



# wwPDB X-ray Structure Validation Summary Report

Jul 22, 2014 – 10:31 AM EDT

PDB ID : 4V4D  
Title : Crystal Structure of Pyrogallol-PhloroglucinolTranshydroxylase from Pelobacter acidigallici complexed with pyrogallol  
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.  
Deposited on : 2004-06-02  
Resolution : 2.20 Å(reported)

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

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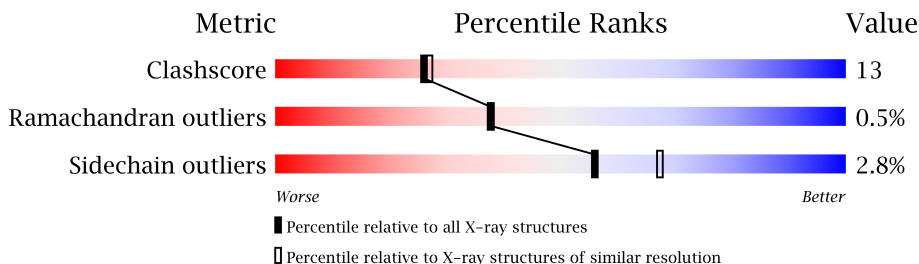
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 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) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.






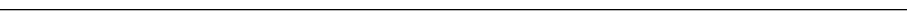











Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)








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  $\geq 3$ , 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	
1	M	875	
1	O	875	
1	Q	875	
1	S	875	
1	U	875	
1	W	875	
2	B	274	
2	D	274	
2	F	274	
2	H	274	
2	J	274	

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Mol	Chain	Length	Quality of chain
2	L	274	
2	N	274	
2	P	274	
2	R	274	
2	T	274	
2	V	274	
2	X	274	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	PYG	A	905	X	-
6	PYG	C	905	X	-
6	PYG	E	905	X	-
6	PYG	G	905	X	-
6	PYG	I	905	X	-
6	PYG	K	905	X	-
6	PYG	M	905	X	-
6	PYG	O	905	X	-
6	PYG	Q	905	X	-
6	PYG	S	905	X	-
6	PYG	U	905	X	-
6	PYG	W	905	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 121808 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	0	0
			6998	4464	1189	1297	48			
1	C	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	E	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	G	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	I	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	K	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	M	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	O	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	Q	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	S	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	U	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	W	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			

There are 12 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

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	INITIATING METHIONINE	UNP P80563
M	1	MET	-	INITIATING METHIONINE	UNP P80563
O	1	MET	-	INITIATING METHIONINE	UNP P80563
Q	1	MET	-	INITIATING METHIONINE	UNP P80563
S	1	MET	-	INITIATING METHIONINE	UNP P80563
U	1	MET	-	INITIATING METHIONINE	UNP P80563
W	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			
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			
2	N	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	P	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	R	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	T	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	V	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	X	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

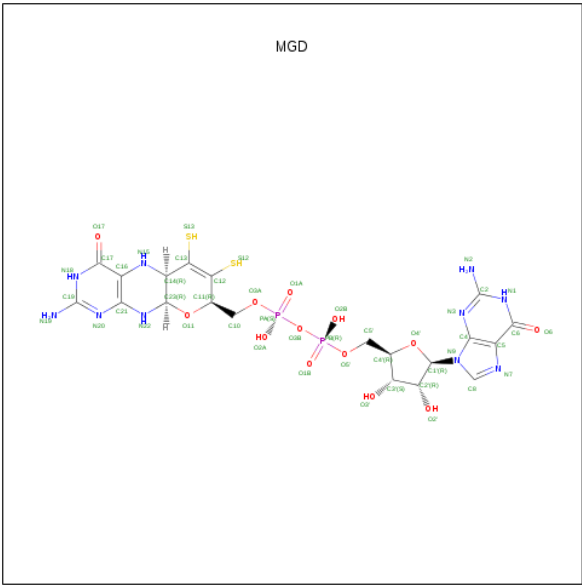
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	W	1	Total 1	Ca 1	0	0
3	N	1	Total 1	Ca 1	0	0
3	X	1	Total 1	Ca 1	0	0
3	S	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	V	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	R	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	U	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	Q	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	T	1	Total 1	Ca 1	0	0
3	O	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

- Molecule 4 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<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Mo 1	0	0
5	Q	1	Total 1	Mo 1	0	0
5	K	1	Total 1	Mo 1	0	0
5	E	1	Total 1	Mo 1	0	0
5	I	1	Total 1	Mo 1	0	0
5	C	1	Total 1	Mo 1	0	0
5	W	1	Total 1	Mo 1	0	0

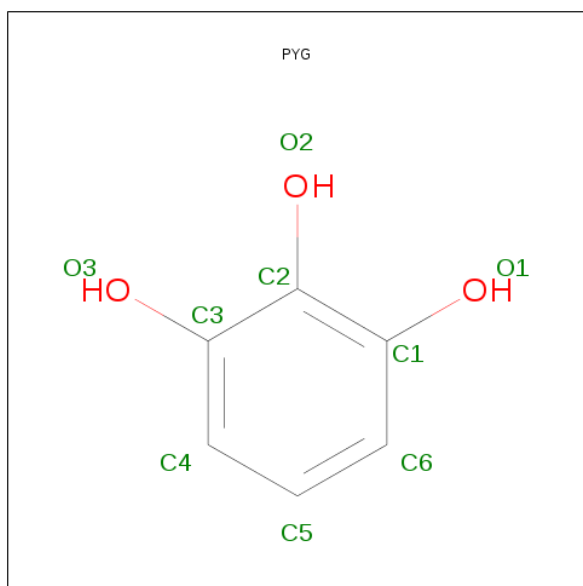
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	U	1	Total	Mo	0	0
			1	1		
5	O	1	Total	Mo	0	0
			1	1		
5	S	1	Total	Mo	0	0
			1	1		
5	M	1	Total	Mo	0	0
			1	1		

- Molecule 6 is BENZENE-1,2,3-TRIOL (three-letter code: PYG) (formula:  $C_6H_6O_3$ ).



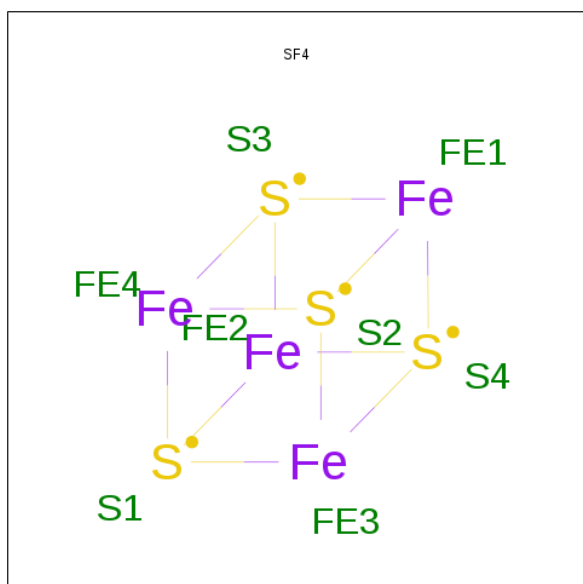
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			9	6	3		
6	E	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			9	6	3		
6	I	1	Total	C	O	0	0
			9	6	3		
6	K	1	Total	C	O	0	0
			9	6	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			9	6	3		
6	O	1	Total	C	O	0	0
			9	6	3		
6	Q	1	Total	C	O	0	0
			9	6	3		
6	S	1	Total	C	O	0	0
			9	6	3		
6	U	1	Total	C	O	0	0
			9	6	3		
6	W	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	R	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	681	Total 681	O 681	0	0
8	B	170	Total 170	O 170	0	0
8	C	681	Total 681	O 681	0	0
8	D	166	Total 166	O 166	0	0
8	E	684	Total 684	O 684	0	0
8	F	163	Total 163	O 163	0	0
8	G	683	Total 683	O 683	0	0
8	H	161	Total 161	O 161	0	0
8	I	671	Total 671	O 671	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	163	Total 163	O 163	0	0
8	K	681	Total 681	O 681	0	0
8	L	165	Total 165	O 165	0	0
8	M	684	Total 684	O 684	0	0
8	N	159	Total 159	O 159	0	0
8	O	672	Total 672	O 672	0	0
8	P	164	Total 164	O 164	0	0
8	Q	690	Total 690	O 690	0	0
8	R	161	Total 161	O 161	0	0
8	S	663	Total 663	O 663	0	0
8	T	163	Total 163	O 163	0	0
8	U	668	Total 668	O 668	0	0
8	V	157	Total 157	O 157	0	0
8	W	675	Total 675	O 675	0	0
8	X	164	Total 164	O 164	0	0

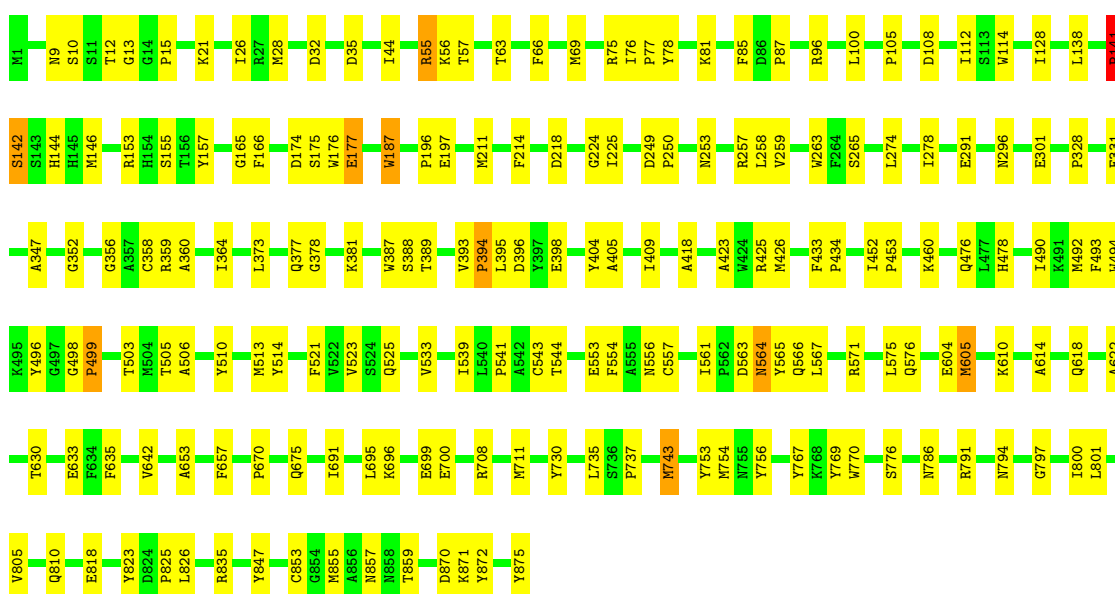
### 3 Residue-property plots

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.

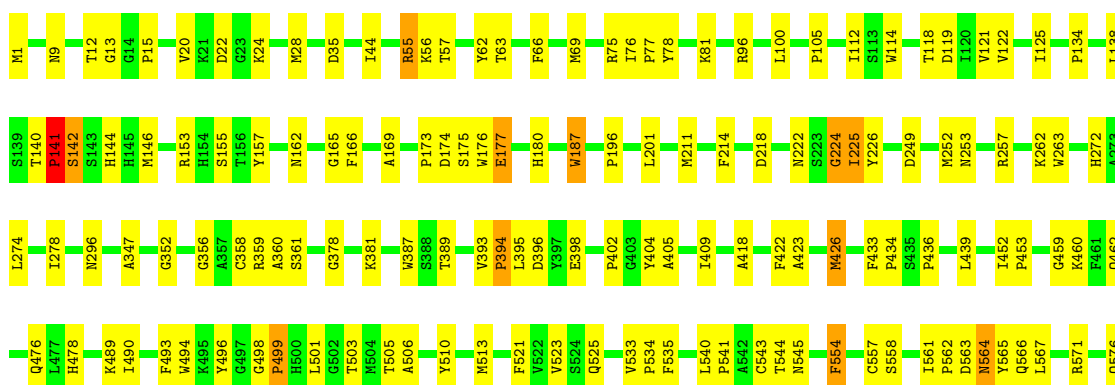
#### • Molecule 1: Pyrogallol hydroxytransferase large subunit

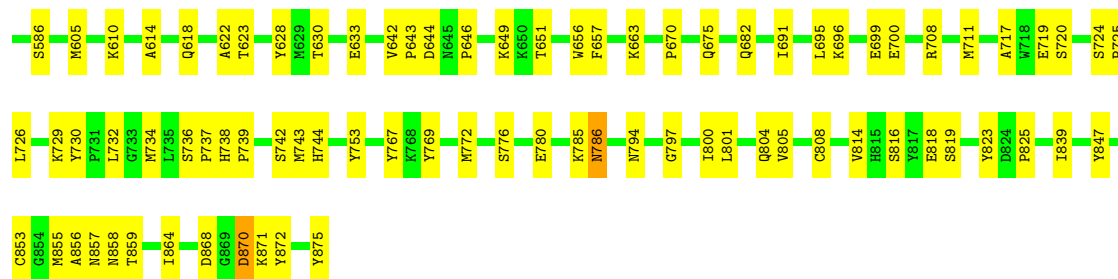
Chain A:



#### • Molecule 1: Pyrogallol hydroxytransferase large subunit

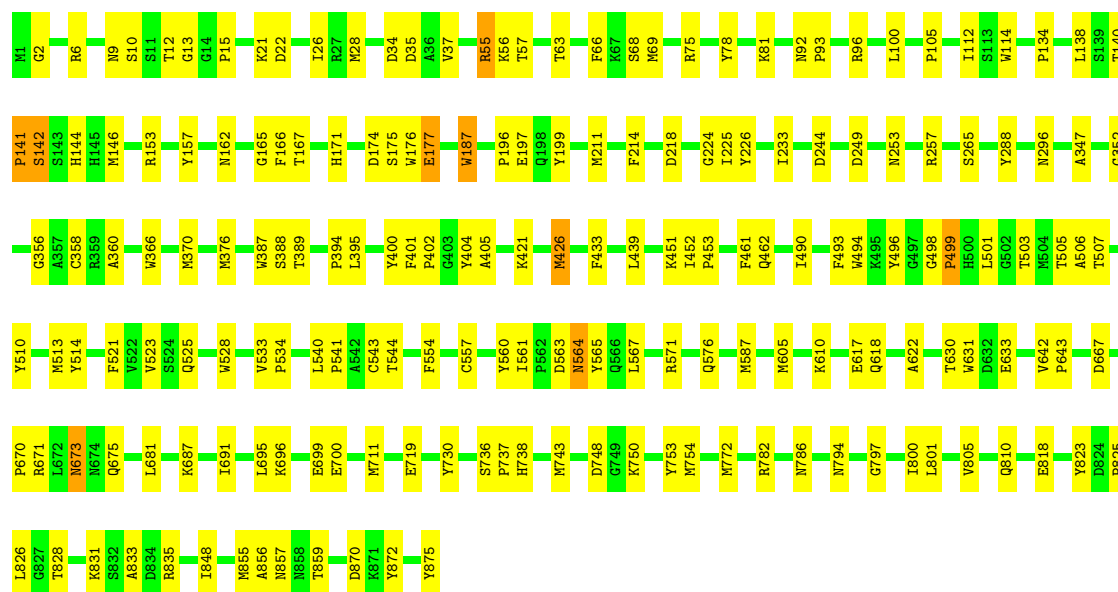
Chain C:





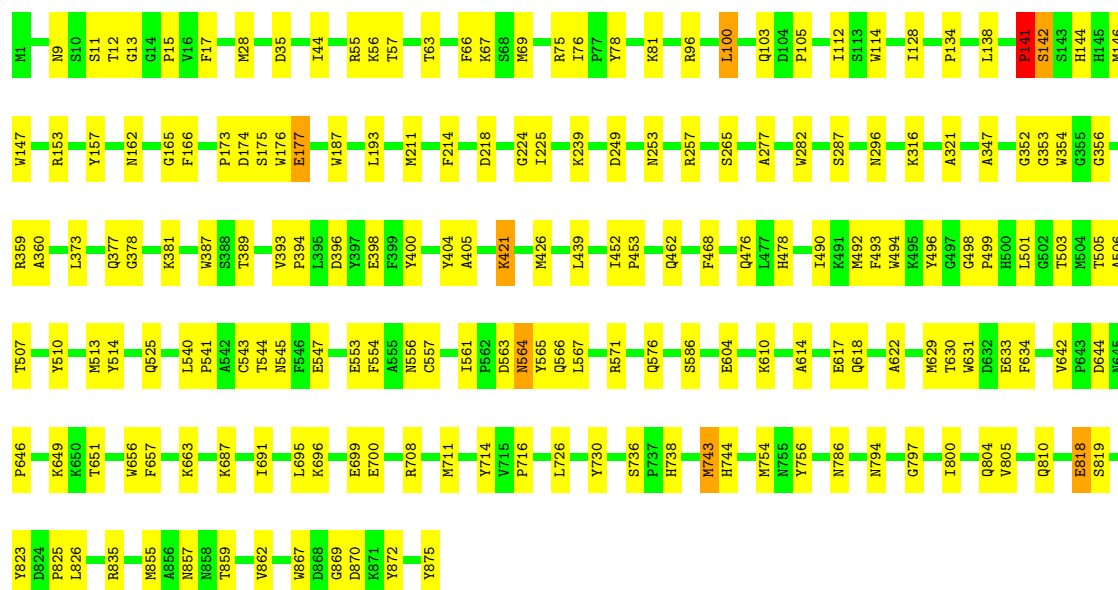
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain E:



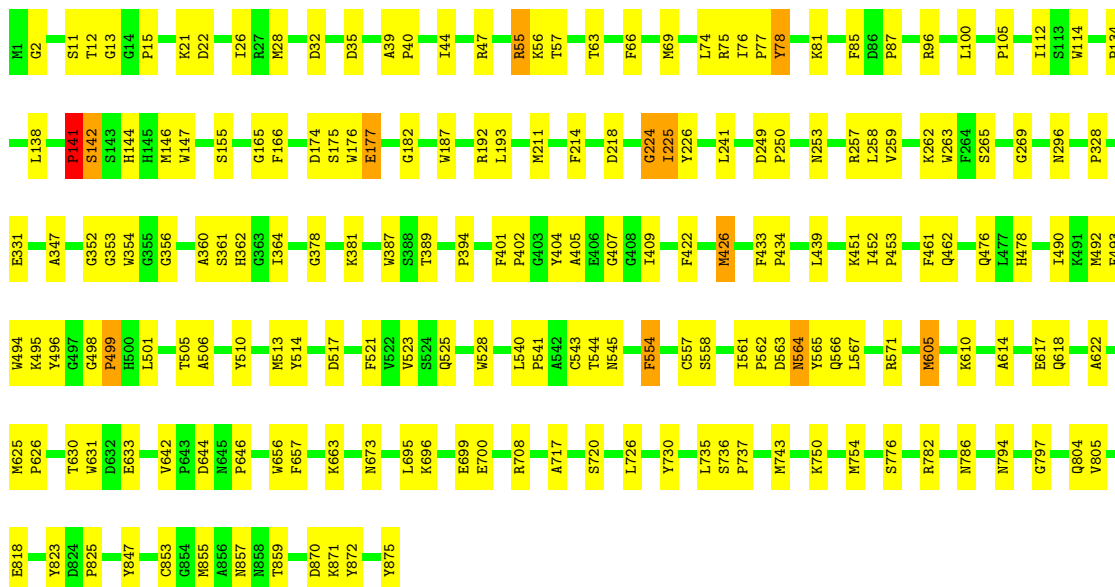
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain G:



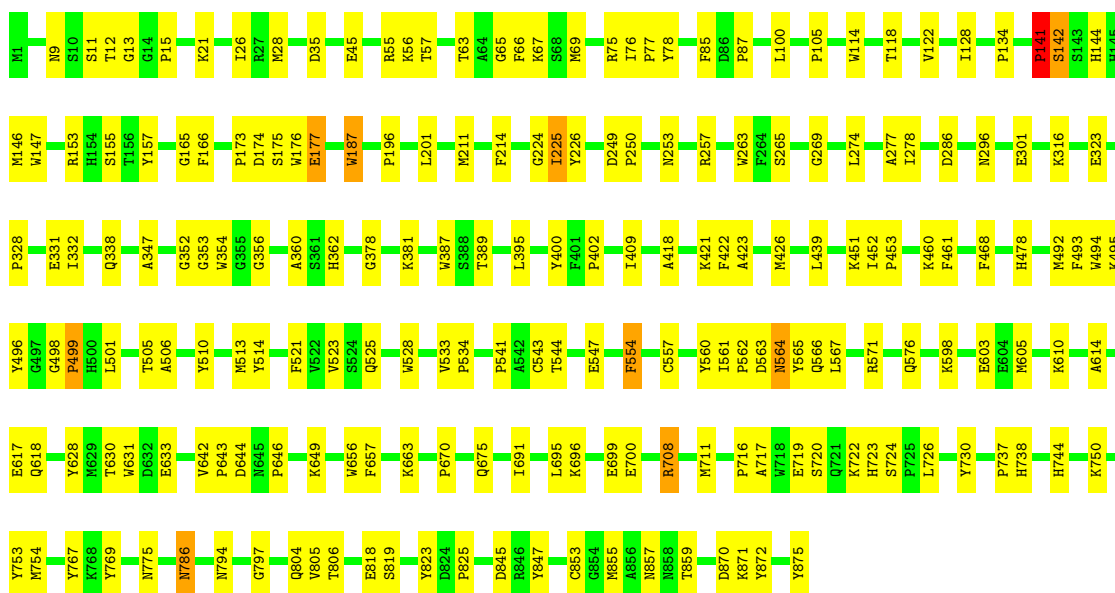
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain I:



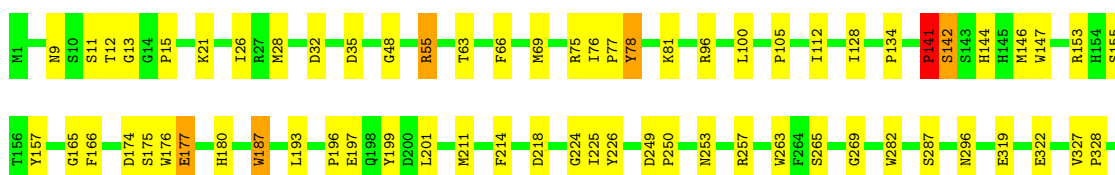
- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain K:

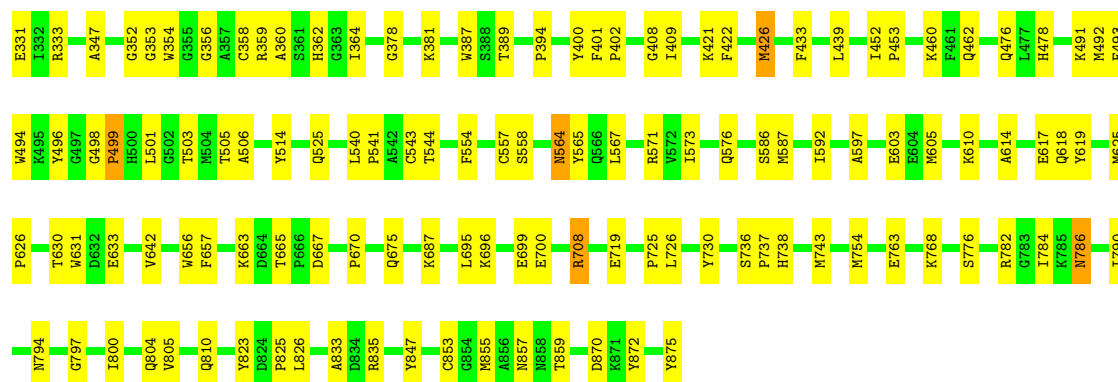


- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain M:

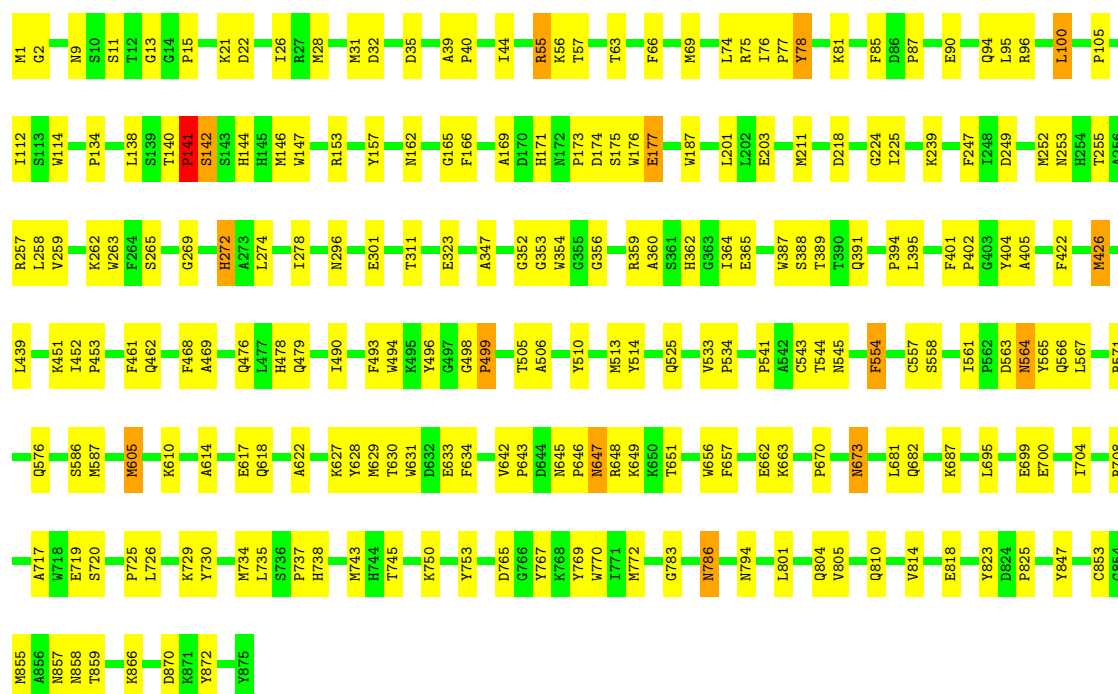






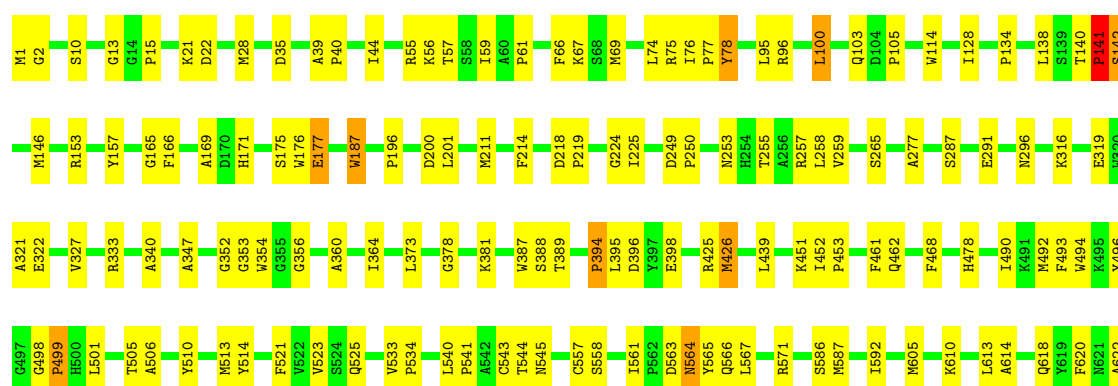
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O:



• Molecule 1: Pyrogallol hydroxytransferase large subunit

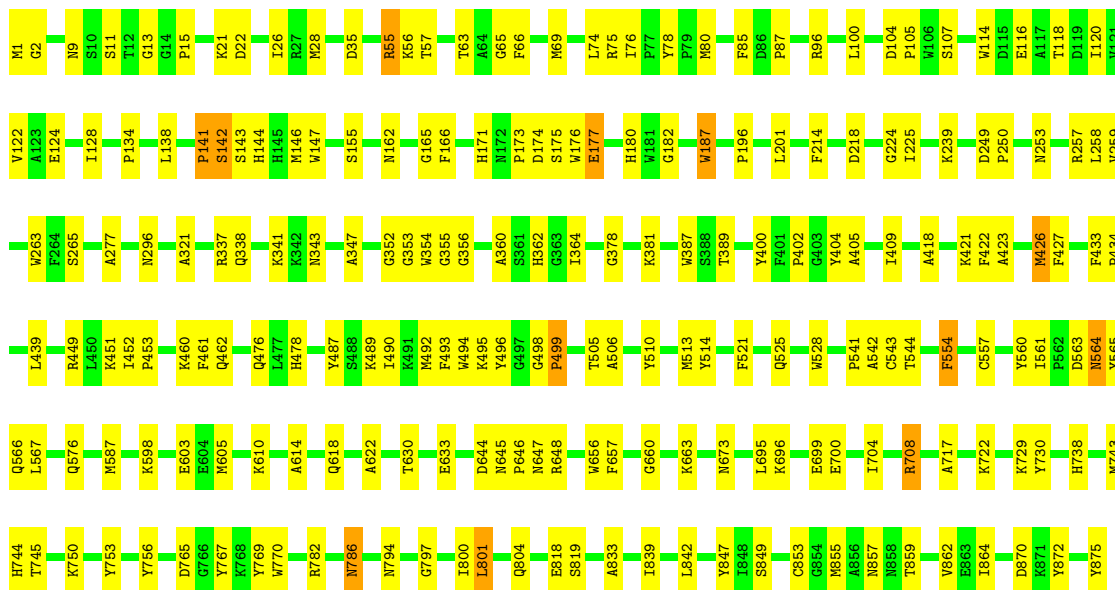
Chain Q:





- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain W:



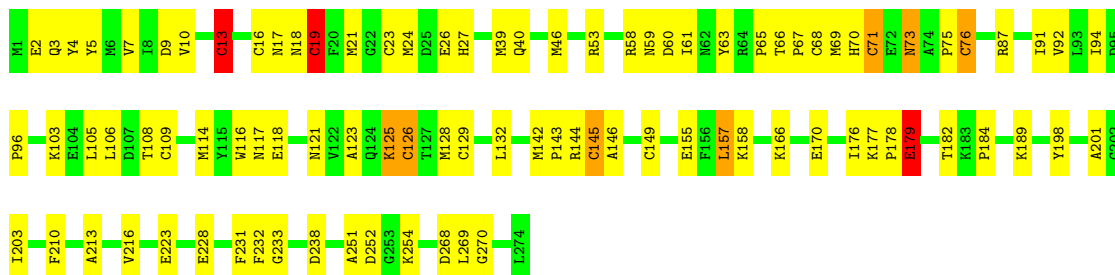
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B:



- Molecule 2: Pyrogallol hydroxytransferase small subunit

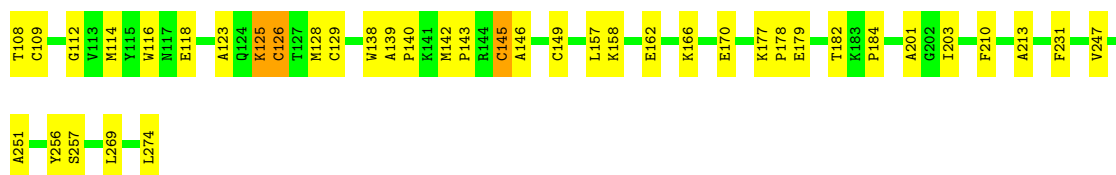
Chain D:



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain F:





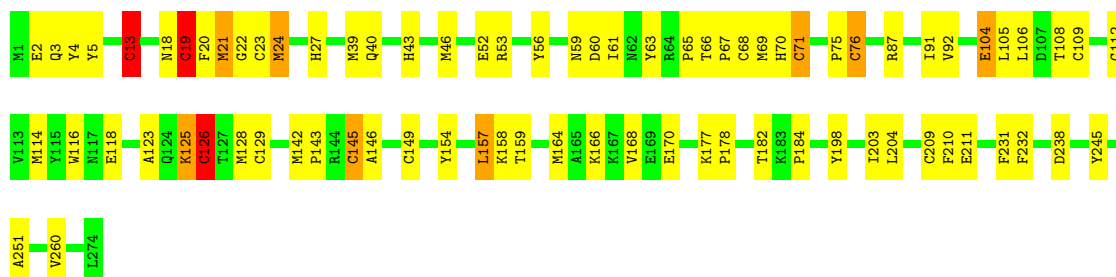
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H:



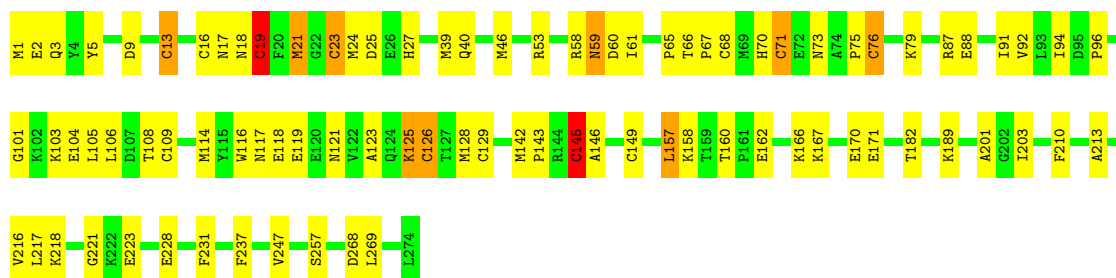
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J:



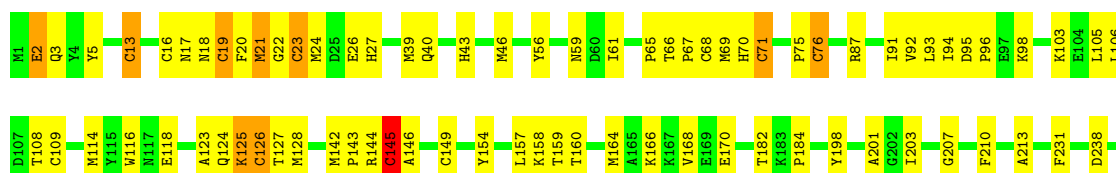
• Molecule 2: Pyrogallol hydroxytransferase small subunit

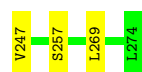
Chain L:



• Molecule 2: Pyrogallol hydroxytransferase small subunit

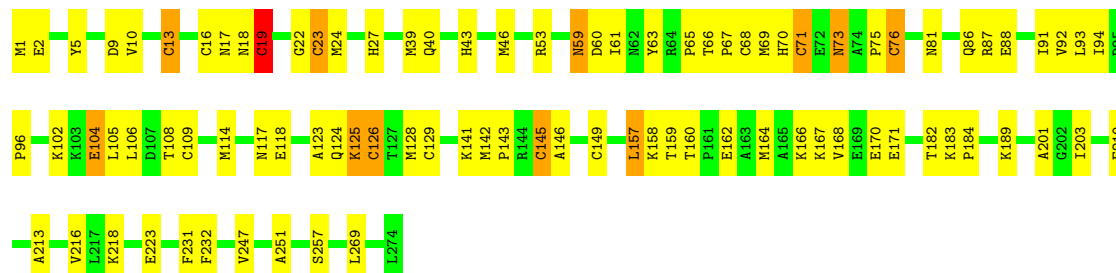
Chain N:





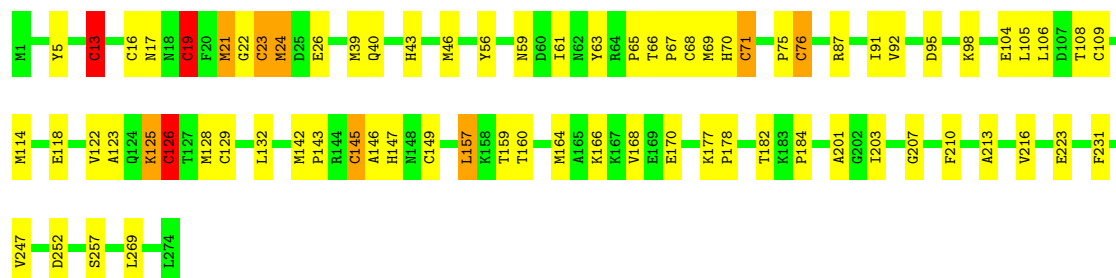
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:



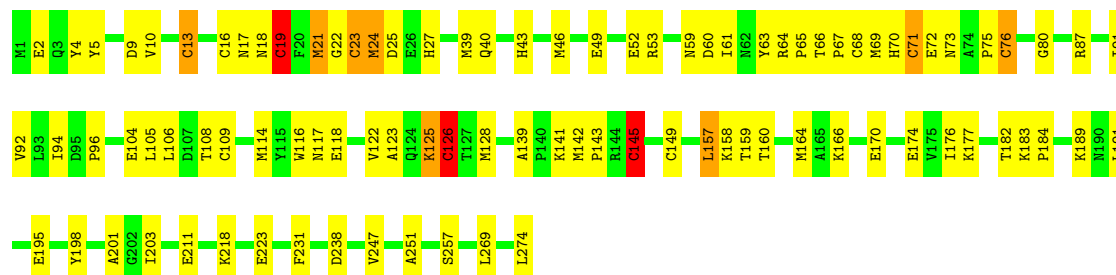
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:



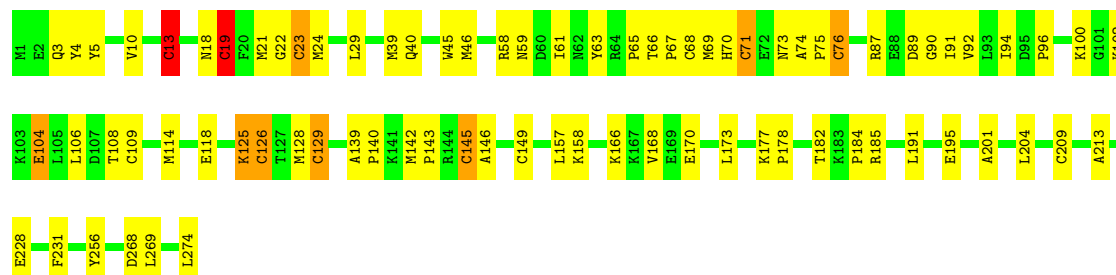
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T:



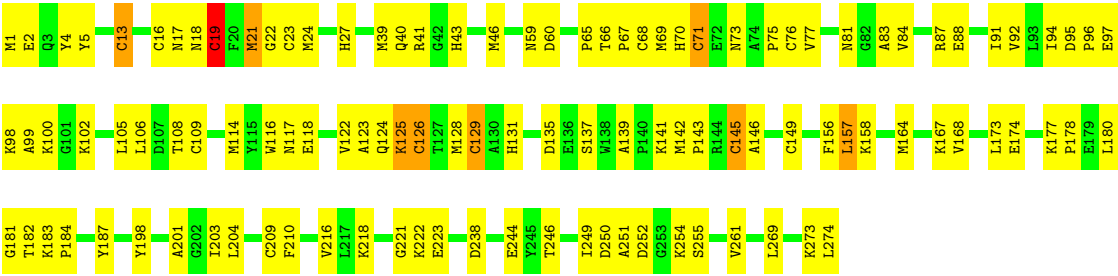
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V:



● Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X:



## 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, $\alpha$ , $\beta$ , $\gamma$	172.47Å 178.14Å 179.05Å 64.11° 64.45° 65.11°	Depositor
Resolution (Å)	24.99 – 2.20	Depositor
% Data completeness (in resolution range)	96.7 (24.99-2.20)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.178 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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, PYG, 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	0.34	0/7219	0.63	3/9786 (0.0%)
1	C	0.33	0/7219	0.61	3/9786 (0.0%)
1	E	0.33	0/7219	0.62	2/9786 (0.0%)
1	G	0.34	0/7219	0.63	3/9786 (0.0%)
1	I	0.33	0/7219	0.62	3/9786 (0.0%)
1	K	0.34	0/7219	0.63	3/9786 (0.0%)
1	M	0.34	0/7219	0.63	3/9786 (0.0%)
1	O	0.34	0/7219	0.62	3/9786 (0.0%)
1	Q	0.34	0/7219	0.63	3/9786 (0.0%)
1	S	0.33	0/7219	0.62	4/9786 (0.0%)
1	U	0.33	0/7219	0.61	2/9786 (0.0%)
1	W	0.33	0/7219	0.61	2/9786 (0.0%)
2	B	0.50	5/2231 (0.2%)	0.68	4/3009 (0.1%)
2	D	0.42	2/2231 (0.1%)	0.63	2/3009 (0.1%)
2	F	0.50	4/2231 (0.2%)	0.67	2/3009 (0.1%)
2	H	0.48	4/2231 (0.2%)	0.68	2/3009 (0.1%)
2	J	0.46	3/2231 (0.1%)	0.66	2/3009 (0.1%)
2	L	0.47	4/2231 (0.2%)	0.68	2/3009 (0.1%)
2	N	0.49	4/2231 (0.2%)	0.67	2/3009 (0.1%)
2	P	0.47	3/2231 (0.1%)	0.65	3/3009 (0.1%)
2	R	0.51	4/2231 (0.2%)	0.67	3/3009 (0.1%)
2	T	0.46	4/2231 (0.2%)	0.65	2/3009 (0.1%)
2	V	0.43	3/2231 (0.1%)	0.64	1/3009 (0.0%)
2	X	0.41	2/2231 (0.1%)	0.62	2/3009 (0.1%)
All	All	0.37	42/113400 (0.0%)	0.63	61/153540 (0.0%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	126	CYS	CB-SG	-9.31	1.66	1.82
2	R	19	CYS	CB-SG	-8.27	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	19	CYS	CB-SG	-8.17	1.68	1.82
2	P	23	CYS	CB-SG	-8.13	1.68	1.82
2	J	19	CYS	CB-SG	-8.10	1.68	1.82

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	352	GLY	N-CA-C	-8.63	91.53	113.10
1	A	352	GLY	N-CA-C	-8.48	91.90	113.10
1	C	352	GLY	N-CA-C	-8.23	92.51	113.10
1	O	352	GLY	N-CA-C	-8.19	92.63	113.10
1	M	352	GLY	N-CA-C	-8.13	92.77	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	6998	0	6632	154	0
1	C	6998	0	6632	186	0
1	E	6998	0	6632	155	0
1	G	6998	0	6632	150	0
1	I	6998	0	6632	158	0
1	K	6998	0	6632	156	0
1	M	6998	0	6632	170	0
1	O	6998	0	6632	194	0
1	Q	6998	0	6632	184	0
1	S	6998	0	6632	169	0
1	U	6998	0	6632	187	0
1	W	6998	0	6632	175	0
2	B	2182	0	2077	77	0
2	D	2182	0	2077	86	0
2	F	2182	0	2077	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2182	0	2077	71	0
2	J	2182	0	2077	73	0
2	L	2182	0	2077	79	0
2	N	2182	0	2077	85	0
2	P	2182	0	2077	84	0
2	R	2182	0	2077	76	0
2	T	2182	0	2077	78	0
2	V	2182	0	2077	62	0
2	X	2182	0	2077	91	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	94	0	44	13	0
4	C	94	0	44	13	0
4	E	94	0	44	14	0
4	G	94	0	44	10	0
4	I	94	0	44	12	0
4	K	94	0	44	13	0
4	M	94	0	44	15	0
4	O	94	0	44	11	0
4	Q	94	0	44	10	0
4	S	94	0	44	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	94	0	44	13	0
4	W	94	0	44	12	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
5	Q	1	0	0	0	0
5	S	1	0	0	0	0
5	U	1	0	0	0	0
5	W	1	0	0	0	0
6	A	9	0	5	1	0
6	C	9	0	5	0	0
6	E	9	0	5	1	0
6	G	9	0	5	0	0
6	I	9	0	5	1	0
6	K	9	0	5	0	0
6	M	9	0	5	1	0
6	O	9	0	5	1	0
6	Q	9	0	5	1	0
6	S	9	0	5	1	0
6	U	9	0	5	1	0
6	W	9	0	5	0	0
7	B	24	0	0	4	0
7	D	24	0	0	4	0
7	F	24	0	0	4	0
7	H	24	0	0	4	0
7	J	24	0	0	4	0
7	L	24	0	0	4	0
7	N	24	0	0	5	0
7	P	24	0	0	4	0
7	R	24	0	0	3	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	5	0
8	A	681	0	0	10	0
8	B	170	0	0	1	0
8	C	681	0	0	14	0
8	D	166	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	684	0	0	8	0
8	F	163	0	0	3	0
8	G	683	0	0	9	0
8	H	161	0	0	0	0
8	I	671	0	0	10	0
8	J	163	0	0	1	0
8	K	681	0	0	9	0
8	L	165	0	0	2	0
8	M	684	0	0	10	0
8	N	159	0	0	4	0
8	O	672	0	0	21	0
8	P	164	0	0	4	0
8	Q	690	0	0	14	0
8	R	161	0	0	1	0
8	S	663	0	0	15	0
8	T	163	0	0	2	0
8	U	668	0	0	12	0
8	V	157	0	0	1	0
8	W	675	0	0	20	0
8	X	164	0	0	7	0
All	All	121808	0	105096	2898	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 13.

The worst 5 of 2898 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.24	1.15
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.23	1.09
2:B:68:CYS:HB2	2:B:126:CYS:HB3	1.36	1.05
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.40	1.04
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.38	1.03

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	873/875 (100%)	815 (93%)	54 (6%)	4 (0%)	38	38
1	C	873/875 (100%)	822 (94%)	46 (5%)	5 (1%)	33	32
1	E	873/875 (100%)	820 (94%)	50 (6%)	3 (0%)	50	53
1	G	873/875 (100%)	823 (94%)	46 (5%)	4 (0%)	38	38
1	I	873/875 (100%)	821 (94%)	49 (6%)	3 (0%)	50	53
1	K	873/875 (100%)	822 (94%)	48 (6%)	3 (0%)	50	53
1	M	873/875 (100%)	825 (94%)	45 (5%)	3 (0%)	50	53
1	O	873/875 (100%)	816 (94%)	51 (6%)	6 (1%)	30	28
1	Q	873/875 (100%)	821 (94%)	48 (6%)	4 (0%)	38	38
1	S	873/875 (100%)	814 (93%)	52 (6%)	7 (1%)	27	24
1	U	873/875 (100%)	820 (94%)	49 (6%)	4 (0%)	38	38
1	W	873/875 (100%)	815 (93%)	55 (6%)	3 (0%)	50	53
2	B	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	43	45
2	D	272/274 (99%)	256 (94%)	14 (5%)	2 (1%)	30	28
2	F	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	43	45
2	H	272/274 (99%)	258 (95%)	11 (4%)	3 (1%)	21	16
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	43	45
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	30	28
2	N	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	43	45
2	P	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	43	45
2	R	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	43	45
2	T	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	43	45
2	V	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	30	28
2	X	272/274 (99%)	245 (90%)	25 (9%)	2 (1%)	30	28
All	All	13740/13788 (100%)	12921 (94%)	752 (6%)	67 (0%)	38	38

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU

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Mol	Chain	Res	Type
1	G	177	GLU
1	I	177	GLU

### 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	729/729 (100%)	715 (98%)	14 (2%)	69	81
1	C	729/729 (100%)	712 (98%)	17 (2%)	63	74
1	E	729/729 (100%)	714 (98%)	15 (2%)	66	78
1	G	729/729 (100%)	717 (98%)	12 (2%)	75	85
1	I	729/729 (100%)	714 (98%)	15 (2%)	66	78
1	K	729/729 (100%)	715 (98%)	14 (2%)	69	81
1	M	729/729 (100%)	714 (98%)	15 (2%)	66	78
1	O	729/729 (100%)	711 (98%)	18 (2%)	60	71
1	Q	729/729 (100%)	715 (98%)	14 (2%)	69	81
1	S	729/729 (100%)	716 (98%)	13 (2%)	71	82
1	U	729/729 (100%)	716 (98%)	13 (2%)	71	82
1	W	729/729 (100%)	713 (98%)	16 (2%)	64	76
2	B	235/235 (100%)	223 (95%)	12 (5%)	33	38
2	D	235/235 (100%)	223 (95%)	12 (5%)	33	38
2	F	235/235 (100%)	223 (95%)	12 (5%)	33	38
2	H	235/235 (100%)	224 (95%)	11 (5%)	36	42
2	J	235/235 (100%)	221 (94%)	14 (6%)	27	29
2	L	235/235 (100%)	222 (94%)	13 (6%)	30	34
2	N	235/235 (100%)	226 (96%)	9 (4%)	44	53
2	P	235/235 (100%)	222 (94%)	13 (6%)	30	34
2	R	235/235 (100%)	223 (95%)	12 (5%)	33	38
2	T	235/235 (100%)	222 (94%)	13 (6%)	30	34
2	V	235/235 (100%)	223 (95%)	12 (5%)	33	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	X	235/235 (100%)	225 (96%)	10 (4%)	40 47
All	All	11568/11568 (100%)	11249 (97%)	319 (3%)	56 67

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	719	GLU
2	N	21	MET
1	W	142	SER
2	L	13	CYS
1	M	78	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 241 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	525	GLN
1	M	701	GLN
1	W	162	ASN
1	K	673	ASN
2	L	81	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 107 ligands modelled in this entry, 35 are monoatomic - leaving 72 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	$\# Z  > 2$
4	MGD	A	902	5	52,52,52	2.52	22 (42%)	73,81,81	4.13	19 (26%)
4	MGD	A	903	5	52,52,52	2.44	18 (34%)	73,81,81	3.23	23 (31%)
6	PYG	A	905	5	9,9,9	4.50	9 (100%)	12,12,12	3.14	4 (33%)
7	SF4	B	302	2	12,12,12	10.85	11 (91%)	0,24,24	0.00	-
7	SF4	B	303	2	12,12,12	11.57	8 (66%)	0,24,24	0.00	-
7	SF4	B	304	2	12,12,12	10.66	8 (66%)	0,24,24	0.00	-
4	MGD	C	902	5	52,52,52	2.54	23 (44%)	73,81,81	3.86	18 (24%)
4	MGD	C	903	5	52,52,52	2.60	19 (36%)	73,81,81	3.50	16 (21%)
6	PYG	C	905	5	9,9,9	4.46	9 (100%)	12,12,12	3.19	5 (41%)
7	SF4	D	302	2	12,12,12	11.19	10 (83%)	0,24,24	0.00	-
7	SF4	D	303	2	12,12,12	11.84	9 (75%)	0,24,24	0.00	-
7	SF4	D	304	2	12,12,12	10.40	8 (66%)	0,24,24	0.00	-
4	MGD	E	902	5	52,52,52	2.47	25 (48%)	73,81,81	4.02	19 (26%)
4	MGD	E	903	5	52,52,52	2.45	18 (34%)	73,81,81	3.19	17 (23%)
6	PYG	E	905	5	9,9,9	4.52	9 (100%)	12,12,12	3.18	4 (33%)
7	SF4	F	302	2	12,12,12	11.06	9 (75%)	0,24,24	0.00	-
7	SF4	F	303	2	12,12,12	11.33	9 (75%)	0,24,24	0.00	-
7	SF4	F	304	2	12,12,12	10.50	9 (75%)	0,24,24	0.00	-
4	MGD	G	902	5	52,52,52	2.51	21 (40%)	73,81,81	3.80	19 (26%)
4	MGD	G	903	5	52,52,52	2.45	19 (36%)	73,81,81	3.04	19 (26%)
6	PYG	G	905	5	9,9,9	4.47	9 (100%)	12,12,12	3.17	4 (33%)
7	SF4	H	302	2	12,12,12	10.66	10 (83%)	0,24,24	0.00	-
7	SF4	H	303	2	12,12,12	11.96	8 (66%)	0,24,24	0.00	-
7	SF4	H	304	2	12,12,12	10.53	10 (83%)	0,24,24	0.00	-
4	MGD	I	902	5	52,52,52	2.42	21 (40%)	73,81,81	3.95	22 (30%)
4	MGD	I	903	5	52,52,52	2.46	18 (34%)	73,81,81	2.91	17 (23%)
6	PYG	I	905	5	9,9,9	4.50	9 (100%)	12,12,12	3.19	5 (41%)
7	SF4	J	301	2	12,12,12	10.51	9 (75%)	0,24,24	0.00	-
7	SF4	J	302	2	12,12,12	11.21	10 (83%)	0,24,24	0.00	-
7	SF4	J	303	2	12,12,12	10.74	9 (75%)	0,24,24	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MGD	K	902	5	52,52,52	2.47	20 (38%)	73,81,81	3.66	20 (27%)
4	MGD	K	903	5	52,52,52	2.42	17 (32%)	73,81,81	3.20	22 (30%)
6	PYG	K	905	5	9,9,9	4.53	9 (100%)	12,12,12	3.20	5 (41%)
7	SF4	L	302	2	12,12,12	10.91	9 (75%)	0,24,24	0.00	-
7	SF4	L	303	2	12,12,12	11.21	8 (66%)	0,24,24	0.00	-
7	SF4	L	304	2	12,12,12	10.47	10 (83%)	0,24,24	0.00	-
4	MGD	M	902	5	52,52,52	2.37	19 (36%)	73,81,81	3.82	19 (26%)
4	MGD	M	903	5	52,52,52	2.49	18 (34%)	73,81,81	3.32	18 (24%)
6	PYG	M	905	5	9,9,9	4.51	9 (100%)	12,12,12	3.18	5 (41%)
7	SF4	N	302	2	12,12,12	10.49	8 (66%)	0,24,24	0.00	-
7	SF4	N	303	2	12,12,12	11.61	8 (66%)	0,24,24	0.00	-
7	SF4	N	304	2	12,12,12	10.86	9 (75%)	0,24,24	0.00	-
4	MGD	O	902	5	52,52,52	2.50	22 (42%)	73,81,81	3.90	18 (24%)
4	MGD	O	903	5	52,52,52	2.48	19 (36%)	73,81,81	3.26	18 (24%)
6	PYG	O	905	5	9,9,9	4.51	9 (100%)	12,12,12	3.22	5 (41%)
7	SF4	P	302	2	12,12,12	10.80	10 (83%)	0,24,24	0.00	-
7	SF4	P	303	2	12,12,12	11.35	10 (83%)	0,24,24	0.00	-
7	SF4	P	304	2	12,12,12	10.03	10 (83%)	0,24,24	0.00	-
4	MGD	Q	902	5	52,52,52	2.45	22 (42%)	73,81,81	3.81	19 (26%)
4	MGD	Q	903	5	52,52,52	2.39	15 (28%)	73,81,81	2.92	18 (24%)
6	PYG	Q	905	5	9,9,9	4.50	9 (100%)	12,12,12	3.16	5 (41%)
7	SF4	R	302	2	12,12,12	10.79	10 (83%)	0,24,24	0.00	-
7	SF4	R	303	2	12,12,12	11.38	10 (83%)	0,24,24	0.00	-
7	SF4	R	304	2	12,12,12	10.67	9 (75%)	0,24,24	0.00	-
4	MGD	S	902	5	52,52,52	2.45	22 (42%)	73,81,81	3.79	18 (24%)
4	MGD	S	903	5	52,52,52	2.43	16 (30%)	73,81,81	3.12	17 (23%)
6	PYG	S	905	5	9,9,9	4.55	9 (100%)	12,12,12	3.15	4 (33%)
7	SF4	T	302	2	12,12,12	10.50	8 (66%)	0,24,24	0.00	-
7	SF4	T	303	2	12,12,12	11.46	9 (75%)	0,24,24	0.00	-
7	SF4	T	304	2	12,12,12	10.29	8 (66%)	0,24,24	0.00	-
4	MGD	U	902	5	52,52,52	2.56	22 (42%)	73,81,81	3.73	19 (26%)
4	MGD	U	903	5	52,52,52	2.49	18 (34%)	73,81,81	3.27	17 (23%)
6	PYG	U	905	5	9,9,9	4.47	9 (100%)	12,12,12	3.18	5 (41%)
7	SF4	V	302	2	12,12,12	11.50	10 (83%)	0,24,24	0.00	-
7	SF4	V	303	2	12,12,12	11.66	8 (66%)	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SF4	V	304	2	12,12,12	10.72	9 (75%)	0,24,24	0.00	-
4	MGD	W	902	5	52,52,52	2.47	22 (42%)	73,81,81	3.65	20 (27%)
4	MGD	W	903	5	52,52,52	2.62	19 (36%)	73,81,81	2.88	17 (23%)
6	PYG	W	905	5	9,9,9	4.50	9 (100%)	12,12,12	3.26	5 (41%)
7	SF4	X	302	2	12,12,12	11.05	10 (83%)	0,24,24	0.00	-
7	SF4	X	303	2	12,12,12	11.31	10 (83%)	0,24,24	0.00	-
7	SF4	X	304	2	12,12,12	10.07	10 (83%)	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
4	MGD	A	902	5	-	0/22/66/66	0/6/6/6
4	MGD	A	903	5	-	0/22/66/66	0/6/6/6
6	PYG	A	905	5	-	0/0/0/0	0/1/1/1
7	SF4	B	302	2	-	0/0/48/48	0/6/5/5
7	SF4	B	303	2	-	0/0/48/48	0/6/5/5
7	SF4	B	304	2	-	0/0/48/48	0/6/5/5
4	MGD	C	902	5	-	0/22/66/66	0/6/6/6
4	MGD	C	903	5	-	0/22/66/66	0/6/6/6
6	PYG	C	905	5	-	0/0/0/0	0/1/1/1
7	SF4	D	302	2	-	0/0/48/48	0/6/5/5
7	SF4	D	303	2	-	0/0/48/48	0/6/5/5
7	SF4	D	304	2	-	0/0/48/48	0/6/5/5
4	MGD	E	902	5	-	0/22/66/66	0/6/6/6
4	MGD	E	903	5	-	0/22/66/66	0/6/6/6
6	PYG	E	905	5	-	0/0/0/0	0/1/1/1
7	SF4	F	302	2	-	0/0/48/48	0/6/5/5
7	SF4	F	303	2	-	0/0/48/48	0/6/5/5
7	SF4	F	304	2	-	0/0/48/48	0/6/5/5
4	MGD	G	902	5	-	0/22/66/66	0/6/6/6
4	MGD	G	903	5	-	0/22/66/66	0/6/6/6
6	PYG	G	905	5	-	0/0/0/0	0/1/1/1
7	SF4	H	302	2	-	0/0/48/48	0/6/5/5
7	SF4	H	303	2	-	0/0/48/48	0/6/5/5
7	SF4	H	304	2	-	0/0/48/48	0/6/5/5
4	MGD	I	902	5	-	0/22/66/66	0/6/6/6
4	MGD	I	903	5	-	0/22/66/66	0/6/6/6
6	PYG	I	905	5	-	0/0/0/0	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	J	301	2	-	0/0/48/48	0/6/5/5
7	SF4	J	302	2	-	0/0/48/48	0/6/5/5
7	SF4	J	303	2	-	0/0/48/48	0/6/5/5
4	MGD	K	902	5	-	0/22/66/66	0/6/6/6
4	MGD	K	903	5	-	0/22/66/66	0/6/6/6
6	PYG	K	905	5	-	0/0/0/0	0/1/1/1
7	SF4	L	302	2	-	0/0/48/48	0/6/5/5
7	SF4	L	303	2	-	0/0/48/48	0/6/5/5
7	SF4	L	304	2	-	0/0/48/48	0/6/5/5
4	MGD	M	902	5	-	0/22/66/66	0/6/6/6
4	MGD	M	903	5	-	0/22/66/66	0/6/6/6
6	PYG	M	905	5	-	0/0/0/0	0/1/1/1
7	SF4	N	302	2	-	0/0/48/48	0/6/5/5
7	SF4	N	303	2	-	0/0/48/48	0/6/5/5
7	SF4	N	304	2	-	0/0/48/48	0/6/5/5
4	MGD	O	902	5	-	0/22/66/66	0/6/6/6
4	MGD	O	903	5	-	0/22/66/66	0/6/6/6
6	PYG	O	905	5	-	0/0/0/0	0/1/1/1
7	SF4	P	302	2	-	0/0/48/48	0/6/5/5
7	SF4	P	303	2	-	0/0/48/48	0/6/5/5
7	SF4	P	304	2	-	0/0/48/48	0/6/5/5
4	MGD	Q	902	5	-	0/22/66/66	0/6/6/6
4	MGD	Q	903	5	-	0/22/66/66	0/6/6/6
6	PYG	Q	905	5	-	0/0/0/0	0/1/1/1
7	SF4	R	302	2	-	0/0/48/48	0/6/5/5
7	SF4	R	303	2	-	0/0/48/48	0/6/5/5
7	SF4	R	304	2	-	0/0/48/48	0/6/5/5
4	MGD	S	902	5	-	0/22/66/66	0/6/6/6
4	MGD	S	903	5	-	0/22/66/66	0/6/6/6
6	PYG	S	905	5	-	0/0/0/0	0/1/1/1
7	SF4	T	302	2	-	0/0/48/48	0/6/5/5
7	SF4	T	303	2	-	0/0/48/48	0/6/5/5
7	SF4	T	304	2	-	0/0/48/48	0/6/5/5
4	MGD	U	902	5	-	0/22/66/66	0/6/6/6
4	MGD	U	903	5	-	0/22/66/66	0/6/6/6
6	PYG	U	905	5	-	0/0/0/0	0/1/1/1
7	SF4	V	302	2	-	0/0/48/48	0/6/5/5
7	SF4	V	303	2	-	0/0/48/48	0/6/5/5
7	SF4	V	304	2	-	0/0/48/48	0/6/5/5
4	MGD	W	902	5	-	0/22/66/66	0/6/6/6
4	MGD	W	903	5	-	0/22/66/66	0/6/6/6
6	PYG	W	905	5	-	0/0/0/0	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	X	302	2	-	0/0/48/48	0/6/5/5
7	SF4	X	303	2	-	0/0/48/48	0/6/5/5
7	SF4	X	304	2	-	0/0/48/48	0/6/5/5

The worst 5 of 913 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	302	SF4	S1-FE4	-21.28	2.18	2.33
7	X	302	SF4	S1-FE4	-21.00	2.19	2.33
7	D	302	SF4	S1-FE4	-20.84	2.19	2.33
7	F	302	SF4	S1-FE4	-20.48	2.19	2.33
7	B	302	SF4	S1-FE4	-20.31	2.19	2.33

The worst 5 of 505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	MGD	C6-C5-N7	-29.98	130.10	134.14
4	E	902	MGD	C6-C5-N7	-29.07	130.23	134.14
4	I	902	MGD	C6-C5-N7	-27.91	130.38	134.14
4	O	902	MGD	C6-C5-N7	-27.77	130.40	134.14
4	C	902	MGD	C6-C5-N7	-27.35	130.46	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.