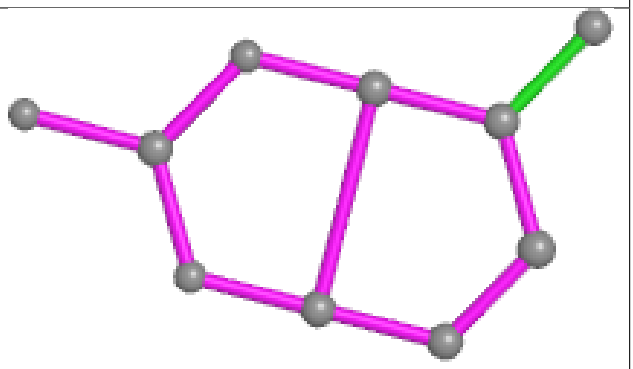


Rings

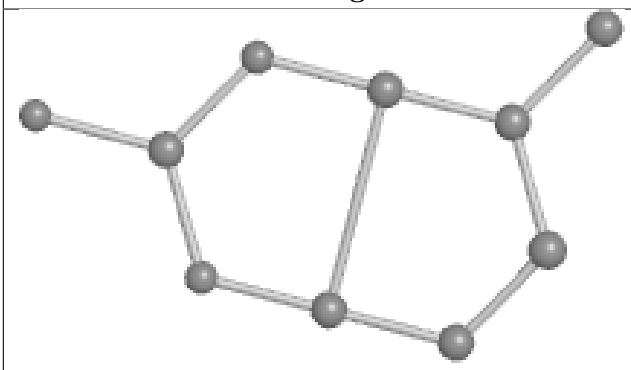
Ligand BYT D 1106



Bond lengths



Bond angles



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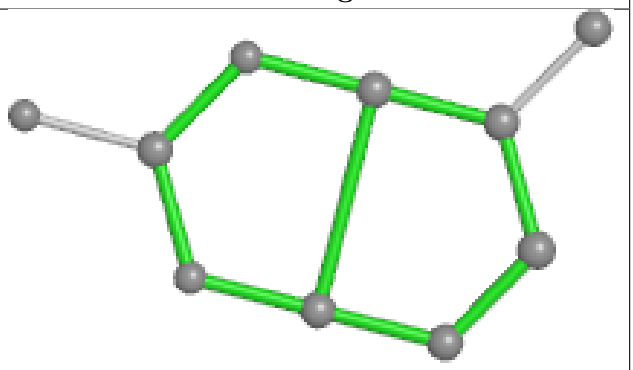
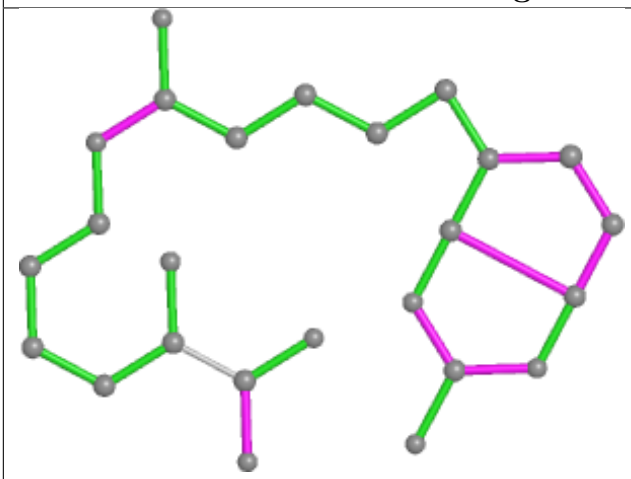
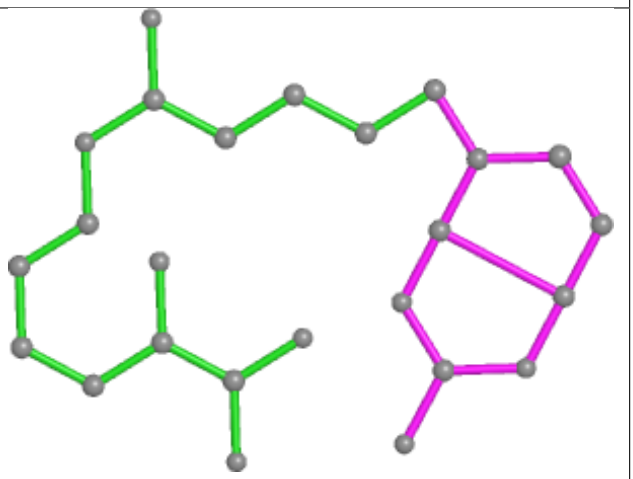


Rings

Ligand BYT A 1105



Bond lengths



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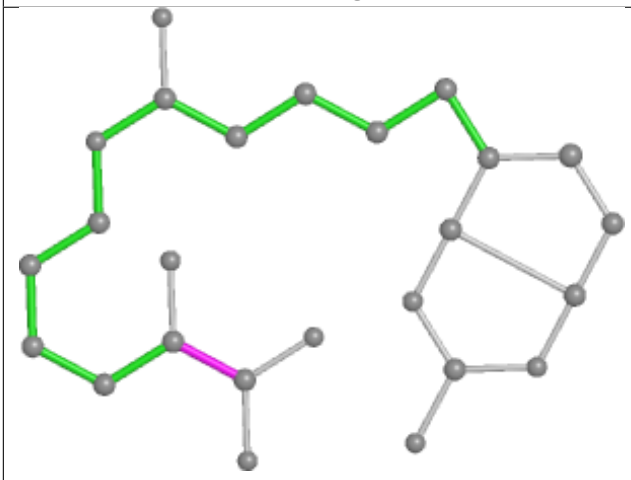
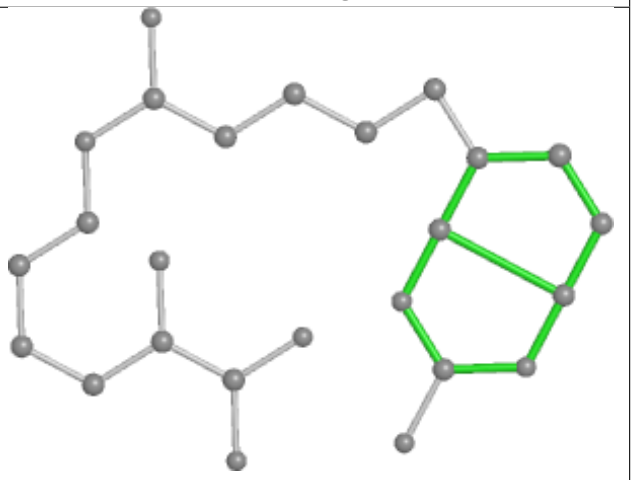
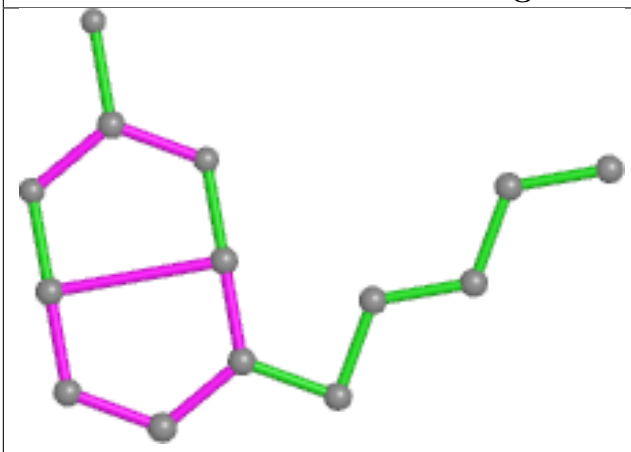


Torsions

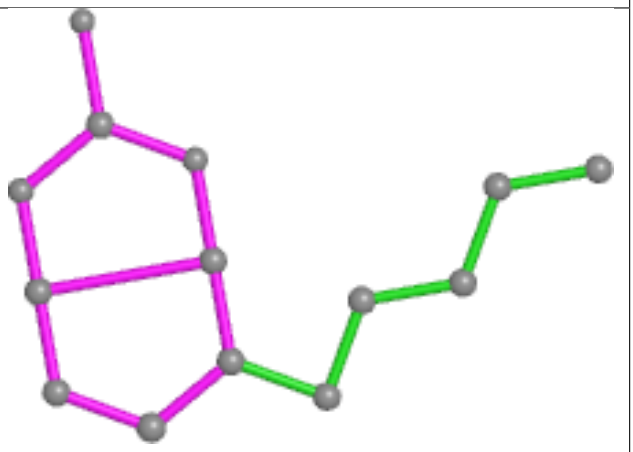


Rings

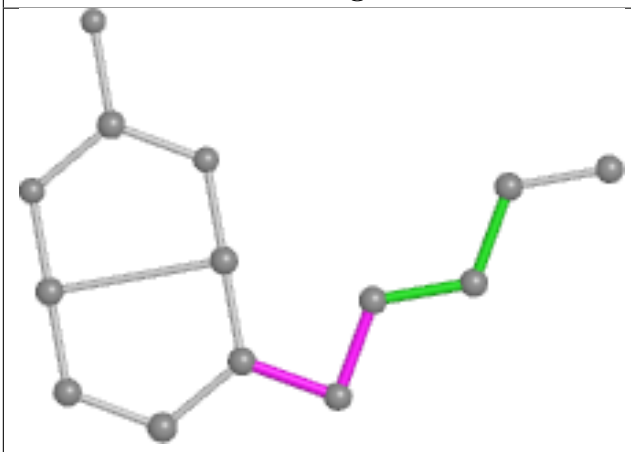
Ligand BYT B 1107



Bond lengths



Bond angles



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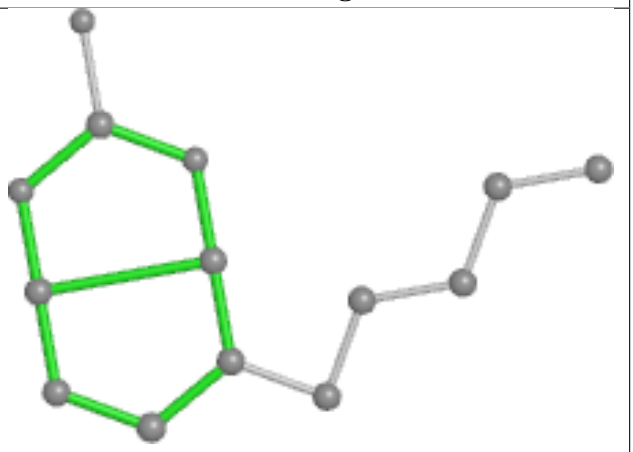
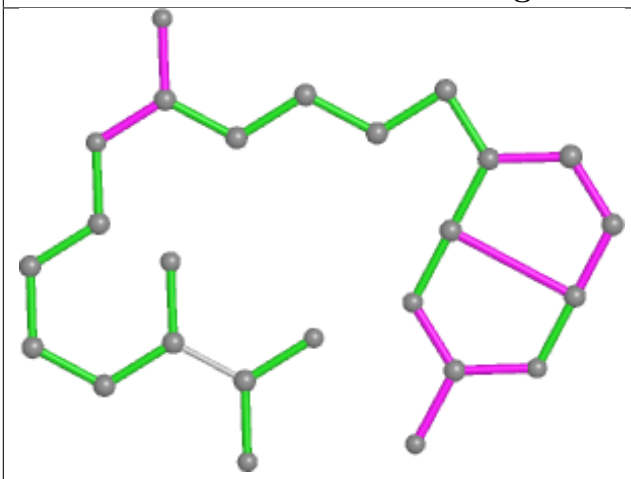
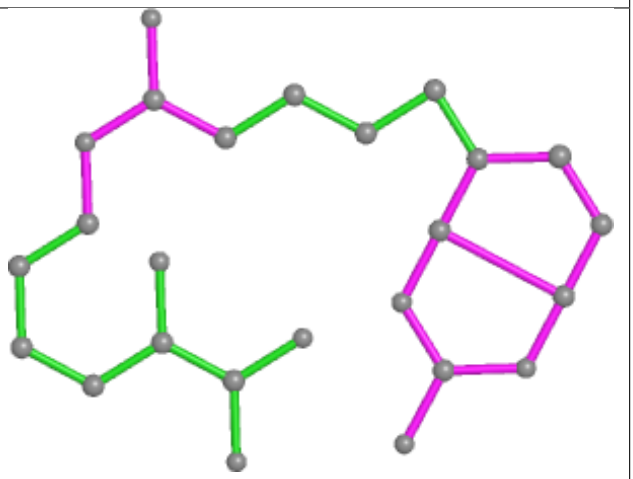


Rings

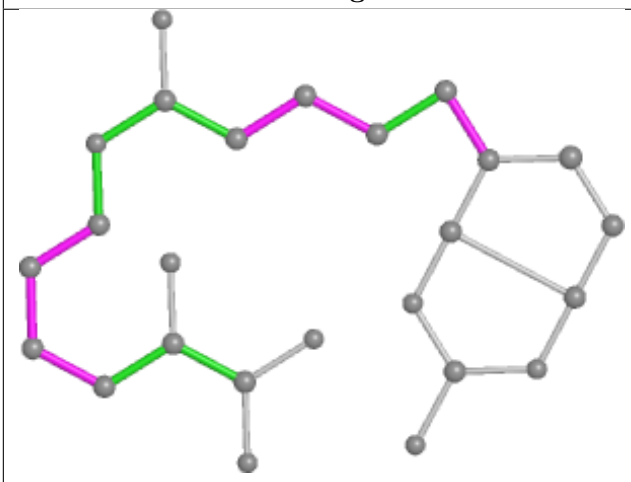
Ligand BYT C 1106



Bond lengths



Bond angles



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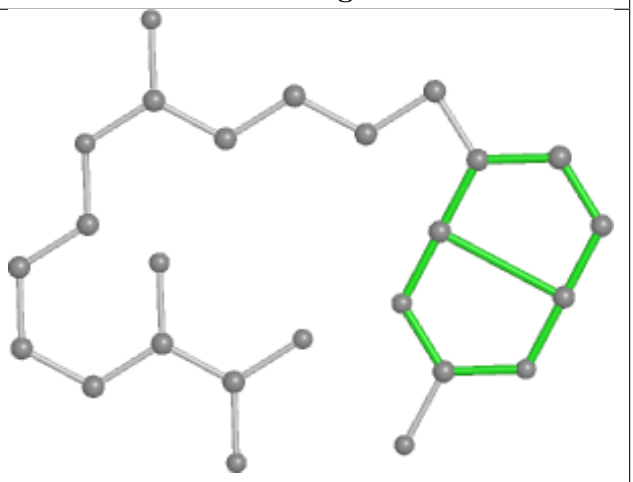
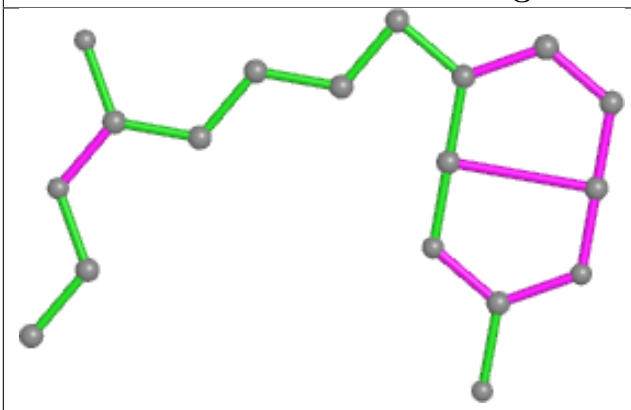


Rings

Ligand BYT A 1106



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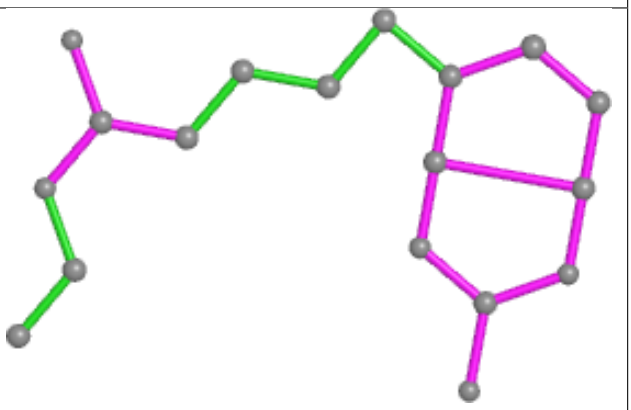
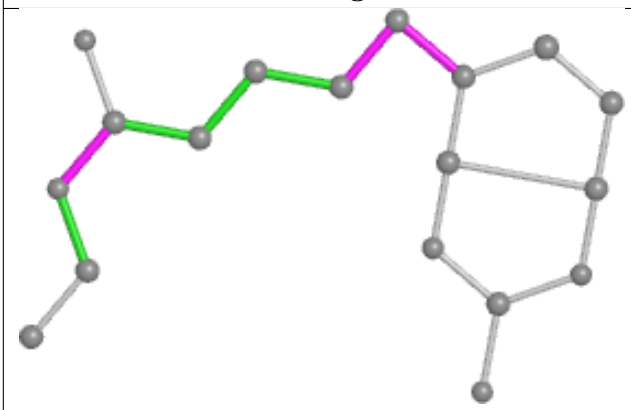
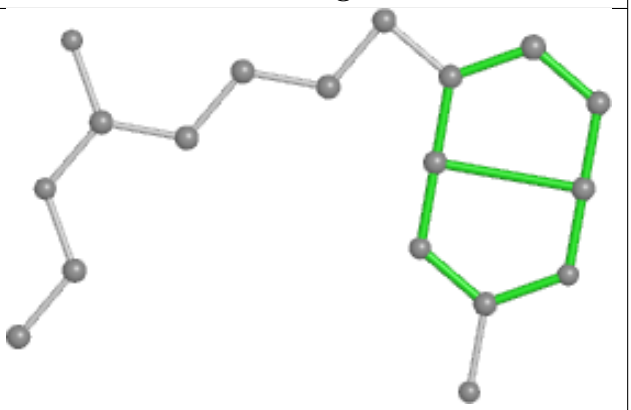


Bond angles

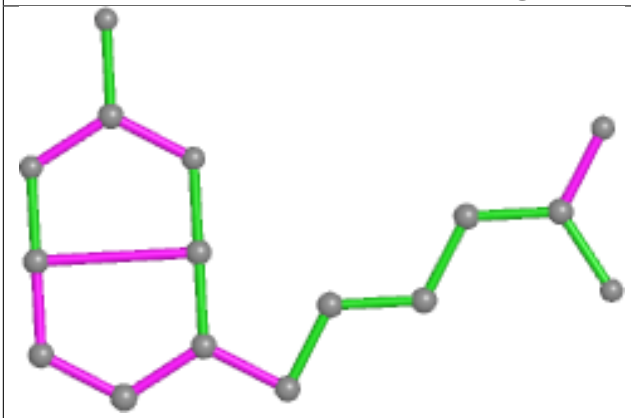


Torsions

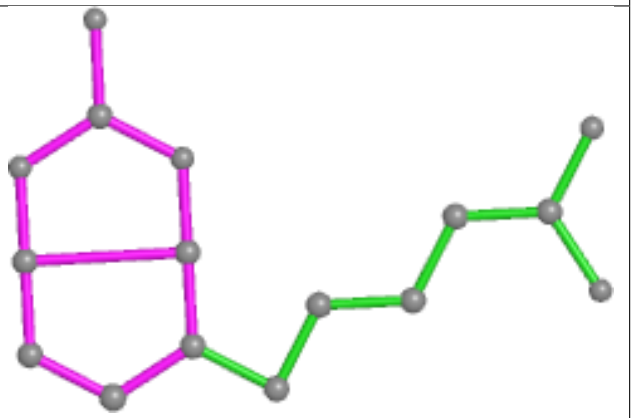


Rings

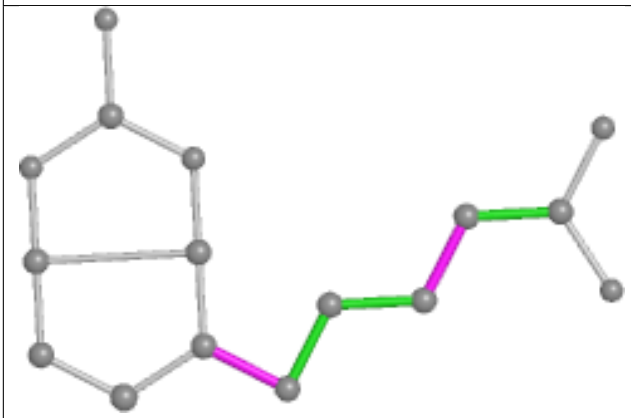
Ligand BYT C 1107



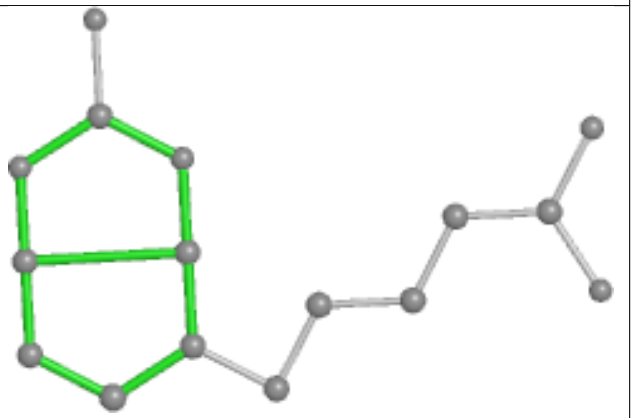
Bond lengths



Bond angles

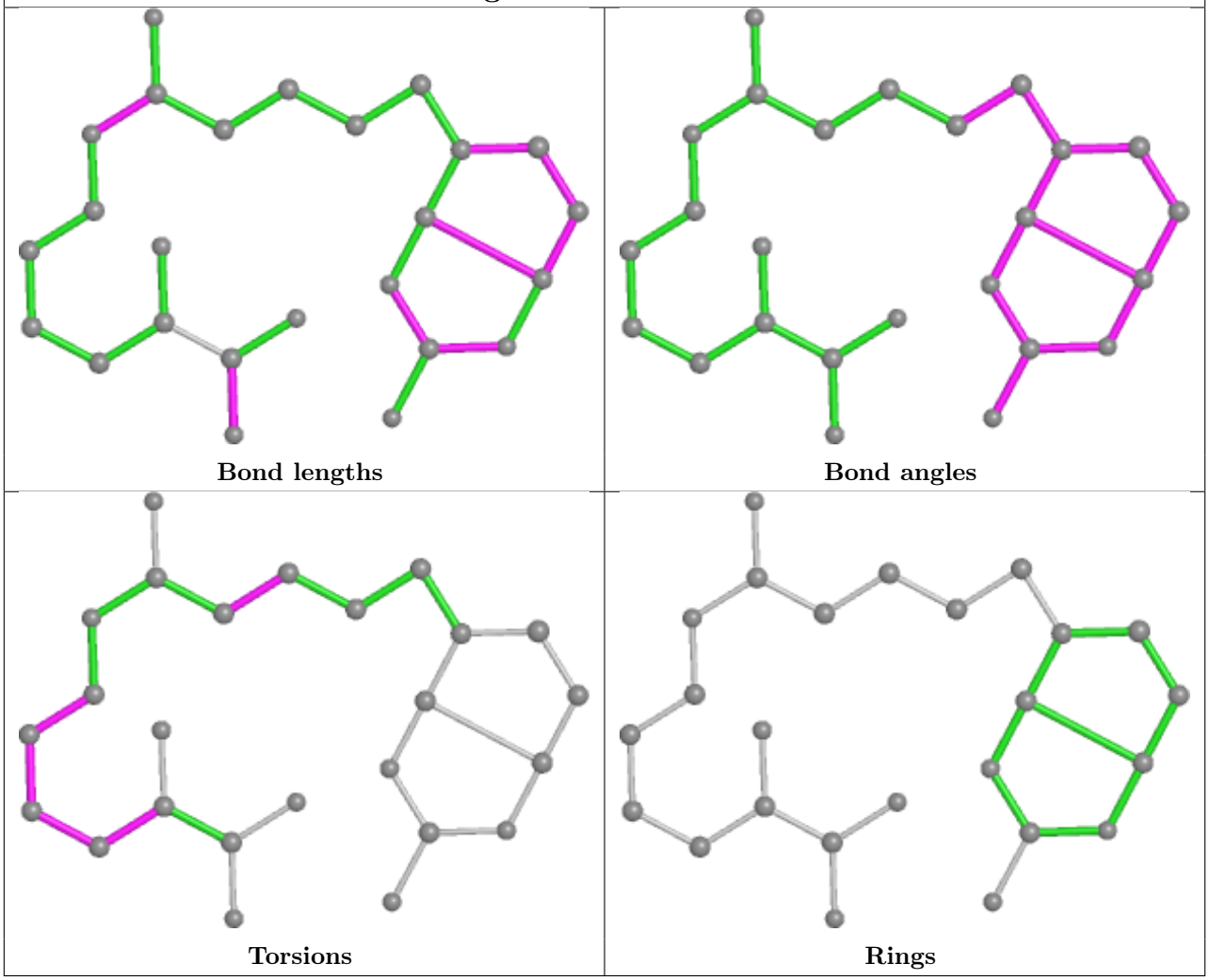


Torsions



Rings

Ligand BYT D 1105



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	A	596/632 (94%)	-0.25	12 (2%)	65	63	30, 45, 68, 130	19 (3%)
1	B	592/632 (93%)	0.19	42 (7%)	16	14	31, 65, 122, 168	13 (2%)
1	C	595/632 (94%)	0.04	29 (4%)	29	28	38, 60, 118, 170	15 (2%)
1	D	592/632 (93%)	0.33	54 (9%)	9	8	46, 77, 115, 158	14 (2%)
All	All	2375/2528 (93%)	0.08	137 (5%)	23	22	30, 60, 113, 170	61 (2%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	628	TYR	9.4
1	D	906	VAL	7.8
1	D	909	ASP	6.8
1	D	907	SER	6.7
1	B	912	VAL	6.1
1	D	905	VAL	6.1
1	D	1044	SER	4.8
1	C	896	VAL	4.7
1	C	900	LEU	4.5
1	D	891[A]	MET	4.5
1	D	908	PRO	4.5
1	A	1029	GLY	4.3
1	C	893	LEU	3.9
1	A	1028	LYS	3.9
1	D	937	LEU	3.9
1	D	896	VAL	3.8
1	D	1067	ALA	3.8
1	D	501	ALA	3.7
1	C	914	PHE	3.7
1	C	874	MET	3.7
1	D	525	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	934	PRO	3.7
1	B	942	LEU	3.7
1	C	1067	ALA	3.7
1	B	900	LEU	3.6
1	D	903	ALA	3.6
1	D	961	LEU	3.5
1	B	909	ASP	3.5
1	D	941	ALA	3.5
1	D	942	LEU	3.5
1	B	963	ALA	3.4
1	D	950	VAL	3.4
1	A	512	ASN	3.4
1	D	914	PHE	3.4
1	D	910	ARG	3.4
1	D	875	PHE	3.3
1	B	904	ASP	3.3
1	C	906	VAL	3.3
1	B	907	SER	3.3
1	D	912	VAL	3.2
1	B	914	PHE	3.2
1	C	908	PRO	3.2
1	C	904	ASP	3.2
1	C	902	VAL	3.2
1	D	900	LEU	3.2
1	D	1051	PHE	3.1
1	B	1067	ALA	3.1
1	C	875	PHE	3.1
1	A	779	GLY	3.1
1	D	630	ASN	3.1
1	C	905	VAL	3.1
1	B	933	TRP	3.0
1	C	948	TYR	3.0
1	B	509	ALA	3.0
1	D	901	THR	3.0
1	B	905	VAL	2.9
1	C	907	SER	2.9
1	B	908	PRO	2.9
1	C	909	ASP	2.8
1	D	911	GLU	2.8
1	B	906	VAL	2.8
1	B	919	VAL	2.8
1	D	933	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	941	ALA	2.8
1	B	944	GLY	2.8
1	B	962	ASP	2.8
1	D	671	ALA	2.7
1	B	1051	PHE	2.7
1	B	897	SER	2.7
1	A	828	LEU	2.7
1	A	554	LEU	2.6
1	C	936	ALA	2.6
1	B	485	VAL	2.6
1	B	896	VAL	2.6
1	B	913	SER	2.6
1	A	835	VAL	2.5
1	B	910	ARG	2.5
1	A	778	SER	2.5
1	B	936	ALA	2.5
1	B	961	LEU	2.5
1	D	904	ASP	2.4
1	D	967	VAL	2.4
1	C	785	CYS	2.4
1	B	659	TRP	2.4
1	C	913	SER	2.4
1	D	975	GLU	2.4
1	B	831	PRO	2.4
1	D	676	LEU	2.4
1	D	500	ASN	2.3
1	B	968	ILE	2.3
1	C	891[A]	MET	2.3
1	D	831	PRO	2.3
1	C	751	THR	2.3
1	D	924	GLY	2.3
1	B	941	ALA	2.3
1	D	931	SER	2.3
1	B	782	SER	2.3
1	C	782	SER	2.3
1	D	959	ALA	2.3
1	D	938	GLN	2.3
1	B	903	ALA	2.2
1	C	857	LEU	2.2
1	B	891[A]	MET	2.2
1	B	950	VAL	2.2
1	A	751	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	831	PRO	2.2
1	B	911	GLU	2.2
1	B	938	GLN	2.2
1	B	554	LEU	2.2
1	D	968	ILE	2.2
1	D	960	ASP	2.2
1	B	948	TYR	2.2
1	C	897	SER	2.2
1	D	629	THR	2.2
1	D	948	TYR	2.1
1	D	976	VAL	2.1
1	A	753	GLY	2.1
1	B	781	THR	2.1
1	D	930	PRO	2.1
1	B	893	LEU	2.1
1	B	981	PHE	2.1
1	C	784	PRO	2.1
1	D	934	PRO	2.1
1	D	1039	VAL	2.1
1	A	782	SER	2.1
1	C	944	GLY	2.1
1	D	972	LEU	2.1
1	D	943	LYS	2.1
1	B	899	ASP	2.1
1	D	631	TYR	2.1
1	C	554	LEU	2.1
1	D	974	ARG	2.1
1	D	947	PRO	2.0
1	D	925	ASP	2.0
1	D	981	PHE	2.0
1	C	553	SER	2.0
1	C	894	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	KCX	A	718	12/13	0.98	0.16	34,37,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	B	718	12/13	0.98	0.15	45,48,50,51	0
1	KCX	D	718	12/13	0.98	0.17	56,62,65,66	0
1	KCX	C	718	12/13	0.99	0.17	49,52,53,55	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	MG	A	1102	1/1	0.81	0.09	60,60,60,60	0
4	CL	D	1103	1/1	0.87	0.09	83,83,83,83	0
3	MG	D	1102	1/1	0.89	0.09	82,82,82,82	0
6	BYT	B	1107	14/25	0.89	0.18	63,75,85,85	1
6	BYT	D	1106	10/25	0.89	0.16	78,81,83,84	0
5	PYR	D	1104	6/6	0.92	0.22	70,77,77,78	0
6	BYT	A	1106	18/25	0.92	0.15	37,46,82,83	1
6	BYT	C	1107	16/25	0.93	0.12	72,78,83,84	0
6	BYT	B	1106	25/25	0.93	0.12	71,77,83,84	0
4	CL	C	1104	1/1	0.94	0.09	70,70,70,70	0
5	PYR	A	1104	6/6	0.94	0.15	41,44,47,47	0
5	PYR	B	1105	6/6	0.94	0.15	63,64,66,67	0
4	CL	B	1104	1/1	0.95	0.11	86,86,86,86	0
7	GOL	B	1101	6/6	0.95	0.33	48,48,50,53	0
6	BYT	D	1105	25/25	0.96	0.12	67,70,76,76	0
6	BYT	C	1106	25/25	0.96	0.11	51,55,61,61	0
5	PYR	C	1105	6/6	0.96	0.18	56,62,65,65	0
7	GOL	C	1102	6/6	0.96	0.21	60,63,69,72	0
3	MG	B	1103	1/1	0.97	0.06	43,43,43,43	0
4	CL	A	1103	1/1	0.97	0.10	47,47,47,47	0
6	BYT	A	1105	25/25	0.98	0.12	40,45,47,48	0
3	MG	C	1103	1/1	0.99	0.07	56,56,56,56	0
2	ZN	A	1101	1/1	0.99	0.14	37,37,37,37	0
2	ZN	C	1101	1/1	1.00	0.16	49,49,49,49	0
2	ZN	D	1101	1/1	1.00	0.14	57,57,57,57	0

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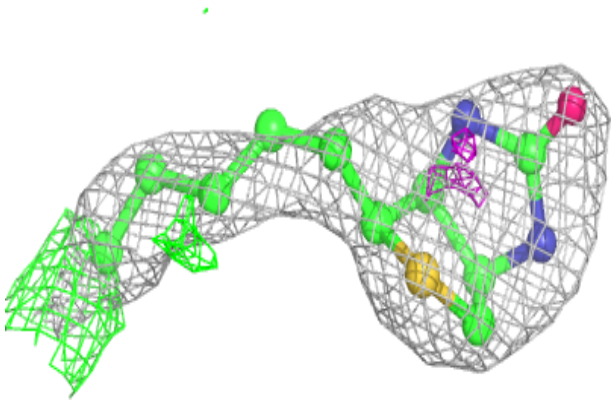
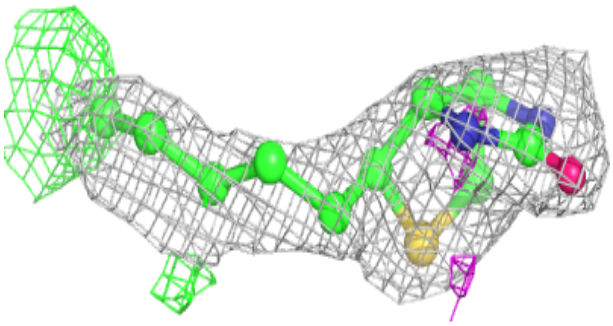
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	1102	1/1	1.00	0.12	46,46,46,46	0

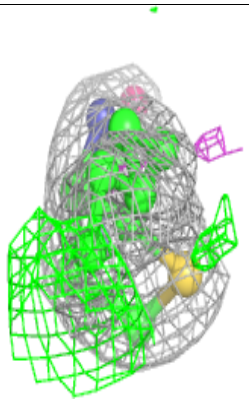
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BYT B 1107:

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

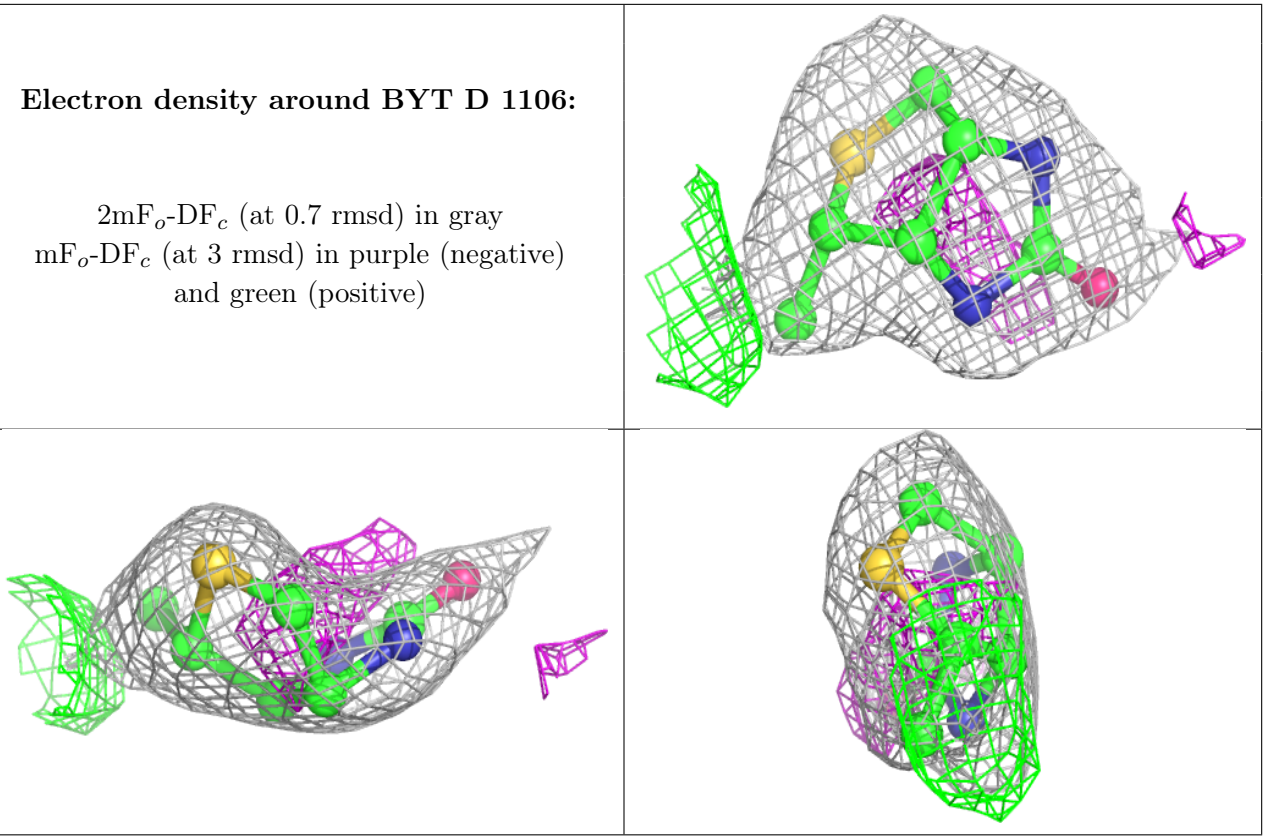






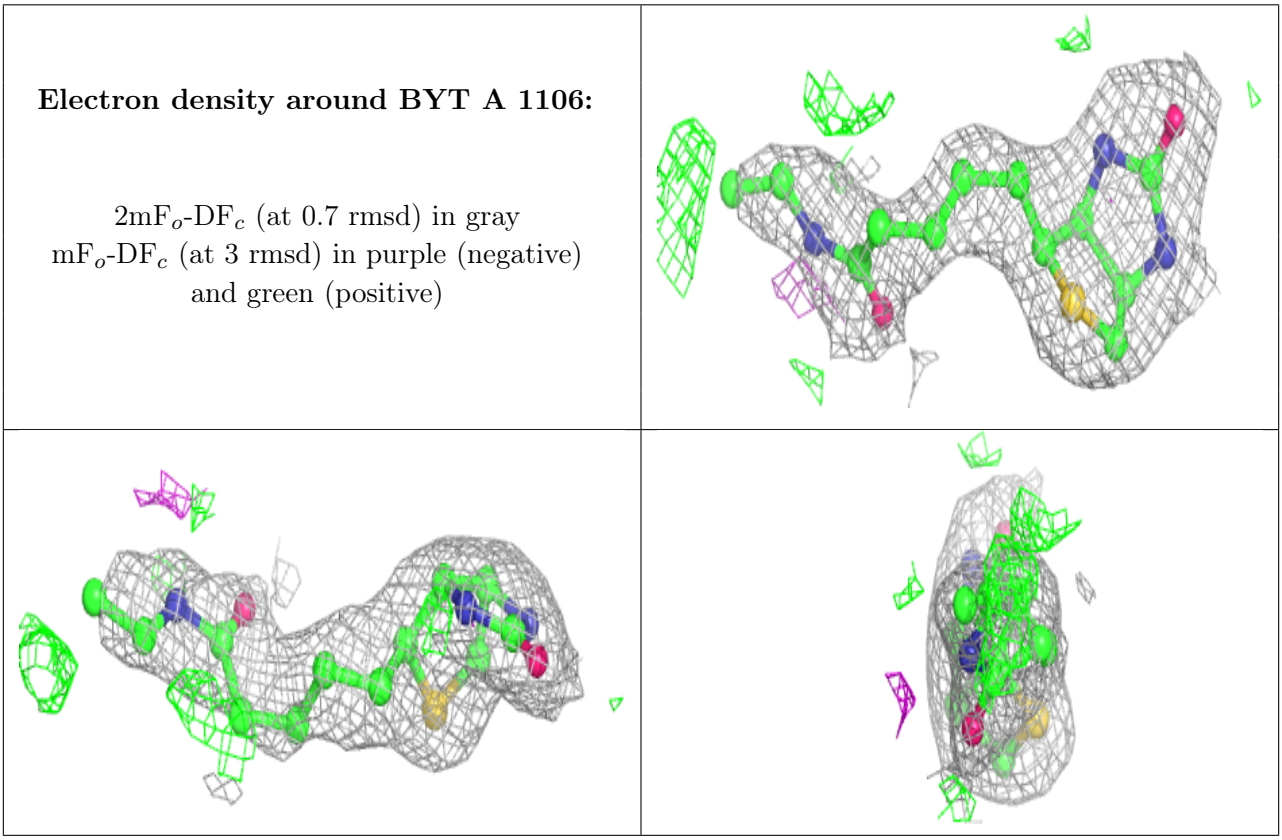
Electron density around BYT D 1106:

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



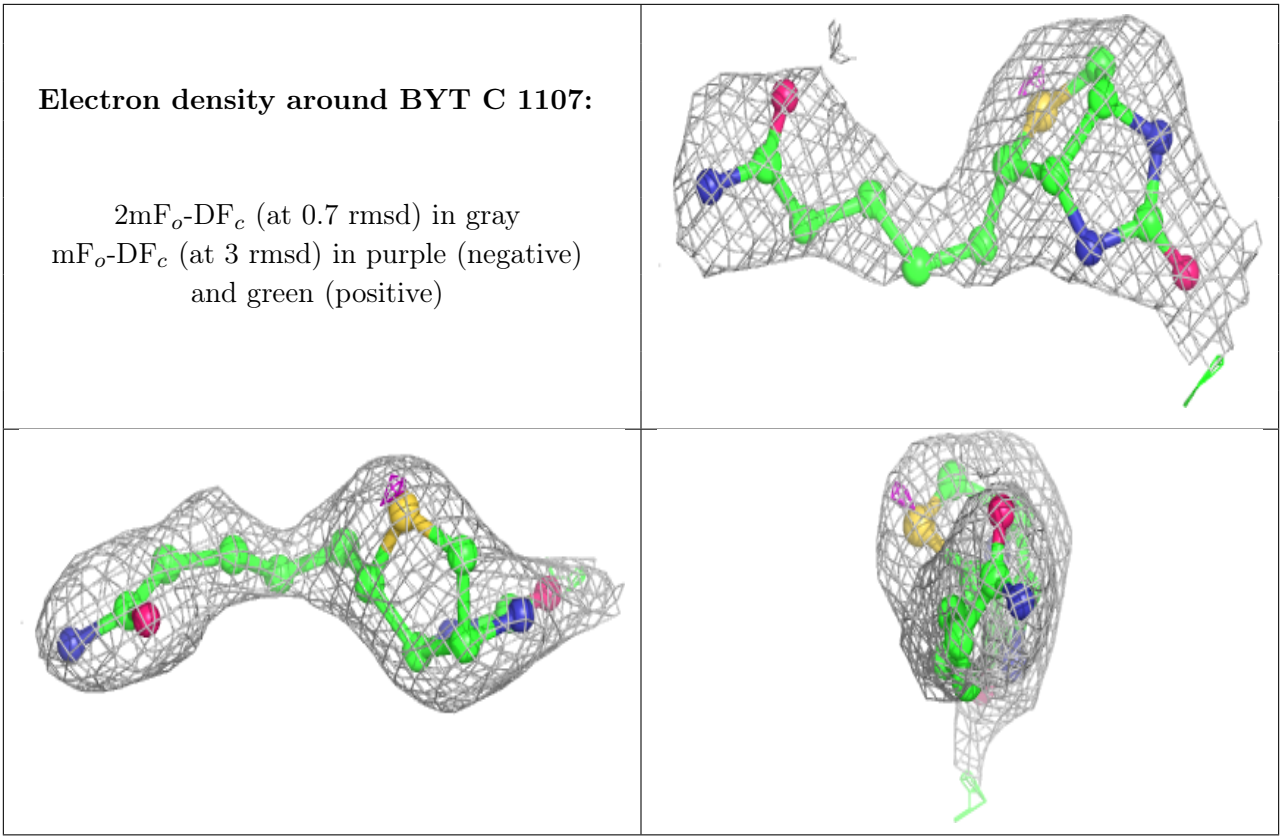
Electron density around BYT A 1106:

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



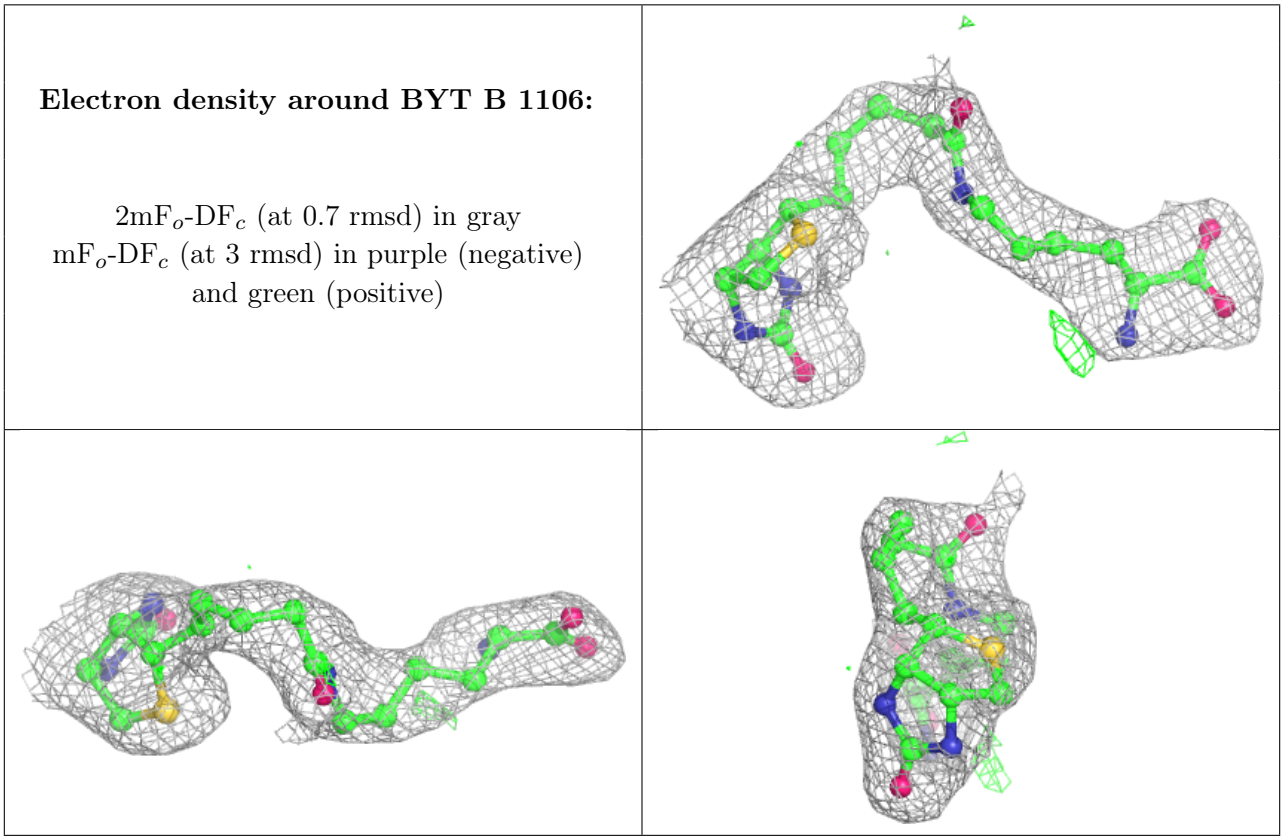
Electron density around BYT C 1107:

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



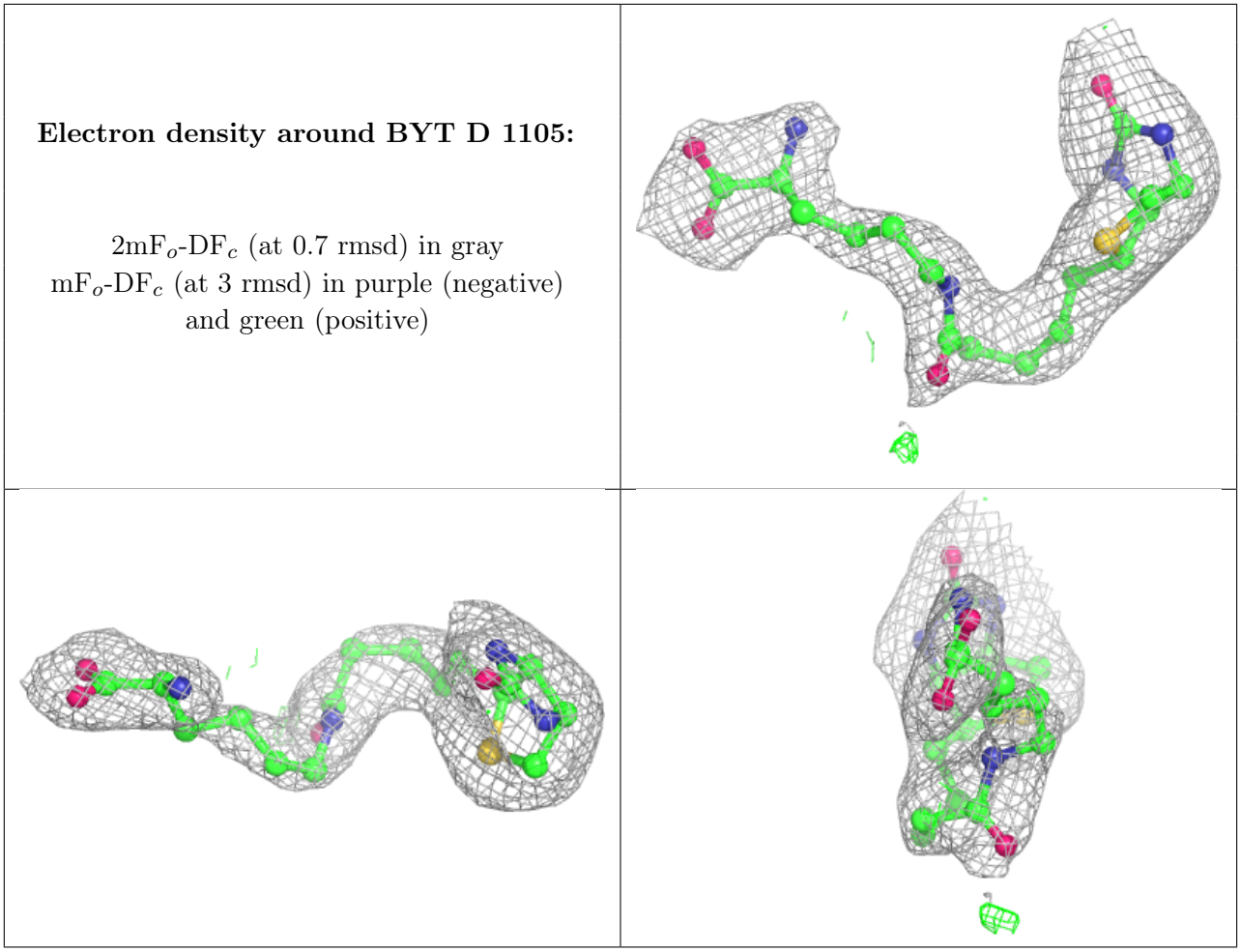
Electron density around BYT B 1106:

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



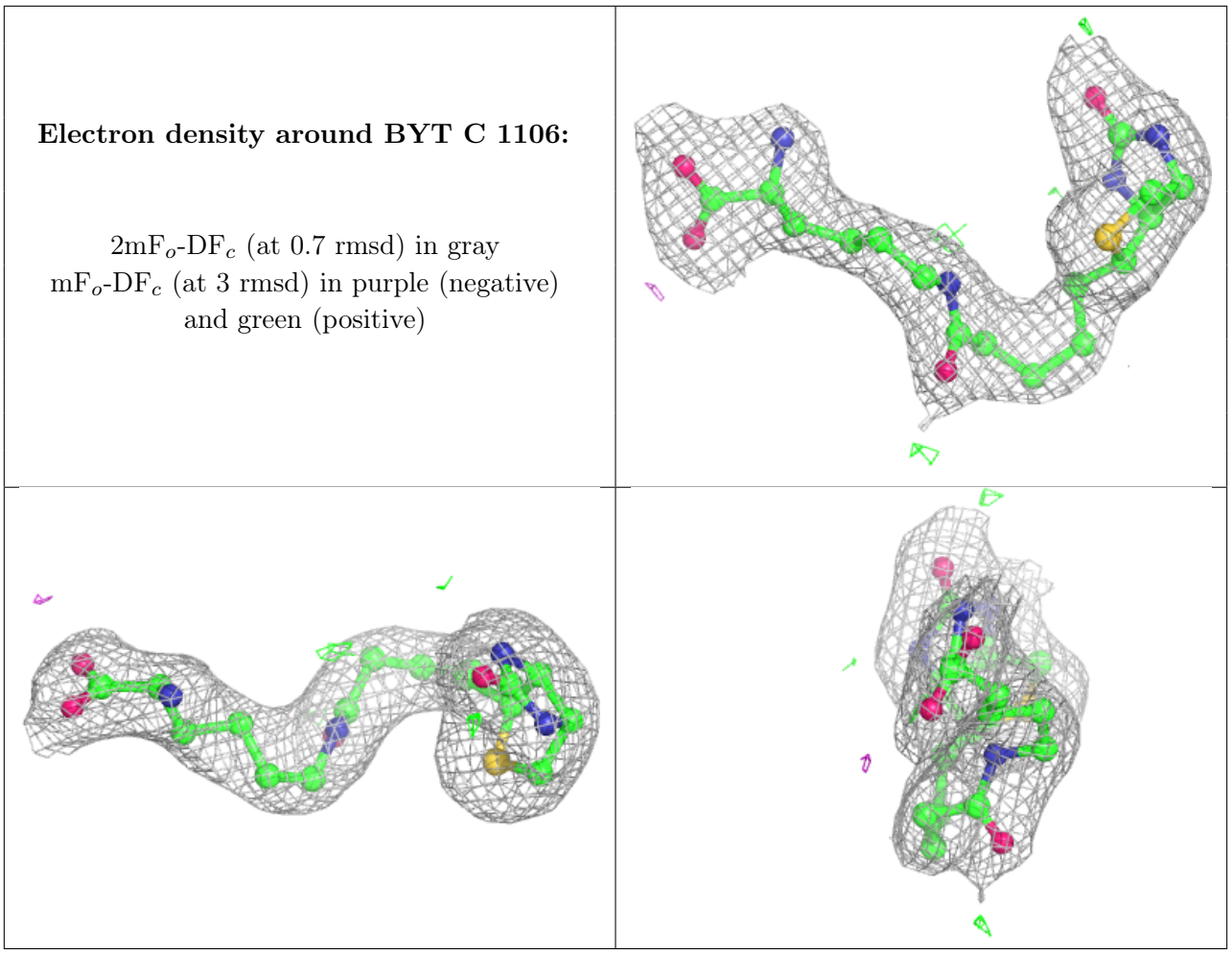
Electron density around BYT D 1105:

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



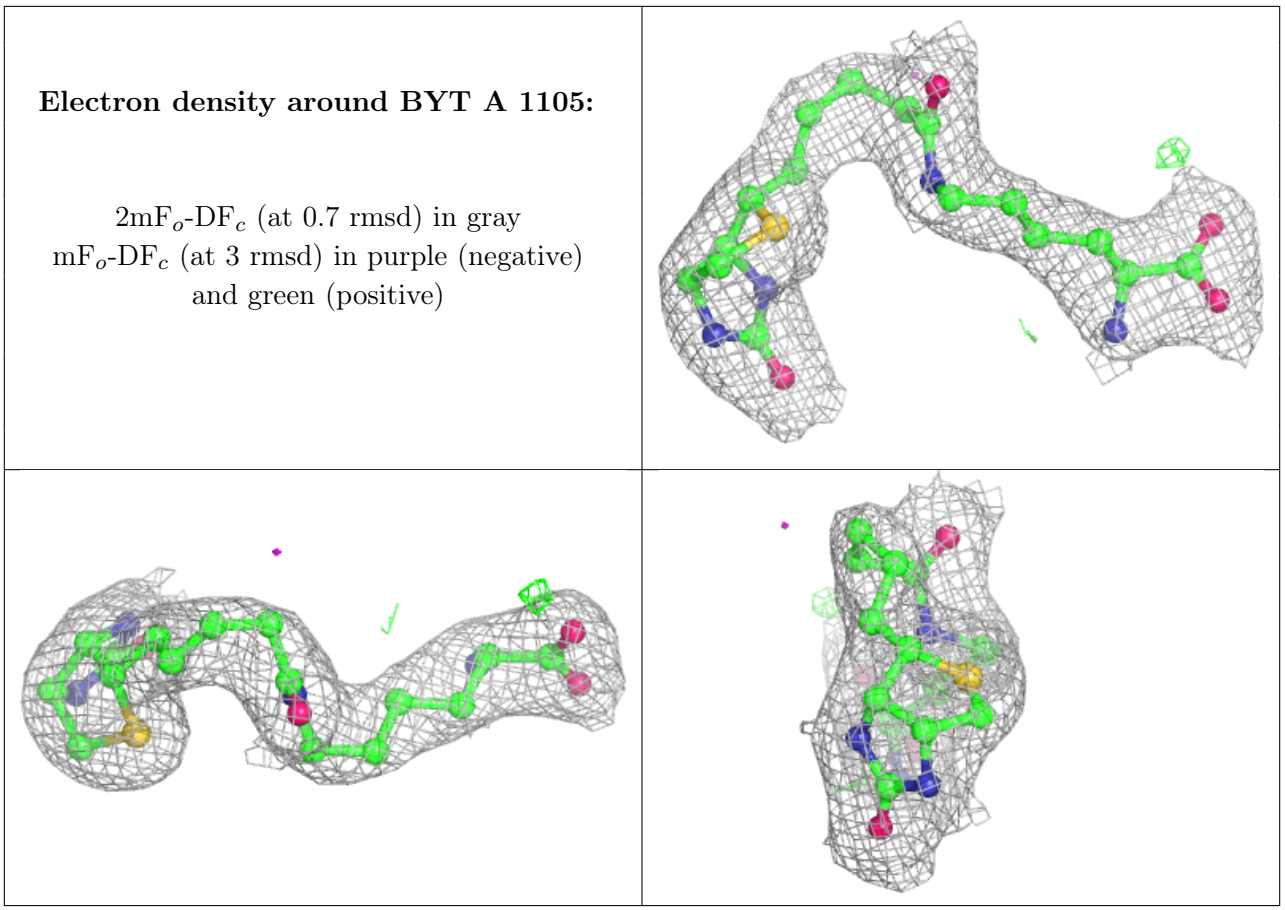
Electron density around BYT C 1106:

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



Electron density around BYT A 1105:

$2mF_o$-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.