



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:45 PM BST

PDB ID : 1TI2
Title : Crystal Structure of Pyrogallol-PhloroglucinolTranshydroxylase from Pelobacter acidigallici
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.35 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

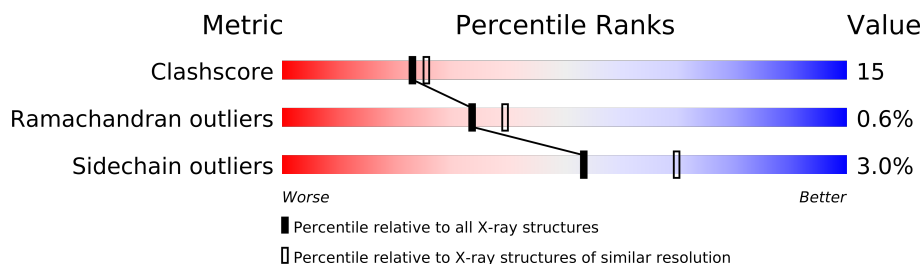
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	
1	C	875	
1	E	875	
1	G	875	
1	I	875	
1	K	875	
2	B	274	
2	D	274	
2	F	274	
2	H	274	
2	J	274	
2	L	274	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 61047 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pyrogallol hydroxytransferase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	C	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	E	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	G	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	I	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	K	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P80563
C	1	MET	-	INITIATING METHIONINE	UNP P80563
E	1	MET	-	INITIATING METHIONINE	UNP P80563
G	1	MET	-	INITIATING METHIONINE	UNP P80563
I	1	MET	-	INITIATING METHIONINE	UNP P80563
K	1	MET	-	INITIATING METHIONINE	UNP P80563

- Molecule 2 is a protein called Pyrogallol hydroxytransferase small subunit.

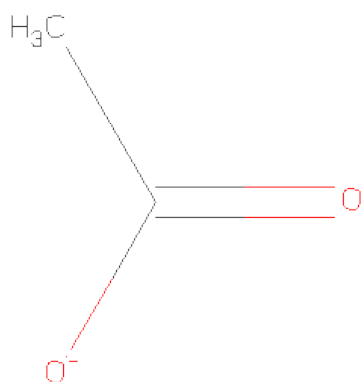
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	D	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	F	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	J	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	L	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

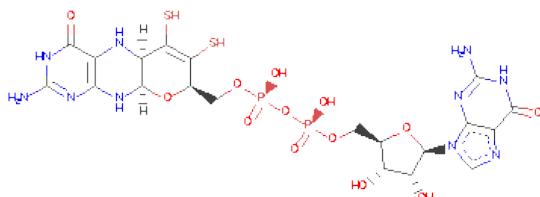


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

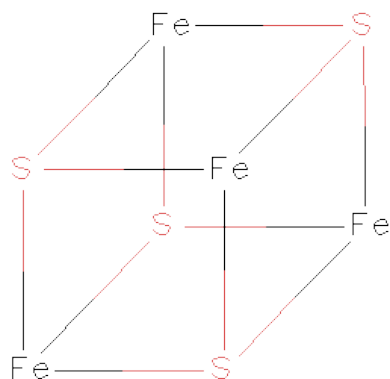


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mo	0	0
			1	1		
6	K	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		
6	I	1	Total	Mo	0	0
			1	1		
6	C	1	Total	Mo	0	0
			1	1		
6	A	1	Total	Mo	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	H	1	Total	Fe	S	0	0
			8	4	4		
7	H	1	Total	Fe	S	0	0
			8	4	4		
7	H	1	Total	Fe	S	0	0
			8	4	4		
7	J	1	Total	Fe	S	0	0
			8	4	4		
7	J	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	688	Total 688	O 688	0	0
8	B	163	Total 163	O 163	0	0
8	C	683	Total 683	O 683	0	0
8	D	168	Total 168	O 168	0	0
8	E	683	Total 683	O 683	0	0
8	F	168	Total 168	O 168	0	0
8	G	689	Total 689	O 689	0	0
8	H	162	Total 162	O 162	0	0
8	I	674	Total 674	O 674	0	0
8	J	168	Total 168	O 168	0	0
8	K	684	Total 684	O 684	0	0
8	L	167	Total 167	O 167	0	0

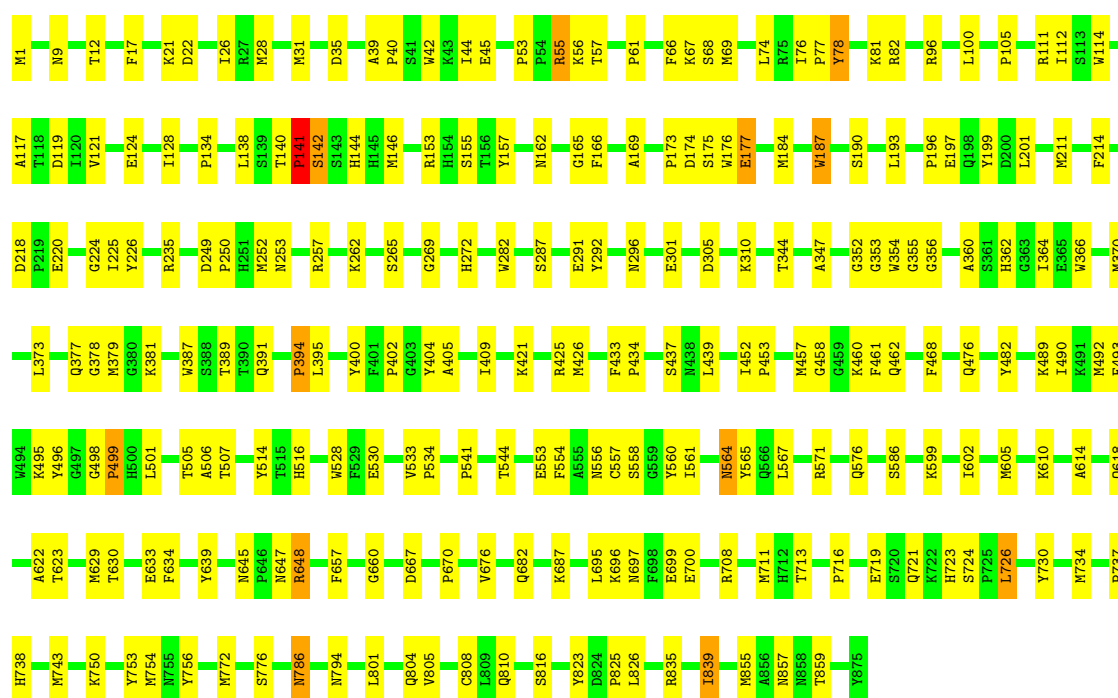
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

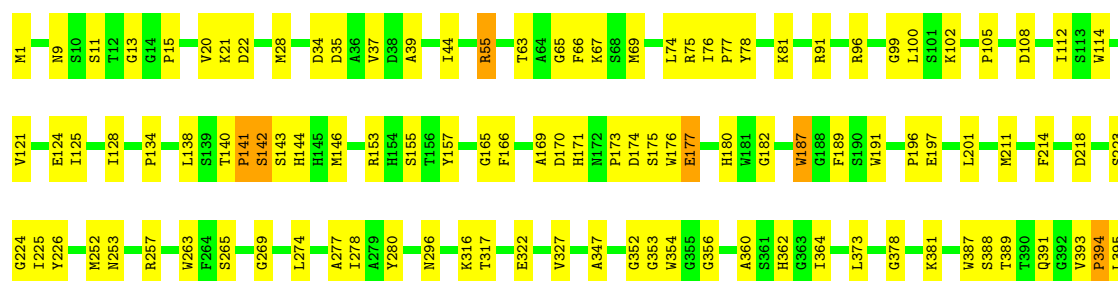
• Molecule 1: Pyrogallol hydroxytransferase large subunit

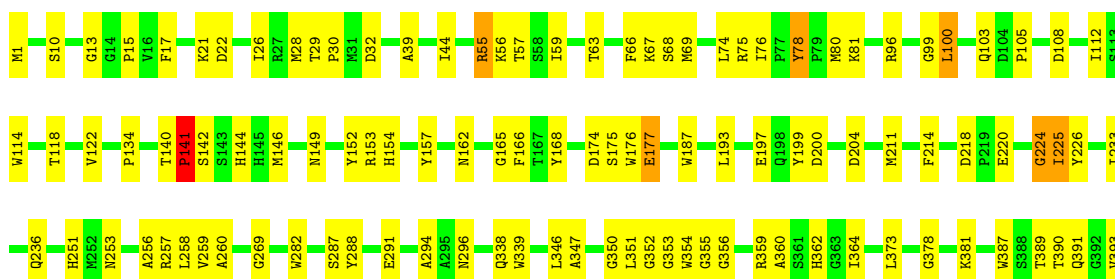
Chain A:

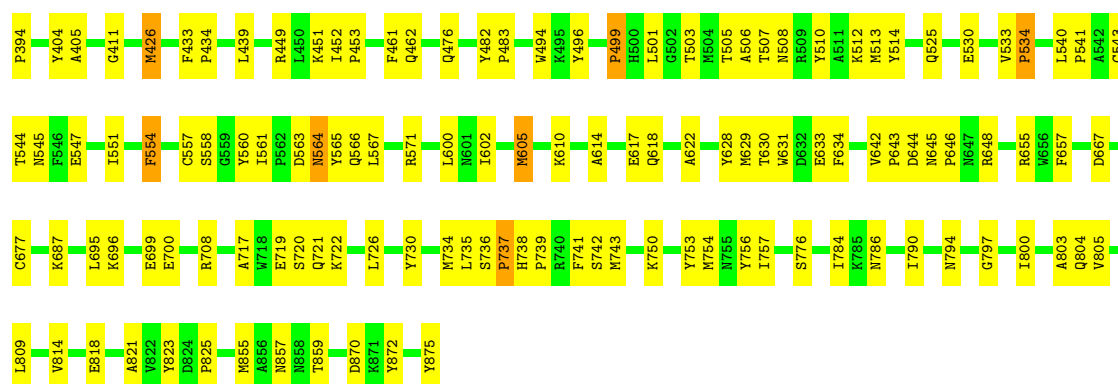


• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain C:

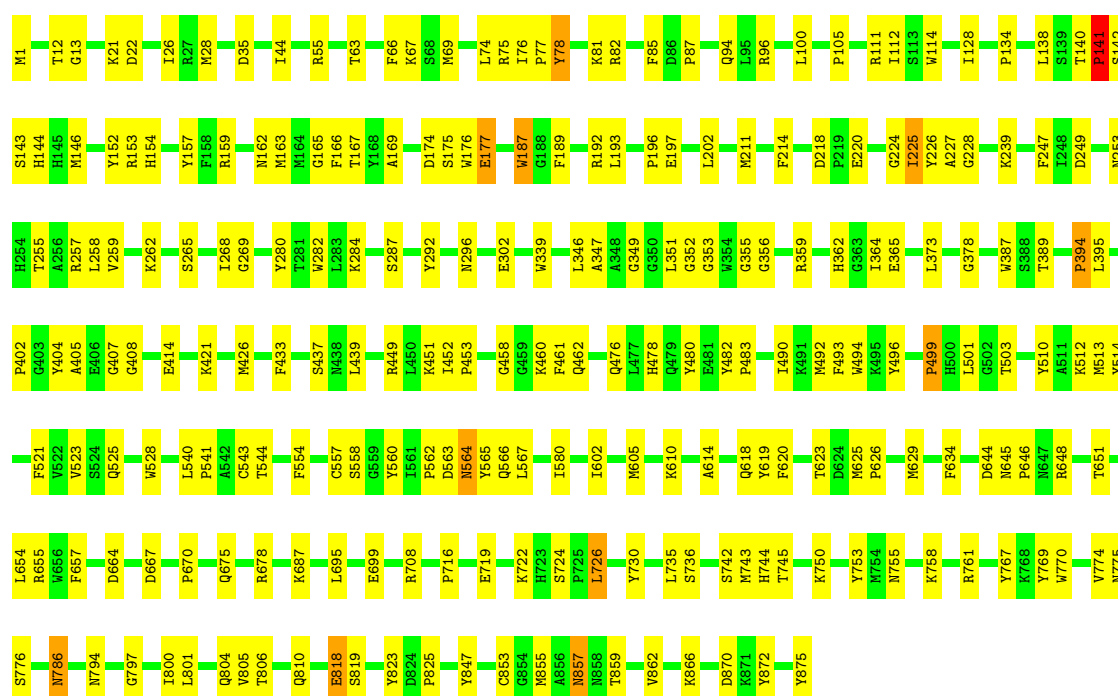






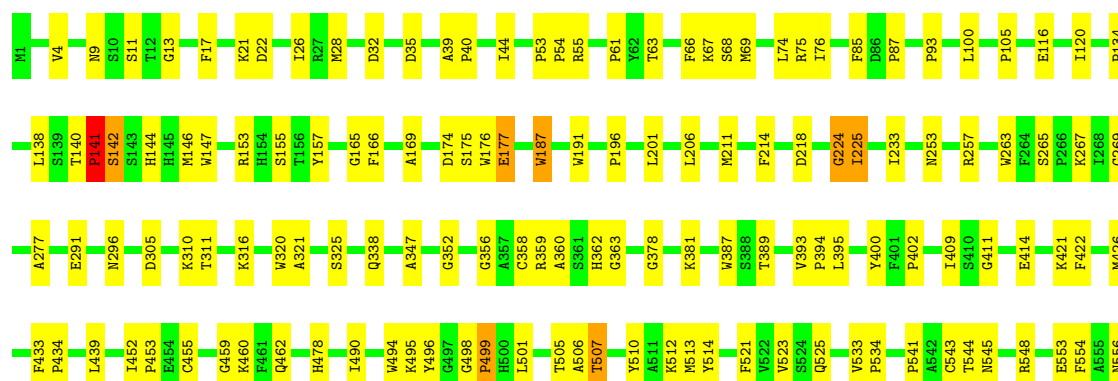
• Molecule 1: Pyrogallol hydroxytransferase large subunit

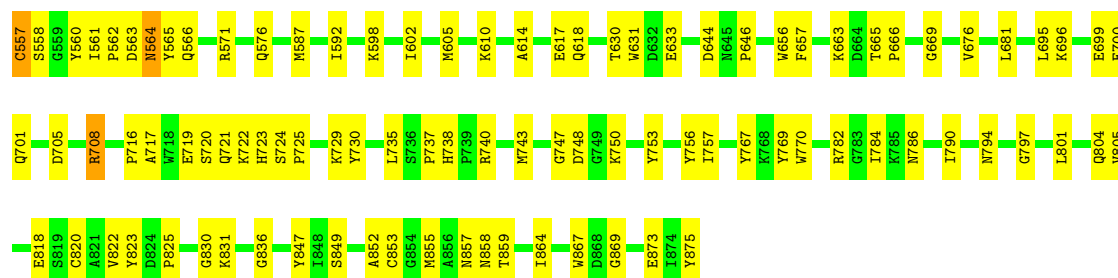
Chain I:



• Molecule 1: Pyrogallol hydroxytransferase large subunit

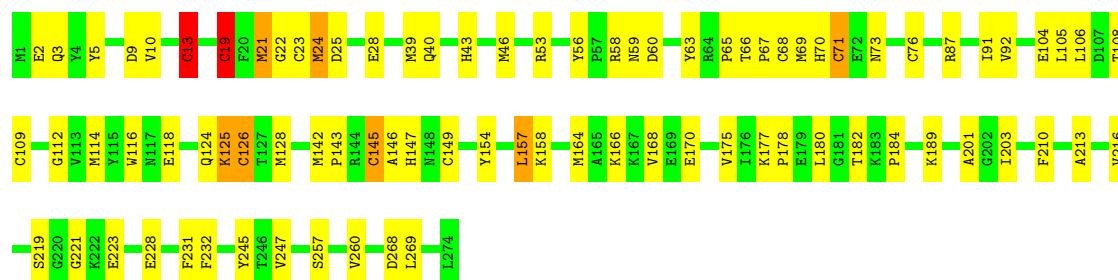
Chain K:





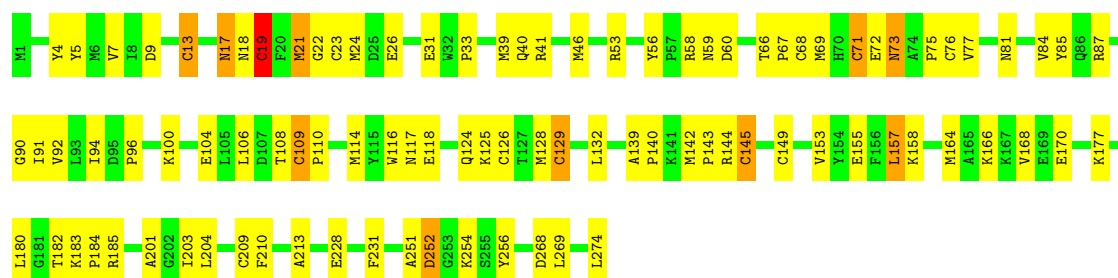
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B:



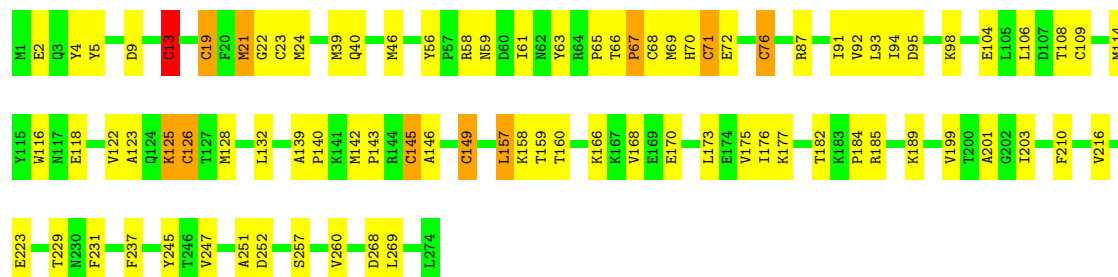
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain D:



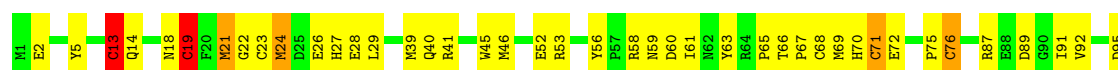
• Molecule 2: Pyrogallol hydroxytransferase small subunit

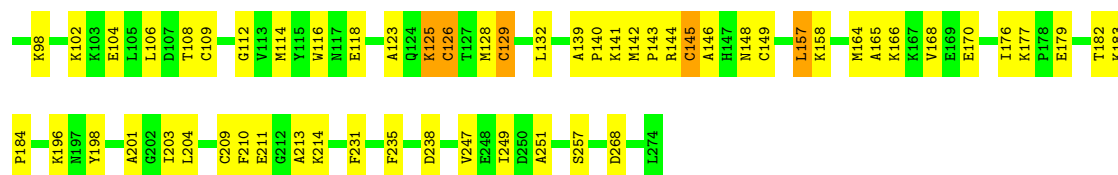
Chain F:



• Molecule 2: Pyrogallol hydroxytransferase small subunit

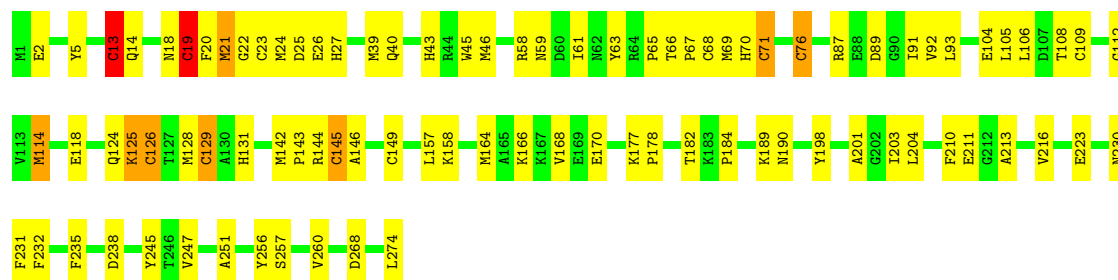
Chain H:





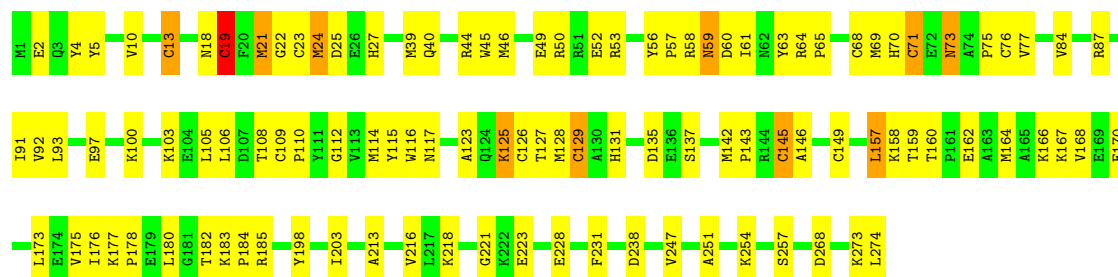
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J: 



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	174.02Å 179.64Å 181.22Å 63.69° 63.98° 64.90°	Depositor
Resolution (Å)	24.98 – 2.35	Depositor
% Data completeness (in resolution range)	86.0 (24.98-2.35)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	61047	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4MO, SF4, ACT, CA, MGD

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	0.36	0/7240	0.63	3/9815 (0.0%)
1	C	0.34	0/7240	0.61	2/9815 (0.0%)
1	E	0.34	0/7240	0.62	2/9815 (0.0%)
1	G	0.35	0/7240	0.62	3/9815 (0.0%)
1	I	0.35	0/7240	0.62	3/9815 (0.0%)
1	K	0.36	0/7240	0.62	3/9815 (0.0%)
2	B	0.45	2/2231 (0.1%)	0.66	2/3009 (0.1%)
2	D	0.38	1/2231 (0.0%)	0.60	1/3009 (0.0%)
2	F	0.44	3/2231 (0.1%)	0.63	1/3009 (0.0%)
2	H	0.43	2/2231 (0.1%)	0.64	1/3009 (0.0%)
2	J	0.44	3/2231 (0.1%)	0.65	2/3009 (0.1%)
2	L	0.40	1/2231 (0.0%)	0.61	1/3009 (0.0%)
All	All	0.37	12/56826 (0.0%)	0.62	24/76944 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	CYS	CB-SG	-7.37	1.69	1.82
2	H	19	CYS	CB-SG	-7.23	1.70	1.82
2	F	19	CYS	CB-SG	-6.99	1.70	1.82
2	L	19	CYS	CB-SG	-6.81	1.70	1.82
2	B	126	CYS	CB-SG	-6.42	1.71	1.82

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLY	N-CA-C	-8.25	92.48	113.10
1	E	352	GLY	N-CA-C	-8.06	92.94	113.10
1	K	352	GLY	N-CA-C	-7.65	93.98	113.10
1	C	352	GLY	N-CA-C	-7.54	94.26	113.10
1	I	352	GLY	N-CA-C	-7.52	94.31	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7018	0	6645	190	0
1	C	7018	0	6645	195	0
1	E	7018	0	6645	163	0
1	G	7018	0	6645	193	0
1	I	7018	0	6645	180	0
1	K	7018	0	6645	193	0
2	B	2182	0	2077	79	0
2	D	2182	0	2077	90	0
2	F	2182	0	2077	73	0
2	H	2182	0	2077	87	0
2	J	2182	0	2077	80	0
2	L	2182	0	2077	105	0
3	A	4	0	3	1	0
3	C	4	0	3	3	0
3	E	4	0	3	2	0
3	G	4	0	3	3	0
3	I	4	0	3	3	0
3	K	4	0	3	4	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
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	94	0	44	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	94	0	44	10	0
5	E	94	0	44	6	0
5	G	94	0	44	9	0
5	I	94	0	44	10	0
5	K	94	0	44	9	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
7	B	24	0	0	3	0
7	D	24	0	0	5	0
7	F	24	0	0	3	0
7	H	24	0	0	5	0
7	J	24	0	0	3	0
7	L	24	0	0	6	0
8	A	688	0	0	18	0
8	B	163	0	0	4	0
8	C	683	0	0	18	0
8	D	168	0	0	5	0
8	E	683	0	0	21	0
8	F	168	0	0	1	0
8	G	689	0	0	17	0
8	H	162	0	0	5	0
8	I	674	0	0	20	0
8	J	168	0	0	4	0
8	K	684	0	0	25	0
8	L	167	0	0	9	0
All	All	61047	0	52614	1590	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 1590 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.33	1.10
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.19	1.09
1:A:557:CYS:H	1:A:564:ASN:HD21	1.07	1.02
1:I:426:MET:HE1	1:I:618:GLN:HG2	1.39	1.01
1:A:426:MET:HE1	1:A:618:GLN:HG2	1.44	1.00

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	875/875 (100%)	821 (94%)	49 (6%)	5 (1%)	33	39
1	C	875/875 (100%)	804 (92%)	65 (7%)	6 (1%)	30	34
1	E	875/875 (100%)	807 (92%)	61 (7%)	7 (1%)	27	31
1	G	875/875 (100%)	820 (94%)	50 (6%)	5 (1%)	33	39
1	I	875/875 (100%)	816 (93%)	54 (6%)	5 (1%)	33	39
1	K	875/875 (100%)	813 (93%)	57 (6%)	5 (1%)	33	39
2	B	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	43	52
2	D	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	43	52
2	F	272/274 (99%)	249 (92%)	22 (8%)	1 (0%)	43	52
2	H	272/274 (99%)	255 (94%)	16 (6%)	1 (0%)	43	52
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	43	52
2	L	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	43	52
All	All	6882/6894 (100%)	6415 (93%)	428 (6%)	39 (1%)	33	39

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU
1	G	177	GLU
1	G	225	ILE

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	731/729 (100%)	712 (97%)	19 (3%)	59	75
1	C	731/729 (100%)	712 (97%)	19 (3%)	59	75
1	E	731/729 (100%)	717 (98%)	14 (2%)	69	84
1	G	731/729 (100%)	711 (97%)	20 (3%)	57	74
1	I	731/729 (100%)	711 (97%)	20 (3%)	57	74
1	K	731/729 (100%)	715 (98%)	16 (2%)	64	81
2	B	235/235 (100%)	225 (96%)	10 (4%)	40	51
2	D	235/235 (100%)	223 (95%)	12 (5%)	33	41
2	F	235/235 (100%)	223 (95%)	12 (5%)	33	41
2	H	235/235 (100%)	221 (94%)	14 (6%)	27	32
2	J	235/235 (100%)	224 (95%)	11 (5%)	36	46
2	L	235/235 (100%)	222 (94%)	13 (6%)	30	36
All	All	5796/5784 (100%)	5616 (97%)	180 (3%)	53	68

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	125	LYS
1	G	605	MET
1	K	820	CYS
2	F	149	CYS
1	G	187	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	786	ASN
1	G	440	ASN
1	K	697	ASN
2	F	27	HIS
2	F	73	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 18 are monoatomic - leaving 36 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	MGD	A	900	6	52,52,52	2.08	15 (28%)	72,81,81	2.52	16 (22%)
5	MGD	A	901	6	52,52,52	2.24	19 (36%)	72,81,81	3.39	17 (23%)
3	ACT	A	903	6	1,3,3	2.91	1 (100%)	0,3,3	0.00	-
7	SF4	B	805	2	12,12,12	10.24	11 (91%)	0,24,24	0.00	-
7	SF4	B	806	2	12,12,12	10.95	8 (66%)	0,24,24	0.00	-
7	SF4	B	807	2	12,12,12	9.08	9 (75%)	0,24,24	0.00	-
5	MGD	C	900	6	52,52,52	2.22	20 (38%)	72,81,81	3.05	19 (26%)
5	MGD	C	901	6	52,52,52	2.22	19 (36%)	72,81,81	3.15	13 (18%)
3	ACT	C	903	6	1,3,3	3.23	1 (100%)	0,3,3	0.00	-
7	SF4	D	805	2	12,12,12	10.14	8 (66%)	0,24,24	0.00	-
7	SF4	D	806	2	12,12,12	10.62	10 (83%)	0,24,24	0.00	-
7	SF4	D	807	2	12,12,12	8.42	8 (66%)	0,24,24	0.00	-
5	MGD	E	900	6	52,52,52	2.21	19 (36%)	72,81,81	2.86	18 (25%)
5	MGD	E	901	6	52,52,52	2.18	17 (32%)	72,81,81	2.94	16 (22%)
3	ACT	E	903	6	1,3,3	3.30	1 (100%)	0,3,3	0.00	-
7	SF4	F	805	2	12,12,12	10.52	11 (91%)	0,24,24	0.00	-
7	SF4	F	806	2	12,12,12	10.63	10 (83%)	0,24,24	0.00	-
7	SF4	F	807	2	12,12,12	9.25	8 (66%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	G	900	6	52,52,52	2.23	20 (38%)	72,81,81	3.31	18 (25%)
5	MGD	G	901	6	52,52,52	2.09	17 (32%)	72,81,81	2.66	14 (19%)
3	ACT	G	903	6	1,3,3	3.69	1 (100%)	0,3,3	0.00	-
7	SF4	H	805	2	12,12,12	10.08	11 (91%)	0,24,24	0.00	-
7	SF4	H	806	2	12,12,12	10.72	10 (83%)	0,24,24	0.00	-
7	SF4	H	807	2	12,12,12	8.96	8 (66%)	0,24,24	0.00	-
5	MGD	I	900	6	52,52,52	2.21	20 (38%)	72,81,81	2.91	19 (26%)
5	MGD	I	901	6	52,52,52	2.13	18 (34%)	72,81,81	2.64	14 (19%)
3	ACT	I	903	6	1,3,3	3.18	1 (100%)	0,3,3	0.00	-
7	SF4	J	805	2	12,12,12	10.75	8 (66%)	0,24,24	0.00	-
7	SF4	J	806	2	12,12,12	10.56	9 (75%)	0,24,24	0.00	-
7	SF4	J	807	2	12,12,12	9.41	9 (75%)	0,24,24	0.00	-
5	MGD	K	900	6	52,52,52	2.05	16 (30%)	72,81,81	2.71	16 (22%)
5	MGD	K	901	6	52,52,52	2.17	16 (30%)	72,81,81	2.59	15 (20%)
3	ACT	K	903	6	1,3,3	3.86	1 (100%)	0,3,3	0.00	-
7	SF4	L	805	2	12,12,12	10.50	11 (91%)	0,24,24	0.00	-
7	SF4	L	806	2	12,12,12	10.68	11 (91%)	0,24,24	0.00	-
7	SF4	L	807	2	12,12,12	8.60	9 (75%)	0,24,24	0.00	-

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	MGD	A	900	6	-	0/22/66/66	0/1/6/6
5	MGD	A	901	6	-	0/22/66/66	0/1/6/6
3	ACT	A	903	6	-	0/0/0/0	0/0/0/0
7	SF4	B	805	2	-	0/0/48/48	0/0/5/5
7	SF4	B	806	2	-	0/0/48/48	0/0/5/5
7	SF4	B	807	2	-	0/0/48/48	0/0/5/5
5	MGD	C	900	6	-	0/22/66/66	0/1/6/6
5	MGD	C	901	6	-	0/22/66/66	0/1/6/6
3	ACT	C	903	6	-	0/0/0/0	0/0/0/0
7	SF4	D	805	2	-	0/0/48/48	0/0/5/5
7	SF4	D	806	2	-	0/0/48/48	0/0/5/5
7	SF4	D	807	2	-	0/0/48/48	0/0/5/5
5	MGD	E	900	6	-	0/22/66/66	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	E	901	6	-	0/22/66/66	0/1/6/6
3	ACT	E	903	6	-	0/0/0/0	0/0/0/0
7	SF4	F	805	2	-	0/0/48/48	0/0/5/5
7	SF4	F	806	2	-	0/0/48/48	0/0/5/5
7	SF4	F	807	2	-	0/0/48/48	0/0/5/5
5	MGD	G	900	6	-	0/22/66/66	0/1/6/6
5	MGD	G	901	6	-	0/22/66/66	0/1/6/6
3	ACT	G	903	6	-	0/0/0/0	0/0/0/0
7	SF4	H	805	2	-	0/0/48/48	0/0/5/5
7	SF4	H	806	2	-	0/0/48/48	0/0/5/5
7	SF4	H	807	2	-	0/0/48/48	0/0/5/5
5	MGD	I	900	6	-	0/22/66/66	0/1/6/6
5	MGD	I	901	6	-	0/22/66/66	0/1/6/6
3	ACT	I	903	6	-	0/0/0/0	0/0/0/0
7	SF4	J	805	2	-	0/0/48/48	0/0/5/5
7	SF4	J	806	2	-	0/0/48/48	0/0/5/5
7	SF4	J	807	2	-	0/0/48/48	0/0/5/5
5	MGD	K	900	6	-	0/22/66/66	0/1/6/6
5	MGD	K	901	6	-	0/22/66/66	0/1/6/6
3	ACT	K	903	6	-	0/0/0/0	0/0/0/0
7	SF4	L	805	2	-	0/0/48/48	0/0/5/5
7	SF4	L	806	2	-	0/0/48/48	0/0/5/5
7	SF4	L	807	2	-	0/0/48/48	0/0/5/5

The worst 5 of 391 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	805	SF4	S1-FE4	-21.31	2.18	2.33
7	F	805	SF4	S1-FE4	-20.51	2.19	2.33
7	F	806	SF4	S1-FE4	-19.84	2.19	2.33
7	B	805	SF4	S1-FE4	-19.83	2.19	2.33
7	L	806	SF4	S1-FE4	-19.52	2.20	2.33

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	MGD	C6-C5-N7	-25.15	130.75	134.14
5	G	900	MGD	C6-C5-N7	-23.41	130.99	134.14
5	C	901	MGD	C6-C5-N7	-23.21	131.01	134.14
5	E	901	MGD	C6-C5-N7	-20.88	131.33	134.14
5	C	900	MGD	C6-C5-N7	-20.19	131.42	134.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.