



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:19 PM GMT

PDB ID : 4V4C
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase 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 X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

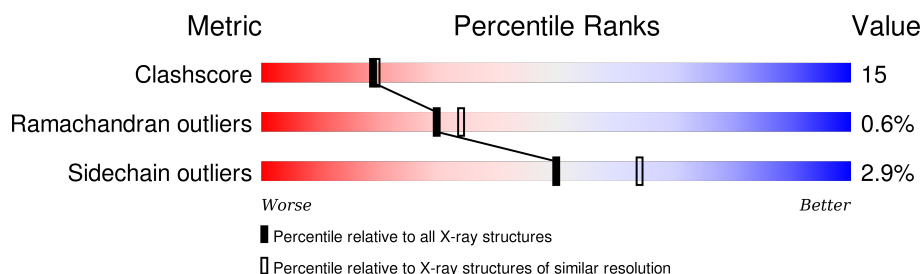
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)

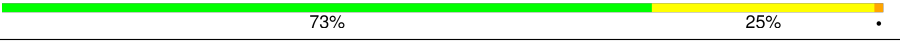










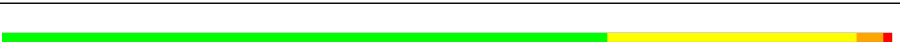




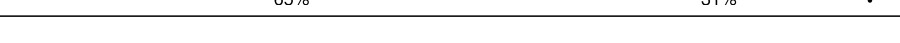
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	 73% 25% .
1	C	875	 70% 28% .
1	E	875	 75% 24% .
1	G	875	 73% 25% .
1	I	875	 73% 26% .
1	K	875	 73% 25% .
1	M	875	 73% 26% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	C	901	-	-	X	-
3	ACT	E	901	-	-	X	-
3	ACT	G	901	-	-	X	-
3	ACT	I	901	-	-	X	-
3	ACT	K	901	-	-	X	-
3	ACT	O	901	-	-	X	-
3	ACT	W	901	-	-	X	-
7	SF4	B	303	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	D	303	-	-	X	-
7	SF4	D	304	-	-	X	-
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	H	304	-	-	X	-
7	SF4	J	303	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	L	304	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	302	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	P	304	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	R	304	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	T	304	-	-	X	-
7	SF4	V	303	-	-	X	-
7	SF4	X	302	-	-	X	-
7	SF4	X	303	-	-	X	-
7	SF4	X	304	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 122057 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 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			
1	M	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	O	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	Q	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	S	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	U	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	W	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	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

Continued on next page...

Continued from previous page...

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 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		
3	M	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	S	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		

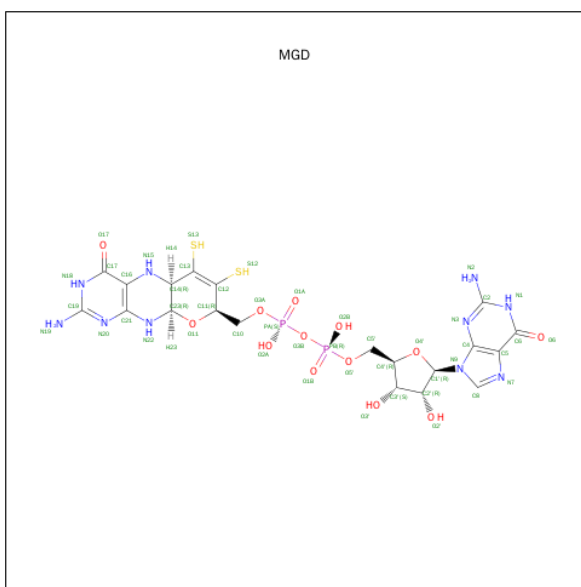
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

Continued on next page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	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-ONE GUANOSINE 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 47	C 20	N 10	O 13	P 2	S 2	0	0
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	C	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	G	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

Continued on next page...

Continued from previous page...

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

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

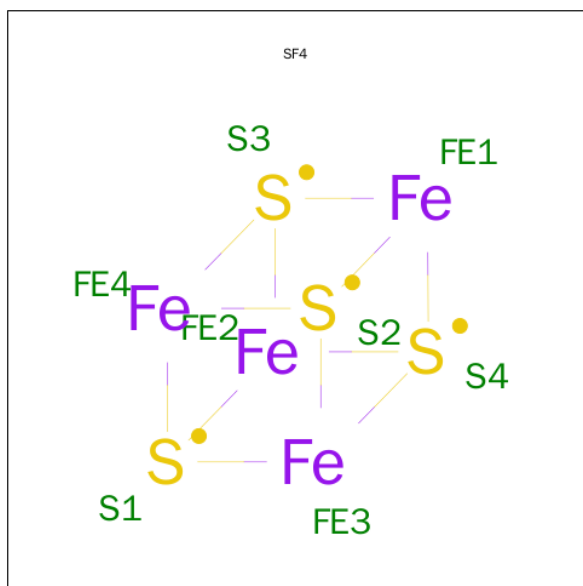
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Mo 1	0	0
6	Q	1	Total 1	Mo 1	0	0
6	K	1	Total 1	Mo 1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
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	688	Total 688	O 688	0	0
8	B	167	Total 167	O 167	0	0
8	C	684	Total 684	O 684	0	0
8	D	167	Total 167	O 167	0	0
8	E	684	Total 684	O 684	0	0
8	F	167	Total 167	O 167	0	0

Continued on next page...

Continued from previous page...

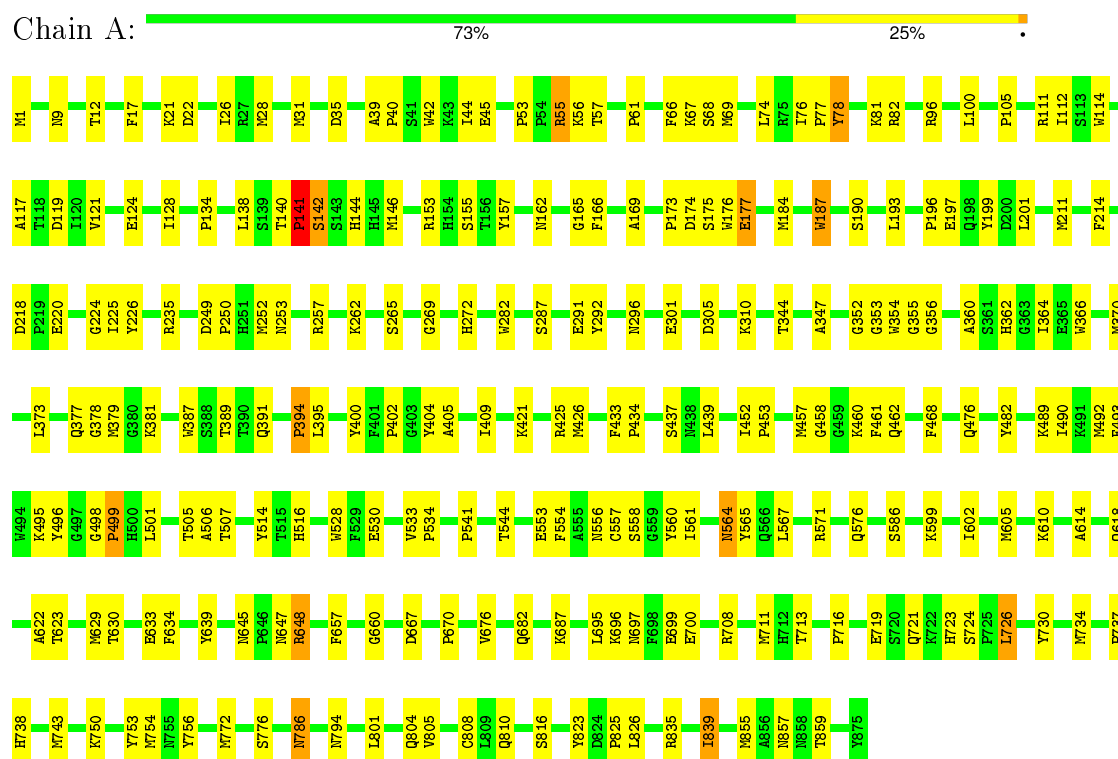
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	689	Total 689	O 689	0	0
8	H	162	Total 162	O 162	0	0
8	I	675	Total 675	O 675	0	0
8	J	170	Total 170	O 170	0	0
8	K	684	Total 684	O 684	0	0
8	L	168	Total 168	O 168	0	0
8	M	683	Total 683	O 683	0	0
8	N	163	Total 163	O 163	0	0
8	O	679	Total 679	O 679	0	0
8	P	163	Total 163	O 163	0	0
8	Q	692	Total 692	O 692	0	0
8	R	166	Total 166	O 166	0	0
8	S	675	Total 675	O 675	0	0
8	T	159	Total 159	O 159	0	0
8	U	667	Total 667	O 667	0	0
8	V	163	Total 163	O 163	0	0
8	W	677	Total 677	O 677	0	0
8	X	165	Total 165	O 165	0	0

3 Residue-property plots

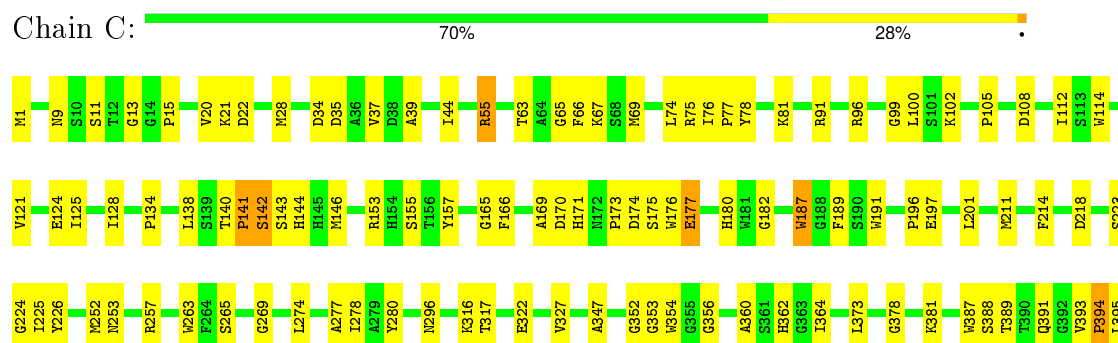
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

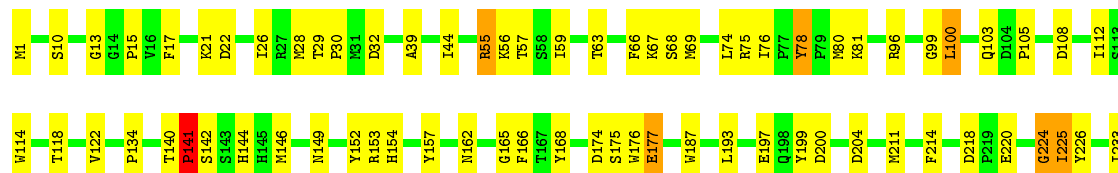
Note EDS was not executed.

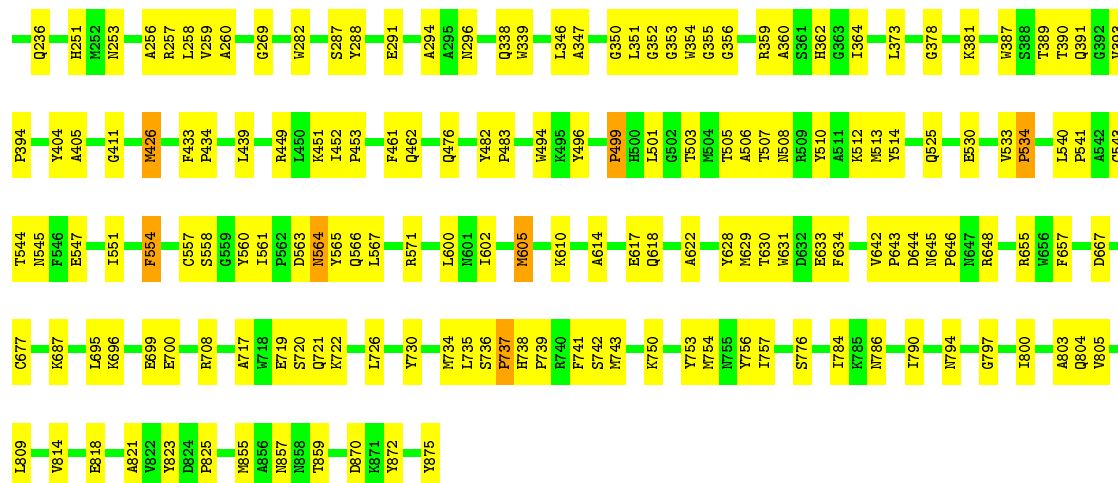
- Molecule 1: Pyrogallol hydroxytransferase large subunit



- Molecule 1: Pyrogallol hydroxytransferase large subunit

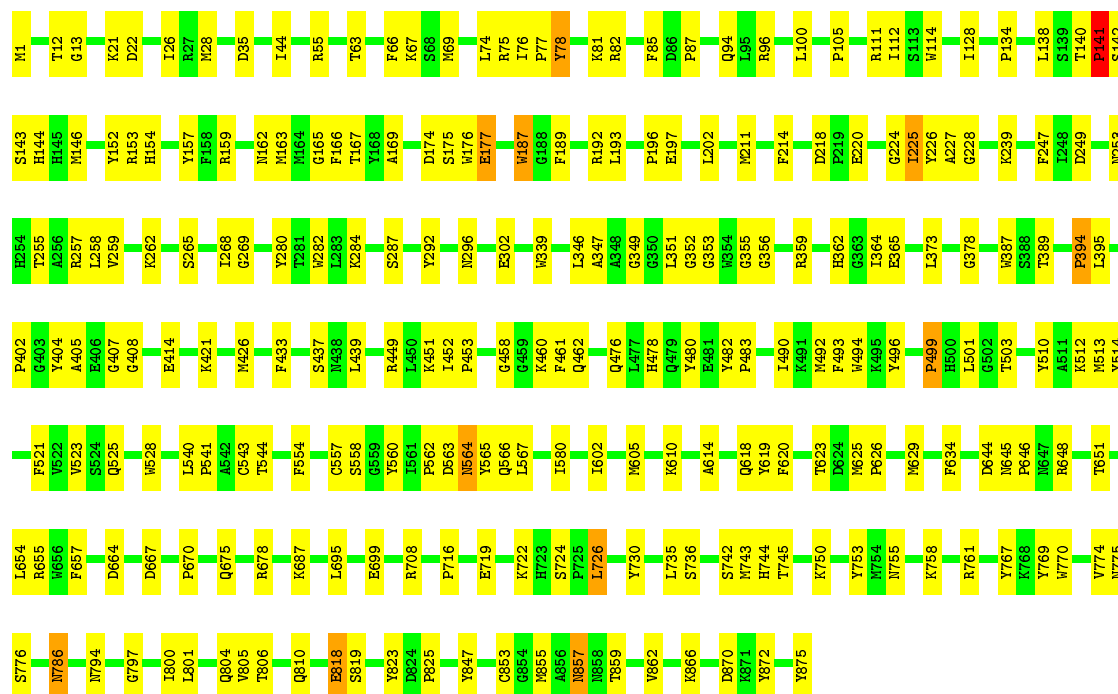


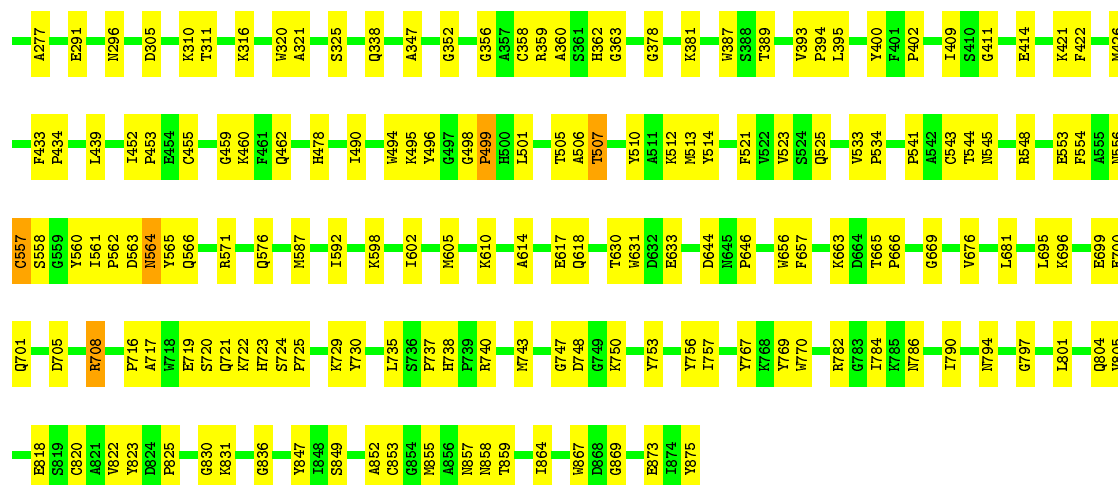




• Molecule 1: Pyrogallol hydroxytransferase large subunit

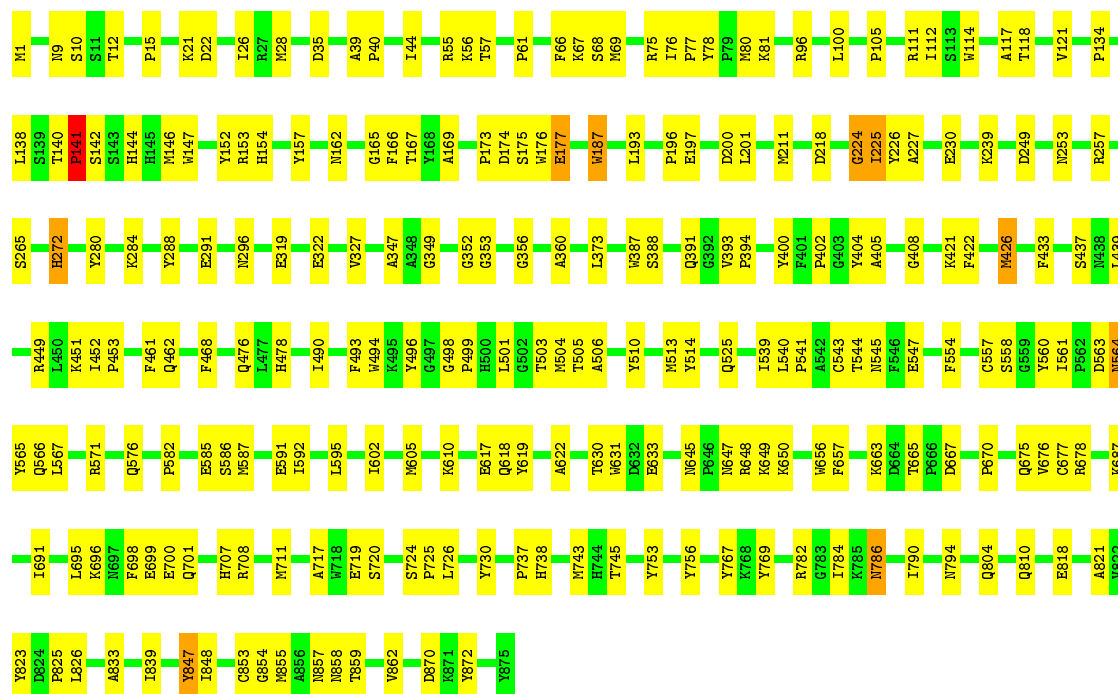
Chain I: 73% 26%





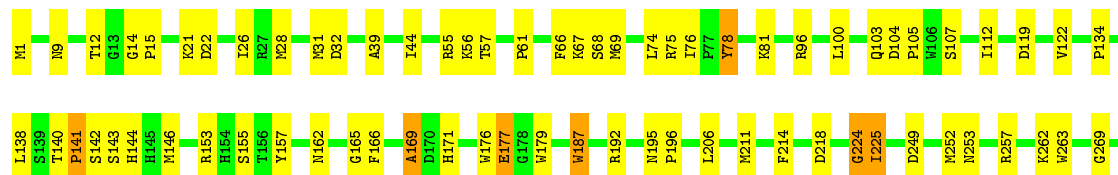
• Molecule 1: Pyrogallol hydroxytransferase large subunit

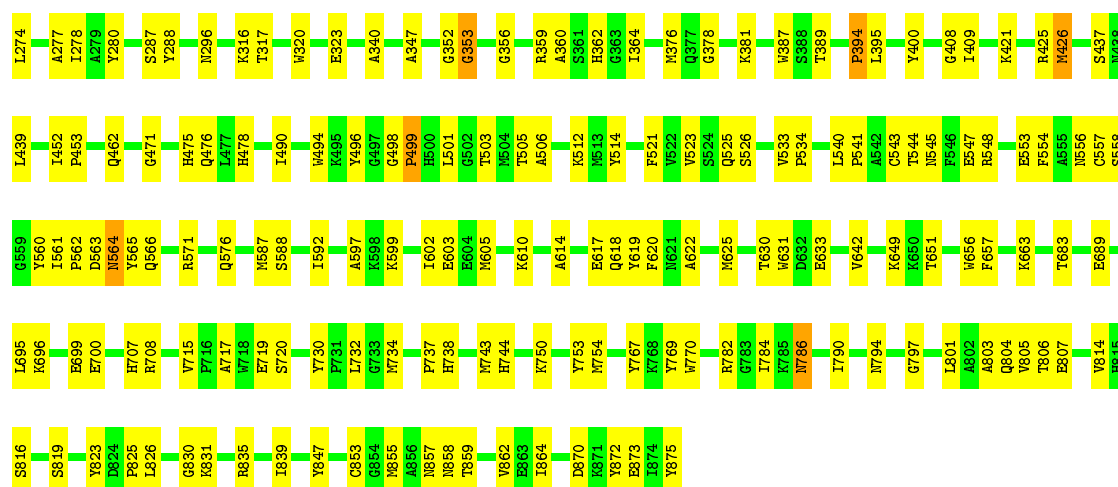
Chain M: 73% 26% .



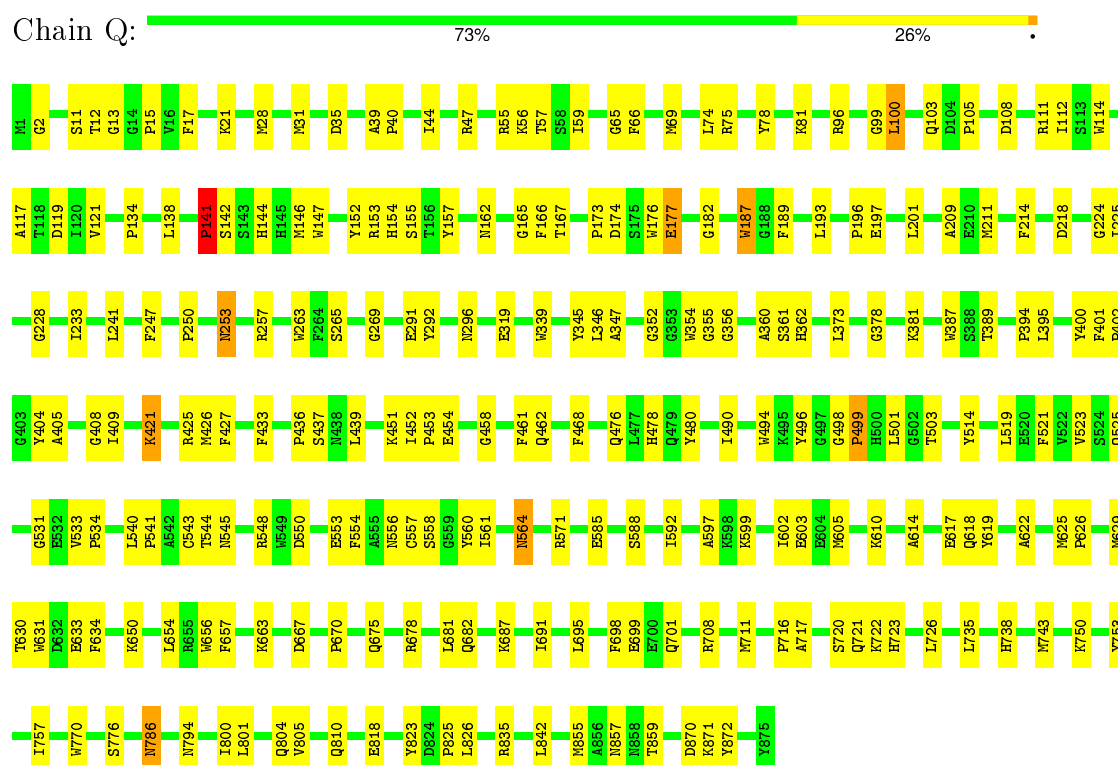
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O: 73% 25% .

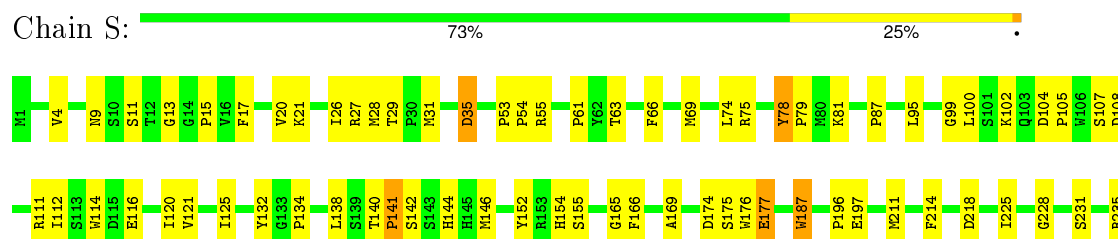


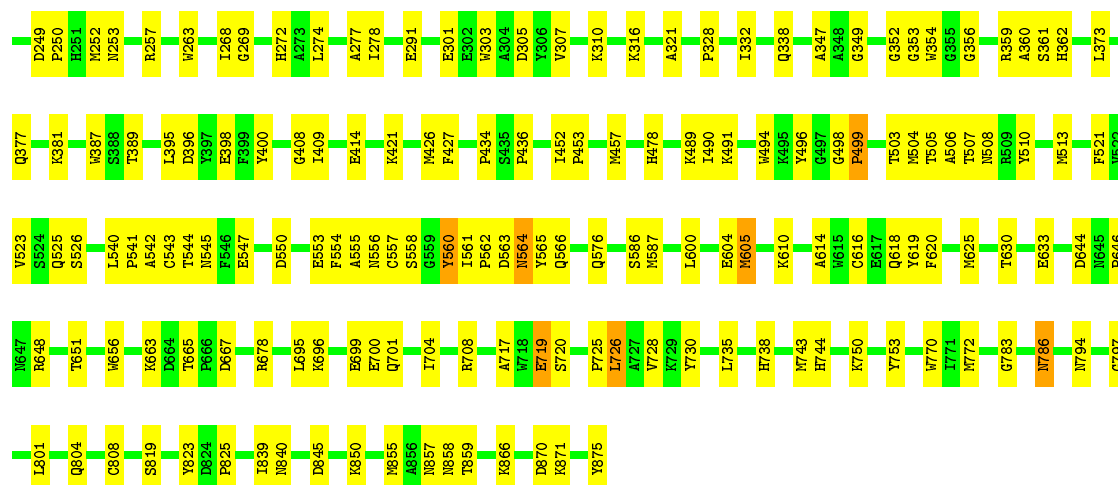


• Molecule 1: Pyrogallol hydroxytransferase large subunit



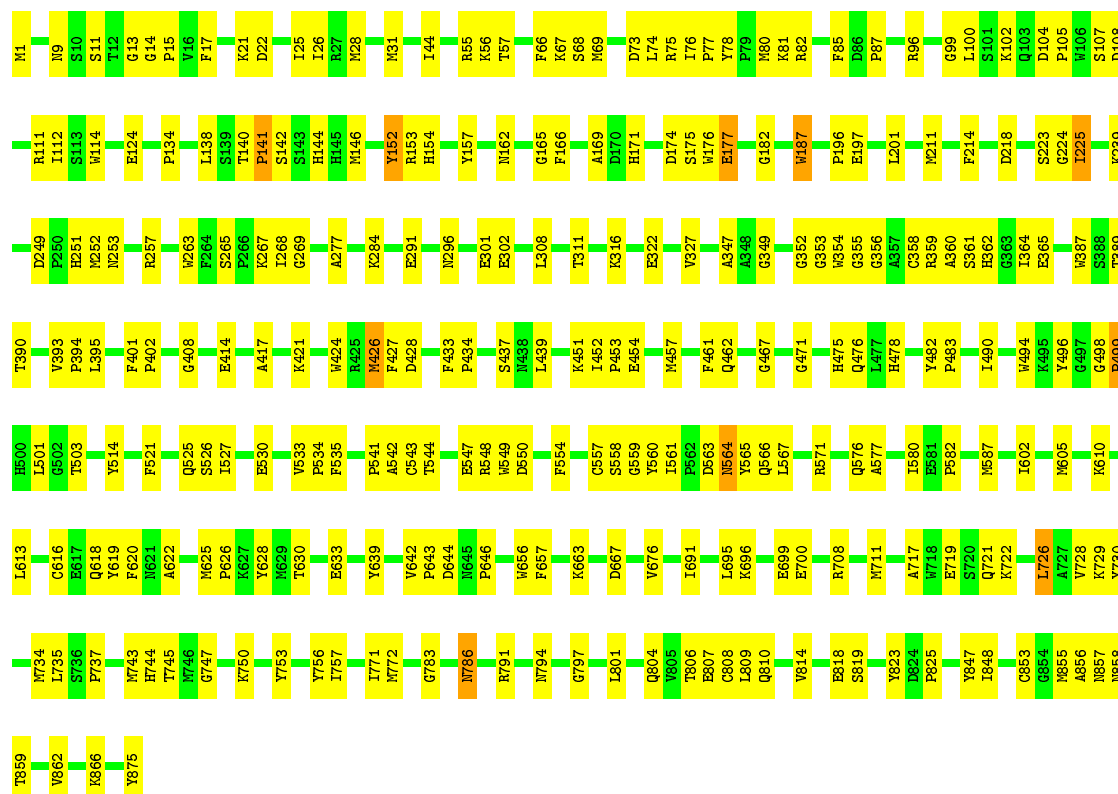
• Molecule 1: Pyrogallol hydroxytransferase large subunit





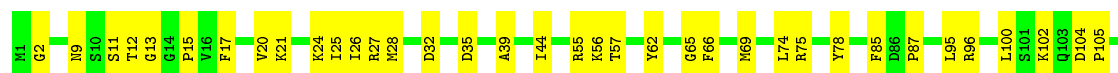
• Molecule 1: Pyrogallol hydroxytransferase large subunit

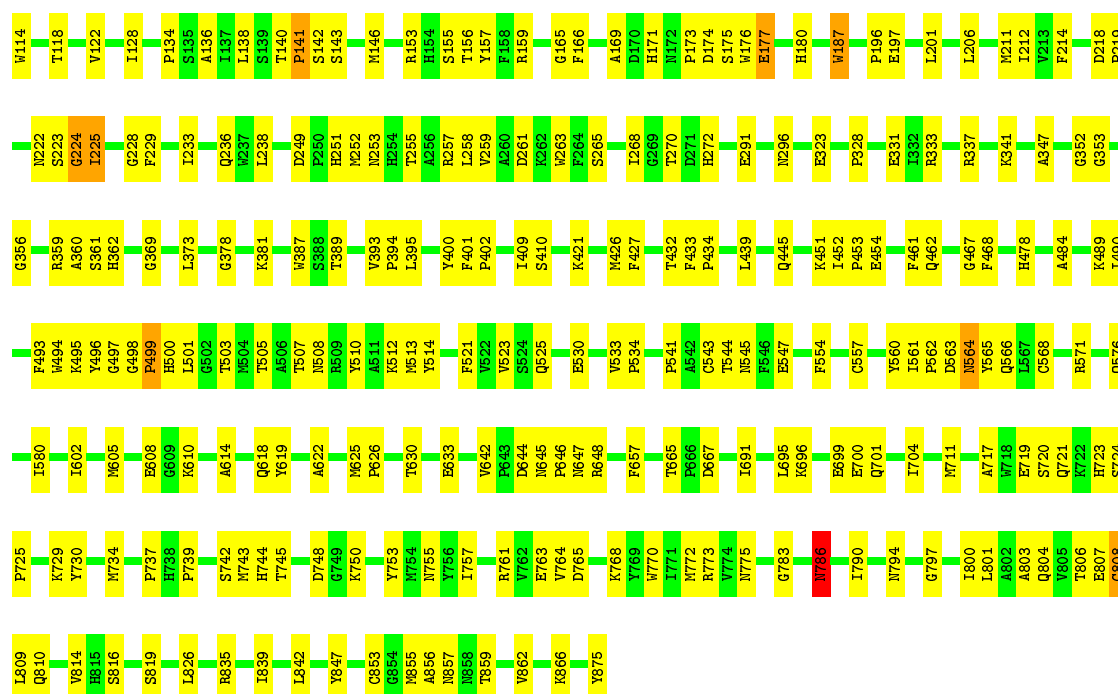
Chain U: 70% 29% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

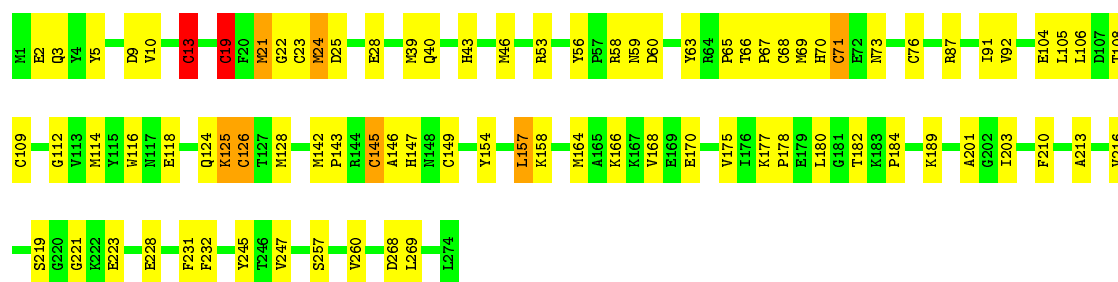
Chain W: 68% 31% .





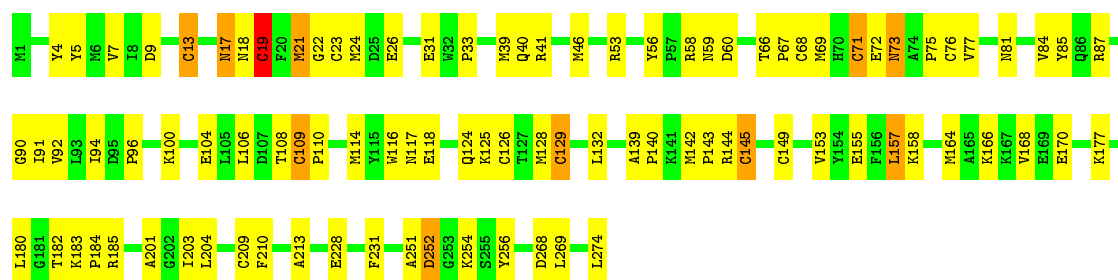
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B: 69% 28%



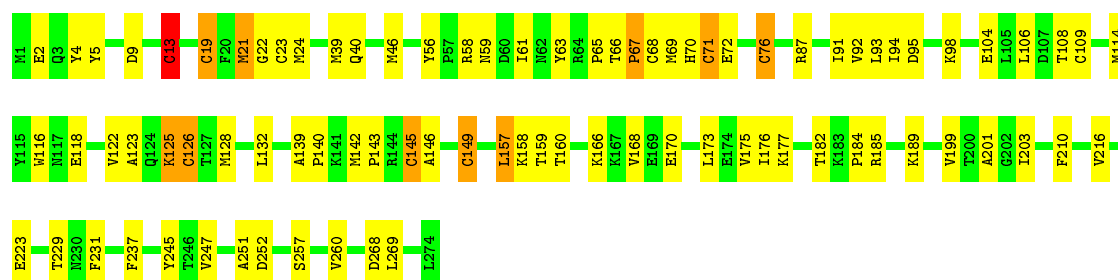
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain D: 65% 31%

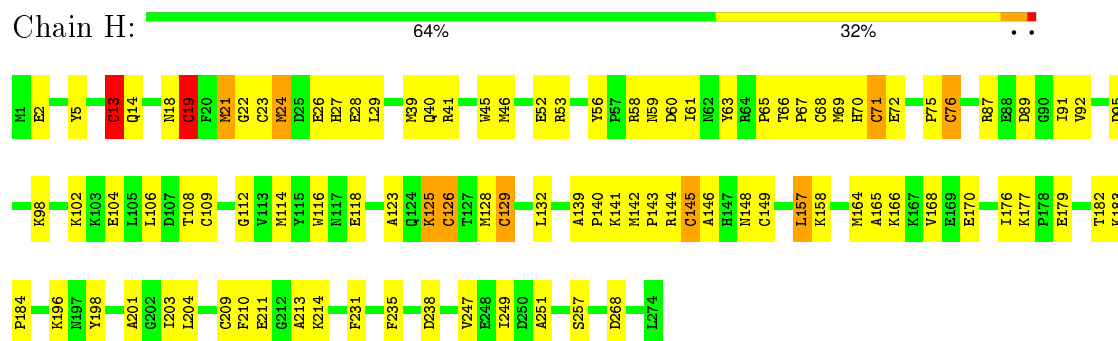


• Molecule 2: Pyrogallol hydroxytransferase small subunit

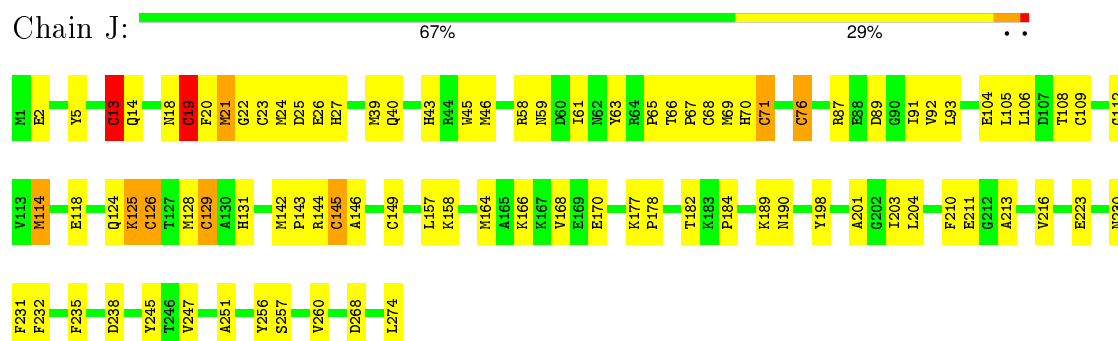
Chain F: 69% 27%



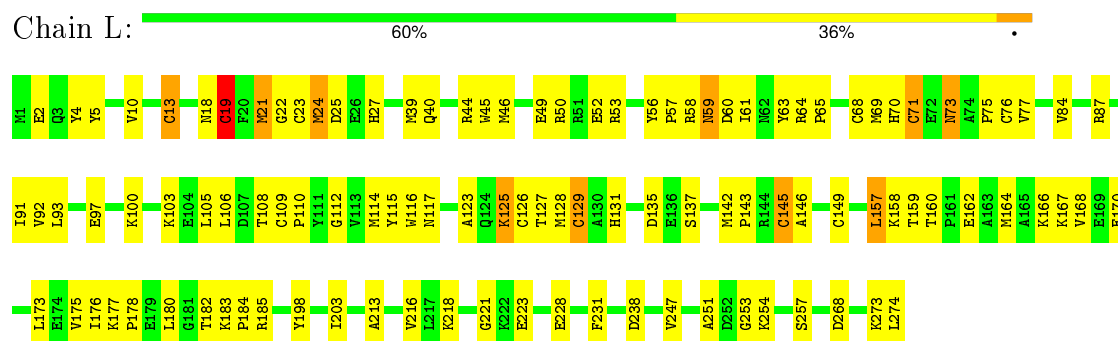
• Molecule 2: Pyrogallol hydroxytransferase small subunit



• Molecule 2: Pyrogallol hydroxytransferase small subunit

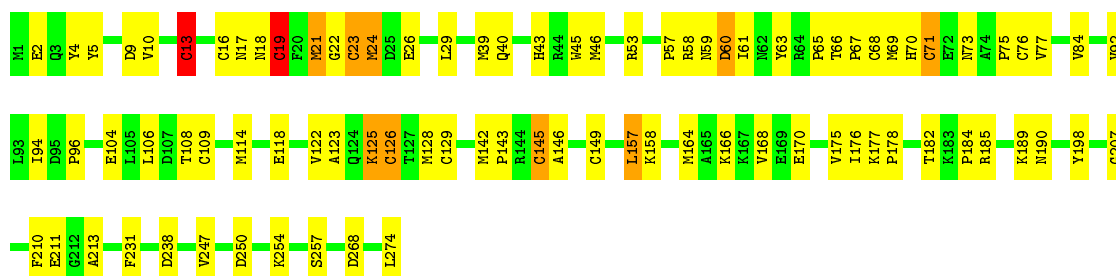


• Molecule 2: Pyrogallol hydroxytransferase small subunit



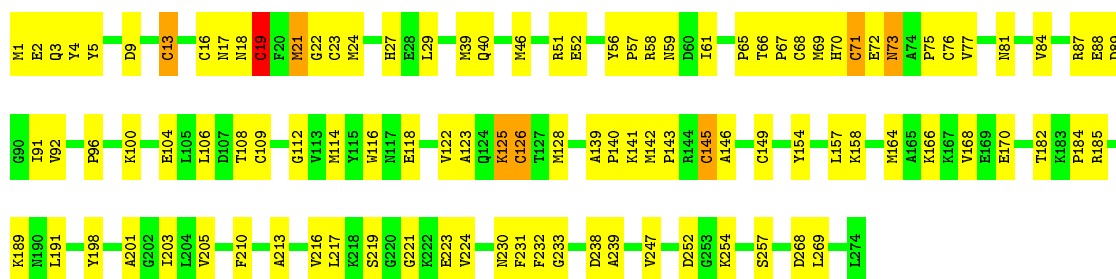
• Molecule 2: Pyrogallol hydroxytransferase small subunit





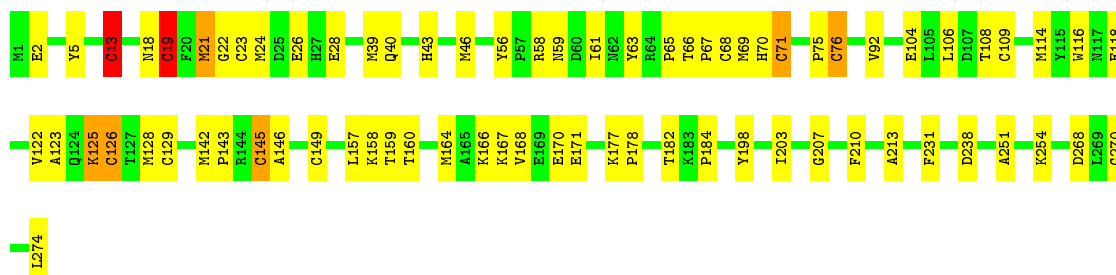
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P: 62% 35%



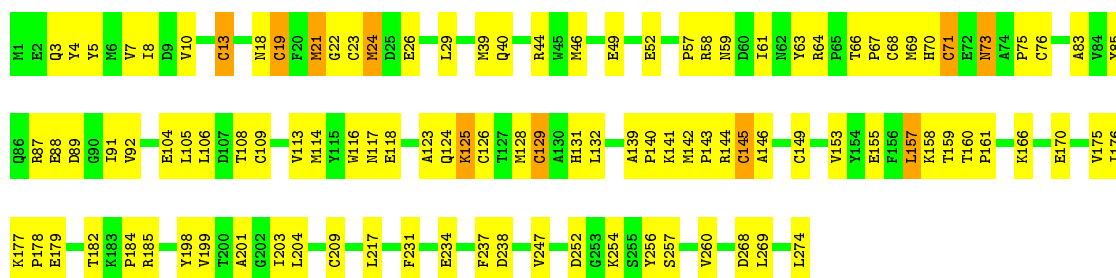
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R: 73% 24%



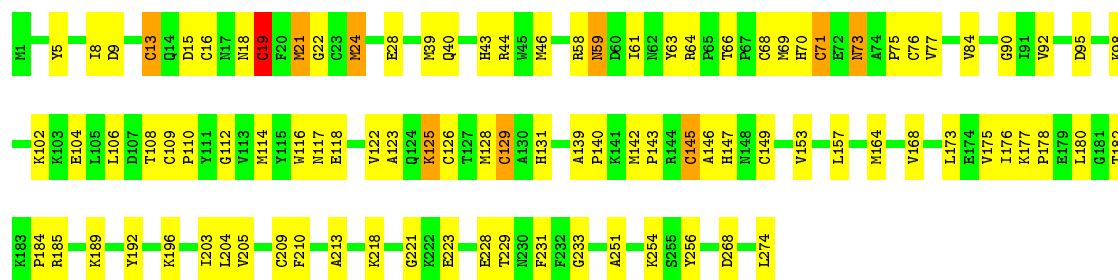
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T: 61% 35%



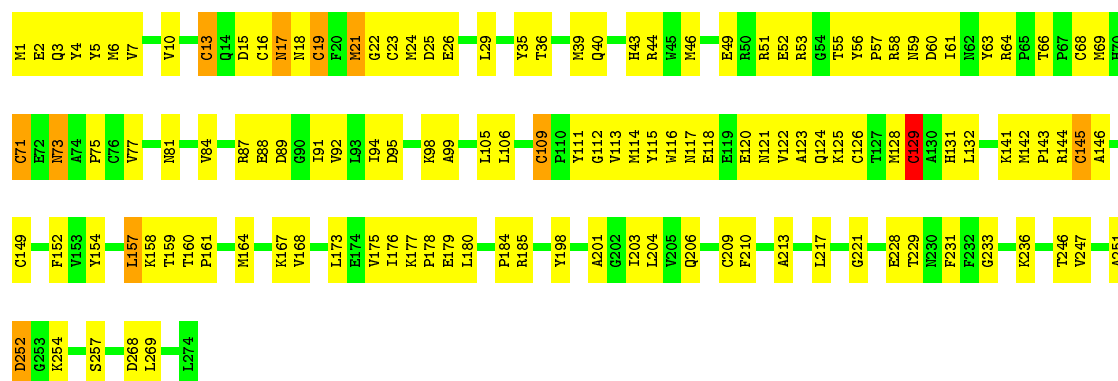
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V: 65% 31%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X: 53% 43% .



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	122057	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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%)
1	M	0.36	0/7240	0.63	3/9815 (0.0%)
1	O	0.34	0/7240	0.62	4/9815 (0.0%)
1	Q	0.35	0/7240	0.62	3/9815 (0.0%)
1	S	0.34	0/7240	0.61	1/9815 (0.0%)
1	U	0.35	0/7240	0.60	1/9815 (0.0%)
1	W	0.33	0/7240	0.59	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%)
2	N	0.47	3/2231 (0.1%)	0.66	2/3009 (0.1%)
2	P	0.40	2/2231 (0.1%)	0.61	1/3009 (0.0%)
2	R	0.44	2/2231 (0.1%)	0.66	2/3009 (0.1%)
2	T	0.37	0/2231	0.59	1/3009 (0.0%)
2	V	0.40	1/2231 (0.0%)	0.61	2/3009 (0.1%)
2	X	0.35	0/2231	0.58	1/3009 (0.0%)
All	All	0.36	20/113652 (0.0%)	0.62	48/153888 (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	M	0	1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	19	CYS	CB-SG	-8.91	1.67	1.82
2	R	19	CYS	CB-SG	-7.56	1.69	1.82
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

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	352	GLY	N-CA-C	-8.47	91.94	113.10
1	O	352	GLY	N-CA-C	-8.36	92.21	113.10
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	Q	352	GLY	N-CA-C	-8.01	93.08	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	847	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
1	M	7018	0	6645	184	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	7018	0	6645	194	0
1	Q	7018	0	6645	179	0
1	S	7018	0	6645	188	0
1	U	7018	0	6645	228	0
1	W	7018	0	6645	228	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	106	0
2	N	2182	0	2077	82	0
2	P	2182	0	2077	102	0
2	R	2182	0	2077	69	0
2	T	2182	0	2077	101	0
2	V	2182	0	2077	87	0
2	X	2182	0	2077	131	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
3	M	4	0	3	1	0
3	O	4	0	3	2	0
3	Q	4	0	3	1	0
3	S	4	0	3	1	0
3	U	4	0	3	1	0
3	W	4	0	3	2	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
4	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
5	A	94	0	44	11	0
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
5	M	94	0	44	9	0
5	O	94	0	44	9	0
5	Q	94	0	44	8	0
5	S	94	0	44	9	0
5	U	94	0	44	13	0
5	W	94	0	44	11	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
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	Q	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	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
7	N	24	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	24	0	0	6	0
7	R	24	0	0	5	0
7	T	24	0	0	7	0
7	V	24	0	0	4	0
7	X	24	0	0	7	0
8	A	688	0	0	18	0
8	B	167	0	0	4	0
8	C	684	0	0	18	0
8	D	167	0	0	5	0
8	E	684	0	0	21	0
8	F	167	0	0	1	0
8	G	689	0	0	17	0
8	H	162	0	0	5	0
8	I	675	0	0	20	0
8	J	170	0	0	4	0
8	K	684	0	0	25	0
8	L	168	0	0	10	0
8	M	683	0	0	16	0
8	N	163	0	0	5	0
8	O	679	0	0	22	0
8	P	163	0	0	5	0
8	Q	692	0	0	19	0
8	R	166	0	0	2	0
8	S	675	0	0	22	0
8	T	159	0	0	4	0
8	U	667	0	0	26	0
8	V	163	0	0	5	0
8	W	677	0	0	27	0
8	X	165	0	0	12	0
All	All	122057	0	105228	3317	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 15.

The worst 5 of 3317 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:K:426:MET:HE1	1:K:618:GLN:HG2	1.33	1.10
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.30	1.10
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.19	1.09
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.37	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.36	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	875/875 (100%)	821 (94%)	49 (6%)	5 (1%)	30	34
1	C	875/875 (100%)	804 (92%)	65 (7%)	6 (1%)	26	29
1	E	875/875 (100%)	807 (92%)	61 (7%)	7 (1%)	24	26
1	G	875/875 (100%)	820 (94%)	50 (6%)	5 (1%)	30	34
1	I	875/875 (100%)	816 (93%)	54 (6%)	5 (1%)	30	34
1	K	875/875 (100%)	813 (93%)	57 (6%)	5 (1%)	30	34
1	M	875/875 (100%)	814 (93%)	57 (6%)	4 (0%)	34	39
1	O	875/875 (100%)	819 (94%)	51 (6%)	5 (1%)	30	34
1	Q	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	21	22
1	S	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	21	22
1	U	875/875 (100%)	808 (92%)	63 (7%)	4 (0%)	34	39
1	W	875/875 (100%)	803 (92%)	65 (7%)	7 (1%)	24	26
2	B	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	39	46
2	D	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	39	46
2	F	272/274 (99%)	249 (92%)	22 (8%)	1 (0%)	39	46
2	H	272/274 (99%)	255 (94%)	16 (6%)	1 (0%)	39	46
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	39	46
2	L	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	39	46
2	N	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	39	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	39	46
2	R	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	39	46
2	T	272/274 (99%)	251 (92%)	20 (7%)	1 (0%)	39	46
2	V	272/274 (99%)	257 (94%)	13 (5%)	2 (1%)	26	29
2	X	272/274 (99%)	239 (88%)	30 (11%)	3 (1%)	17	17
All	All	13764/13788 (100%)	12807 (93%)	873 (6%)	84 (1%)	30	34

5 of 84 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%)	54	68
1	C	731/729 (100%)	712 (97%)	19 (3%)	54	68
1	E	731/729 (100%)	717 (98%)	14 (2%)	65	79
1	G	731/729 (100%)	711 (97%)	20 (3%)	52	67
1	I	731/729 (100%)	711 (97%)	20 (3%)	52	67
1	K	731/729 (100%)	715 (98%)	16 (2%)	60	75
1	M	731/729 (100%)	715 (98%)	16 (2%)	60	75
1	O	731/729 (100%)	719 (98%)	12 (2%)	70	83
1	Q	731/729 (100%)	715 (98%)	16 (2%)	60	75
1	S	731/729 (100%)	715 (98%)	16 (2%)	60	75
1	U	731/729 (100%)	713 (98%)	18 (2%)	55	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	W	731/729 (100%)	717 (98%)	14 (2%)	65 79
2	B	235/235 (100%)	225 (96%)	10 (4%)	35 45
2	D	235/235 (100%)	223 (95%)	12 (5%)	29 36
2	F	235/235 (100%)	223 (95%)	12 (5%)	29 36
2	H	235/235 (100%)	221 (94%)	14 (6%)	24 28
2	J	235/235 (100%)	224 (95%)	11 (5%)	32 41
2	L	235/235 (100%)	222 (94%)	13 (6%)	27 32
2	N	235/235 (100%)	221 (94%)	14 (6%)	24 28
2	P	235/235 (100%)	226 (96%)	9 (4%)	40 52
2	R	235/235 (100%)	224 (95%)	11 (5%)	32 41
2	T	235/235 (100%)	222 (94%)	13 (6%)	27 32
2	V	235/235 (100%)	223 (95%)	12 (5%)	29 36
2	X	235/235 (100%)	221 (94%)	14 (6%)	24 28
All	All	11592/11568 (100%)	11247 (97%)	345 (3%)	50 62

5 of 345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	499	PRO
1	M	743	MET
1	W	55	ARG
1	K	560[B]	TYR
2	L	125	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	564	ASN
1	M	697	ASN
1	W	162	ASN
1	K	673	ASN
1	M	154	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 108 ligands modelled in this entry, 36 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	$\# Z > 2$
3	ACT	A	901	6	1,3,3	2.99	1 (100%)	0,3,3	0.00	-
5	MGD	A	903	6	38,52,52	2.49	13 (34%)	43,81,81	2.70	14 (32%)
5	MGD	A	904	6	38,52,52	2.63	12 (31%)	43,81,81	2.34	14 (32%)
7	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	C	901	6	1,3,3	3.32	1 (100%)	0,3,3	0.00	-
5	MGD	C	903	6	38,52,52	2.70	14 (36%)	43,81,81	2.75	14 (32%)
5	MGD	C	904	6	38,52,52	2.68	13 (34%)	43,81,81	2.25	12 (27%)
7	SF4	D	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	D	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	D	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	E	901	6	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
5	MGD	E	903	6	38,52,52	2.59	14 (36%)	43,81,81	2.68	14 (32%)
5	MGD	E	904	6	38,52,52	2.80	13 (34%)	43,81,81	2.28	13 (30%)
7	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	F	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	F	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	G	901	6	1,3,3	3.78	1 (100%)	0,3,3	0.00	-
5	MGD	G	903	6	38,52,52	2.65	14 (36%)	43,81,81	2.67	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	G	904	6	38,52,52	2.60	13 (34%)	43,81,81	2.32	11 (25%)
7	SF4	H	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	H	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	H	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	I	901	6	1,3,3	3.26	1 (100%)	0,3,3	0.00	-
5	MGD	I	903	6	38,52,52	2.74	12 (31%)	43,81,81	2.74	15 (34%)
5	MGD	I	904	6	38,52,52	2.66	14 (36%)	43,81,81	2.72	13 (30%)
7	SF4	J	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	J	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	J	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	K	901	6	1,3,3	3.96	1 (100%)	0,3,3	0.00	-
5	MGD	K	903	6	38,52,52	2.43	10 (26%)	43,81,81	2.73	14 (32%)
5	MGD	K	904	6	38,52,52	2.64	13 (34%)	43,81,81	2.28	10 (23%)
7	SF4	L	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	M	901	6	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
5	MGD	M	903	6	38,52,52	2.53	13 (34%)	43,81,81	2.72	16 (37%)
5	MGD	M	904	6	38,52,52	2.58	14 (36%)	43,81,81	2.40	13 (30%)
7	SF4	N	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	N	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	N	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	O	901	6	1,3,3	3.64	1 (100%)	0,3,3	0.00	-
5	MGD	O	903	6	38,52,52	2.64	14 (36%)	43,81,81	2.69	13 (30%)
5	MGD	O	904	6	38,52,52	2.70	13 (34%)	43,81,81	2.32	11 (25%)
7	SF4	P	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	P	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	P	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	Q	901	6	1,3,3	3.05	1 (100%)	0,3,3	0.00	-
5	MGD	Q	903	6	38,52,52	2.61	13 (34%)	43,81,81	2.72	15 (34%)
5	MGD	Q	904	6	38,52,52	2.63	13 (34%)	43,81,81	2.34	12 (27%)
7	SF4	R	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	R	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	R	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	S	901	6	1,3,3	3.92	1 (100%)	0,3,3	0.00	-
5	MGD	S	903	6	38,52,52	2.51	14 (36%)	43,81,81	2.69	14 (32%)
5	MGD	S	904	6	38,52,52	2.68	13 (34%)	43,81,81	2.27	11 (25%)
7	SF4	T	302	2	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	T	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	T	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	U	901	6	1,3,3	3.77	1 (100%)	0,3,3	0.00	-
5	MGD	U	903	6	38,52,52	2.57	13 (34%)	43,81,81	2.67	14 (32%)
5	MGD	U	904	6	38,52,52	2.75	12 (31%)	43,81,81	2.23	10 (23%)
7	SF4	V	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	V	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	V	304	2	0,12,12	0.00	-	0,24,24	0.00	-
3	ACT	W	901	6	1,3,3	4.17	1 (100%)	0,3,3	0.00	-
5	MGD	W	903	6	38,52,52	2.67	15 (39%)	43,81,81	2.65	13 (30%)
5	MGD	W	904	6	38,52,52	2.67	13 (34%)	43,81,81	2.27	12 (27%)
7	SF4	X	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	X	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	X	304	2	0,12,12	0.00	-	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
3	ACT	A	901	6	-	0/0/0/0	0/0/0/0
5	MGD	A	903	6	-	0/18/66/66	0/6/6/6
5	MGD	A	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	C	901	6	-	0/0/0/0	0/0/0/0
5	MGD	C	903	6	-	0/18/66/66	0/6/6/6
5	MGD	C	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	E	901	6	-	0/0/0/0	0/0/0/0
5	MGD	E	903	6	-	0/18/66/66	0/6/6/6
5	MGD	E	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	G	901	6	-	0/0/0/0	0/0/0/0
5	MGD	G	903	6	-	0/18/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	G	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	I	901	6	-	0/0/0/0	0/0/0/0
5	MGD	I	903	6	-	0/18/66/66	0/6/6/6
5	MGD	I	904	6	-	0/18/66/66	0/6/6/6
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
7	SF4	J	304	2	-	0/0/48/48	0/6/5/5
3	ACT	K	901	6	-	0/0/0/0	0/0/0/0
5	MGD	K	903	6	-	0/18/66/66	0/6/6/6
5	MGD	K	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	M	901	6	-	0/0/0/0	0/0/0/0
5	MGD	M	903	6	-	0/18/66/66	0/6/6/6
5	MGD	M	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	O	901	6	-	0/0/0/0	0/0/0/0
5	MGD	O	903	6	-	0/18/66/66	0/6/6/6
5	MGD	O	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	Q	901	6	-	0/0/0/0	0/0/0/0
5	MGD	Q	903	6	-	0/18/66/66	0/6/6/6
5	MGD	Q	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	S	901	6	-	0/0/0/0	0/0/0/0
5	MGD	S	903	6	-	0/18/66/66	0/6/6/6
5	MGD	S	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	U	901	6	-	0/0/0/0	0/0/0/0
5	MGD	U	903	6	-	0/18/66/66	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	U	904	6	-	0/18/66/66	0/6/6/6
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
3	ACT	W	901	6	-	0/0/0/0	0/0/0/0
5	MGD	W	903	6	-	0/18/66/66	0/6/6/6
5	MGD	W	904	6	-	0/18/66/66	0/6/6/6
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 327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	904	MGD	C2-N2	2.01	1.38	1.34
5	M	903	MGD	C2-N2	2.01	1.38	1.34
5	C	904	MGD	C4-N3	2.01	1.38	1.35
5	G	904	MGD	C23-N22	2.05	1.49	1.44
5	C	903	MGD	C2-N2	2.05	1.38	1.34

The worst 5 of 313 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	904	MGD	C5-C6-N1	-7.91	112.77	123.59
5	K	904	MGD	C5-C6-N1	-7.78	112.95	123.59
5	O	904	MGD	C5-C6-N1	-7.77	112.97	123.59
5	S	904	MGD	C5-C6-N1	-7.75	112.99	123.59
5	I	904	MGD	O11-C23-C14	-7.67	103.72	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

69 monomers are involved in 196 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ACT	1	0
5	A	903	MGD	6	0
5	A	904	MGD	5	0
7	B	303	SF4	2	0
7	B	304	SF4	1	0
3	C	901	ACT	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	903	MGD	5	0
5	C	904	MGD	5	0
7	D	302	SF4	1	0
7	D	303	SF4	2	0
7	D	304	SF4	2	0
3	E	901	ACT	2	0
5	E	903	MGD	3	0
5	E	904	MGD	3	0
7	F	303	SF4	2	0
7	F	304	SF4	1	0
3	G	901	ACT	3	0
5	G	903	MGD	5	0
5	G	904	MGD	4	0
7	H	302	SF4	1	0
7	H	303	SF4	2	0
7	H	304	SF4	2	0
3	I	901	ACT	3	0
5	I	903	MGD	4	0
5	I	904	MGD	6	0
7	J	302	SF4	1	0
7	J	303	SF4	2	0
3	K	901	ACT	4	0
5	K	903	MGD	6	0
5	K	904	MGD	3	0
7	L	302	SF4	1	0
7	L	303	SF4	2	0
7	L	304	SF4	3	0
3	M	901	ACT	1	0
5	M	903	MGD	3	0
5	M	904	MGD	6	0
7	N	302	SF4	1	0
7	N	303	SF4	2	0
7	N	304	SF4	1	0
3	O	901	ACT	2	0
5	O	903	MGD	4	0
5	O	904	MGD	5	0
7	P	302	SF4	2	0
7	P	303	SF4	2	0
7	P	304	SF4	2	0
3	Q	901	ACT	1	0
5	Q	903	MGD	4	0
5	Q	904	MGD	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	302	SF4	1	0
7	R	303	SF4	2	0
7	R	304	SF4	2	0
3	S	901	ACT	1	0
5	S	903	MGD	4	0
5	S	904	MGD	5	0
7	T	302	SF4	1	0
7	T	303	SF4	2	0
7	T	304	SF4	4	0
3	U	901	ACT	1	0
5	U	903	MGD	6	0
5	U	904	MGD	7	0
7	V	302	SF4	1	0
7	V	303	SF4	2	0
7	V	304	SF4	1	0
3	W	901	ACT	2	0
5	W	903	MGD	5	0
5	W	904	MGD	6	0
7	X	302	SF4	2	0
7	X	303	SF4	2	0
7	X	304	SF4	3	0

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 ⓘ

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.