Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:55 PM GMT

PDB ID	:	3VC1
Title	:	Crystal structure of geranyl diphosphate C-methyltransferase from Streptomyces coelicolor A3(2) in complex with Mg2+, geranyl-S-thiolodiphosphate, and S-adenosyl-L-homocysteine
Authors	:	Koksal, M.; Christianson, D.W.
Deposited on	:	2012-01-03
Resolution	:	1.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

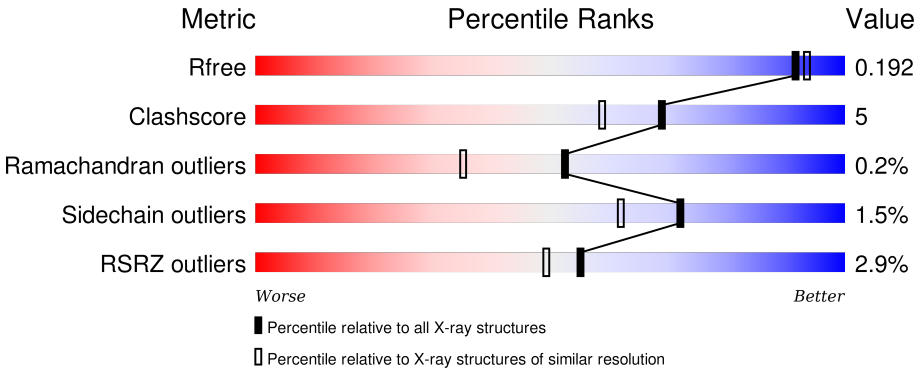
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	2% 80% 8% 11%
1	B	312	81% 8% 11%
1	C	312	% 79% 10% 11%
1	D	312	3% 83% 9% 8%
1	E	312	2% 81% 8% 11%

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Mol	Chain	Length	Quality of chain
1	F	312	8% 75% 13% • 11%
1	G	312	4% 80% 8% • 11%
1	H	312	% 81% 7% • 11%
1	I	312	3% 80% 8% • 11%
1	J	312	3% 79% 9% 12%
1	K	312	4% 80% 9% • 11%
1	L	312	2% 80% 9% 11%

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
2	MG	D	301	-	-	-	X
2	MG	G	301	-	-	-	X
5	GOL	A	304	-	-	X	X
5	GOL	B	304	-	-	-	X
5	GOL	C	304	-	-	-	X
5	GOL	C	305	-	-	-	X
5	GOL	E	305[A]	-	-	X	-
5	GOL	E	306	-	-	-	X
5	GOL	G	304	-	-	-	X
5	GOL	H	304	-	-	-	X
5	GOL	I	304	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29215 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 Geranyl diphosphate 2-C-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2209	1378	407	414	10			
1	B	278	Total	C	N	O	S	0	3	0
			2217	1383	408	416	10			
1	C	278	Total	C	N	O	S	0	3	0
			2217	1383	408	416	10			
1	D	288	Total	C	N	O	S	0	5	0
			2293	1428	423	432	10			
1	E	278	Total	C	N	O	S	0	1	0
			2214	1381	408	415	10			
1	F	278	Total	C	N	O	S	0	2	0
			2216	1383	408	415	10			
1	G	278	Total	C	N	O	S	0	4	0
			2220	1387	408	415	10			
1	H	278	Total	C	N	O	S	0	2	0
			2216	1383	408	415	10			
1	I	278	Total	C	N	O	S	0	2	0
			2219	1384	410	415	10			
1	J	276	Total	C	N	O	S	0	2	0
			2204	1375	406	413	10			
1	K	278	Total	C	N	O	S	0	3	0
			2219	1384	408	417	10			
1	L	278	Total	C	N	O	S	0	1	0
			2214	1381	408	415	10			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
A	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
A	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
A	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
A	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
A	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
A	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
A	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
A	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
A	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
A	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
A	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
A	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
A	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
A	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
A	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
A	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
A	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
A	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
B	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
B	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
B	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
B	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
B	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
B	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
B	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
B	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
B	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
B	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
B	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
B	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
B	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
B	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
C	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
C	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
C	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
C	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
C	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
C	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
C	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
C	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
C	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
C	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
C	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
C	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
C	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
C	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
D	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
D	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
D	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
D	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
D	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
D	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
D	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
D	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
D	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
D	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
D	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
D	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
D	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
D	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
E	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
E	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
E	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
E	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
E	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
E	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
E	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
E	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
E	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
E	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
E	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
E	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
E	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
E	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
F	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
F	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
F	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
F	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
F	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
F	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
F	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
F	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
F	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
F	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
F	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
F	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
F	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
F	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
G	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
G	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
G	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
G	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
G	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
G	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
G	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
G	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
G	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
G	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
G	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
G	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
G	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
H	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
H	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
H	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
H	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
H	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
H	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
H	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
H	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
H	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
H	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
H	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
H	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
H	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
H	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
I	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
I	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
I	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
I	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
I	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
I	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
I	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
I	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
I	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
I	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
I	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
I	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
I	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
J	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
J	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
J	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
J	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
J	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
J	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
J	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
J	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
J	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
J	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
J	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
J	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
J	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
J	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
K	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
K	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
K	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
K	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
K	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
K	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
K	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
K	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
L	-18	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
L	-17	SER	-	EXPRESSION TAG	UNP Q9F1Y5
L	-16	SER	-	EXPRESSION TAG	UNP Q9F1Y5
L	-15	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-14	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-13	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-12	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-11	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-10	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-9	SER	-	EXPRESSION TAG	UNP Q9F1Y5
L	-8	SER	-	EXPRESSION TAG	UNP Q9F1Y5
L	-7	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
L	-6	LEU	-	EXPRESSION TAG	UNP Q9F1Y5
L	-5	VAL	-	EXPRESSION TAG	UNP Q9F1Y5
L	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
L	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
L	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
L	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
L	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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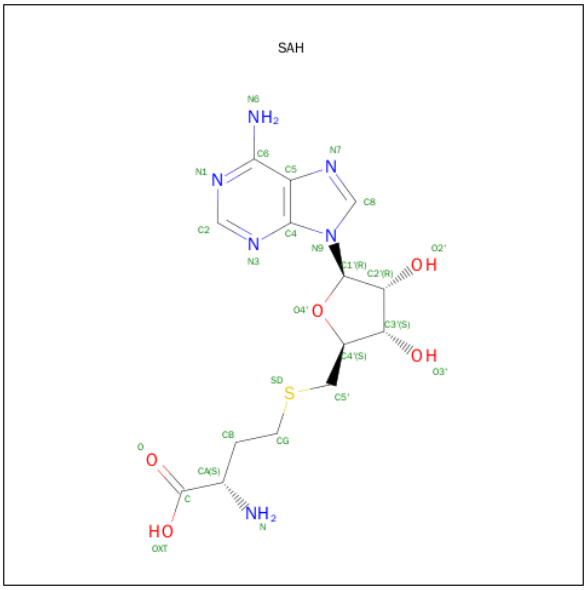
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0
3	C	1	Total C N O S 26 14 6 5 1	0	0
3	D	1	Total C N O S 26 14 6 5 1	0	0
3	E	1	Total C N O S 26 14 6 5 1	0	0
3	F	1	Total C N O S 26 14 6 5 1	0	0

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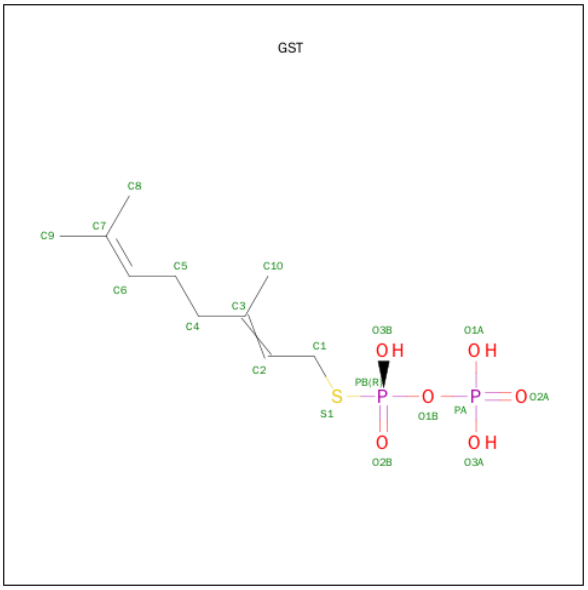
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	J	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	L	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is GERANYL S-THIOLODIPHOSPHATE (three-letter code: GST) (formula: $C_{10}H_{20}O_6P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	B	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	C	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	D	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	E	1	Total	C	O	P	S	0	0
			19	10	6	2	1		

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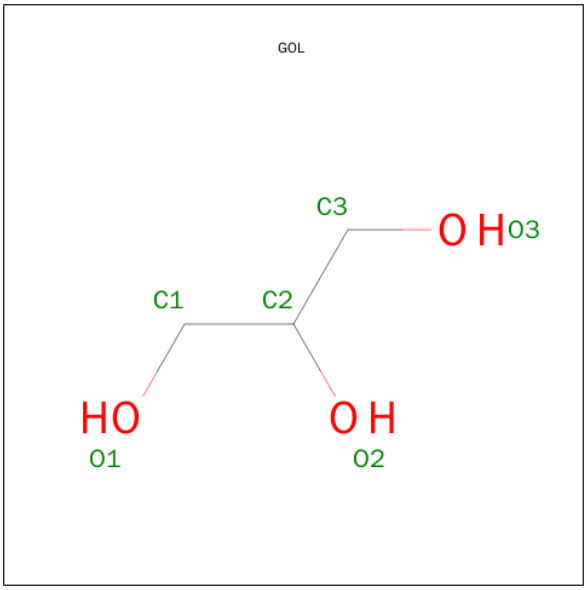
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	G	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	H	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	I	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	J	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	K	1	Total	C	O	P	S	0	0
			19	10	6	2	1		
4	L	1	Total	C	O	P	S	0	0
			19	10	6	2	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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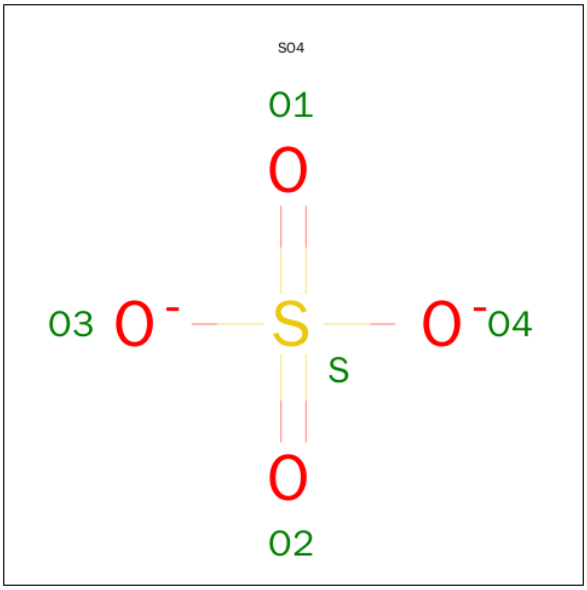
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	1
			12	6	6		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

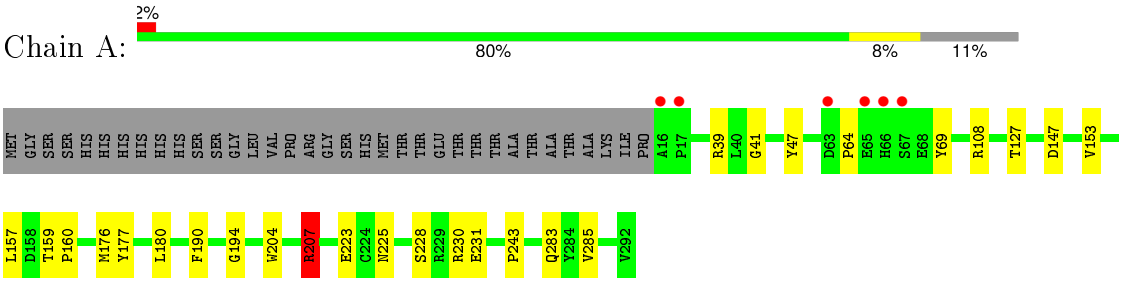
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	185	Total O 185 185	0	0
7	B	175	Total O 175 175	0	0
7	C	151	Total O 151 151	0	0
7	D	182	Total O 182 182	0	0
7	E	165	Total O 165 165	0	0
7	F	99	Total O 99 99	0	0
7	G	157	Total O 157 157	0	0
7	H	187	Total O 187 187	0	0
7	I	161	Total O 161 161	0	0
7	J	157	Total O 157 157	0	0
7	K	133	Total O 133 133	0	0
7	L	152	Total O 152 152	0	0

3 Residue-property plots (i)

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.

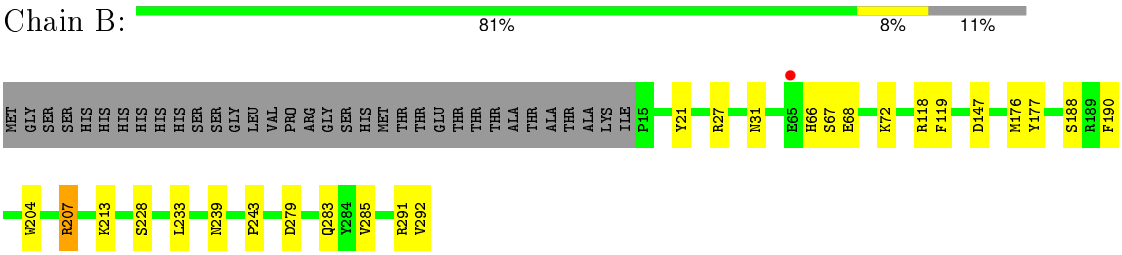
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain A:



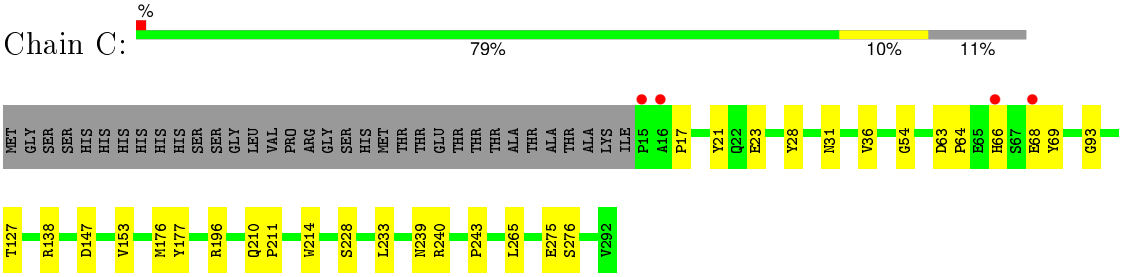
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain B:



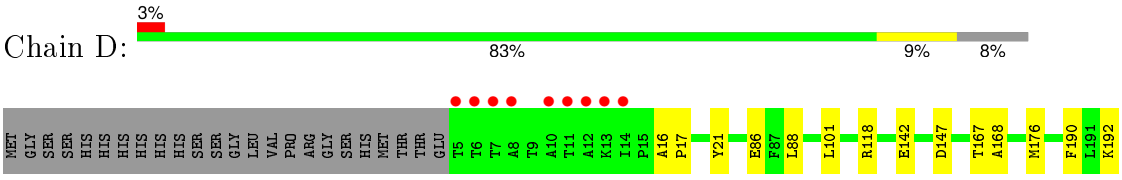
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain C:



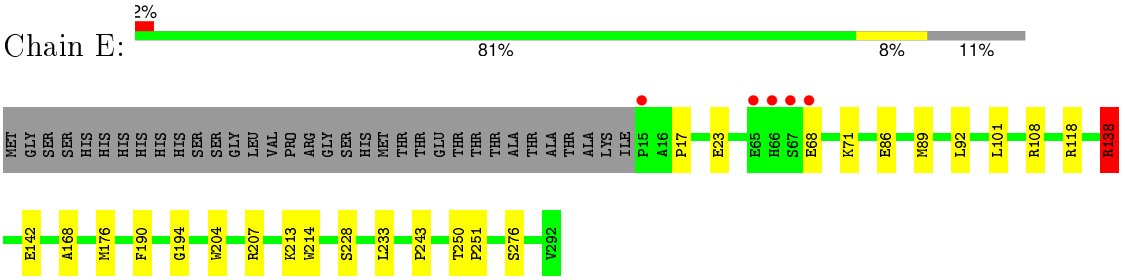
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain D:



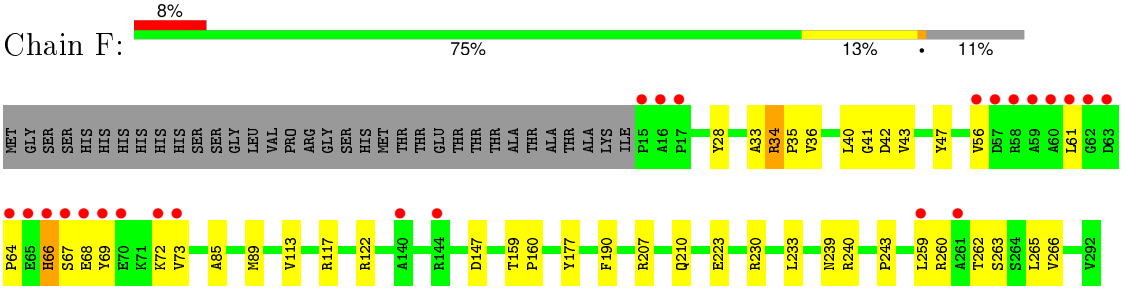
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain E:



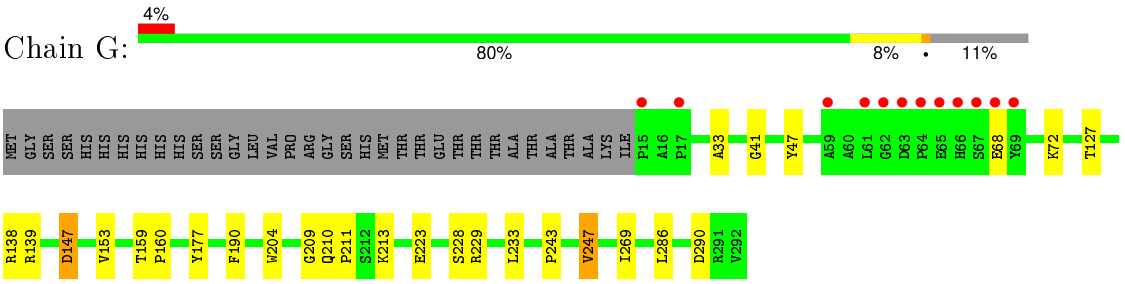
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain F:



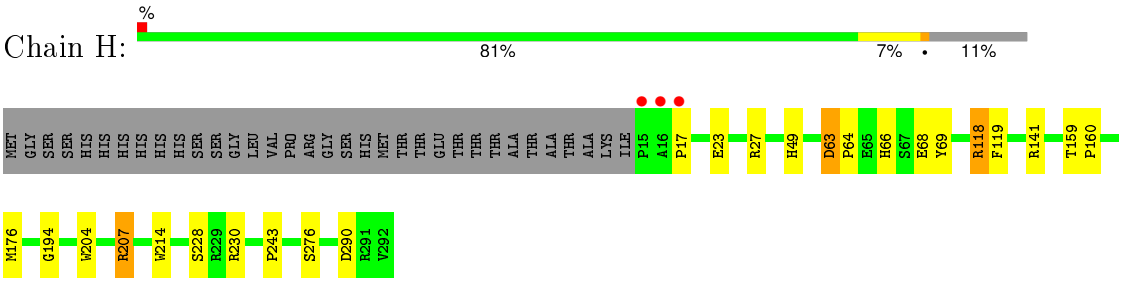
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain G:



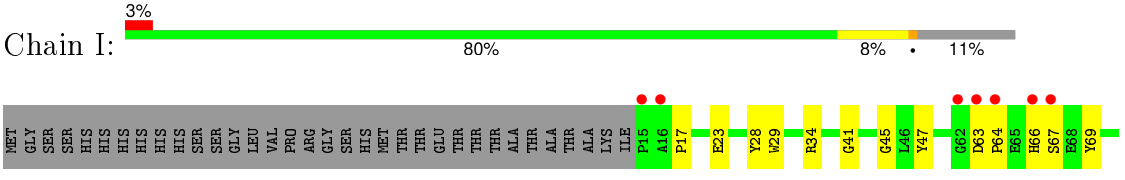
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

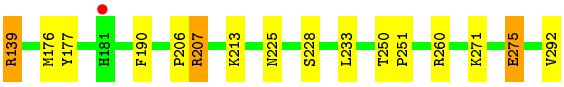
Chain H:



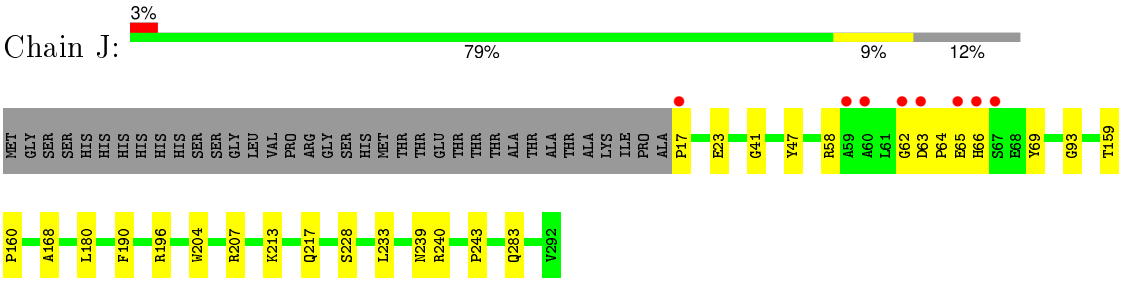
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain I:

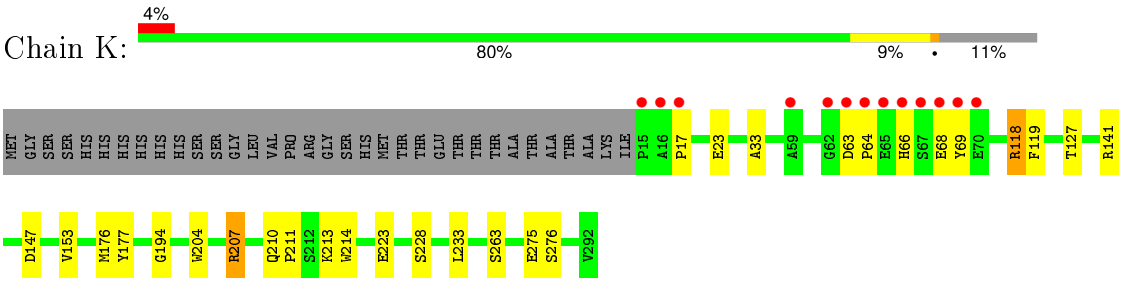




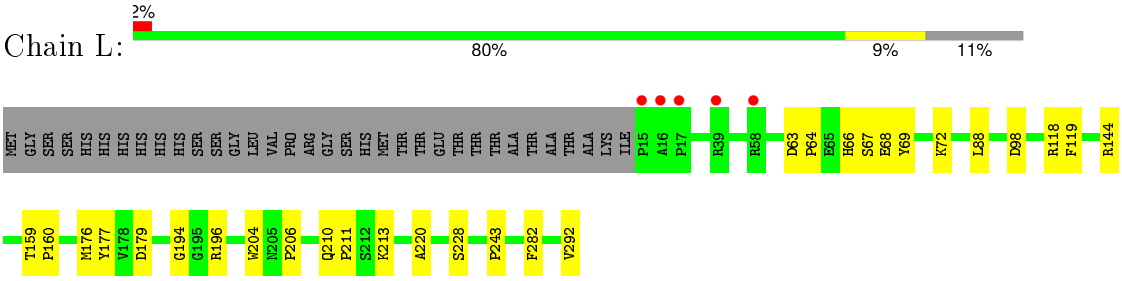
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.03Å 102.90Å 203.58Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	46.28 – 1.82 46.28 – 1.82	Depositor EDS
% Data completeness (in resolution range)	92.0 (46.28-1.82) 92.0 (46.28-1.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.167 , 0.194 0.167 , 0.192	Depositor DCC
R_{free} test set	1998 reflections (0.62%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 348782 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	29215	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SAH, GST, SO4

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	0.78	0/2269	0.82	4/3078 (0.1%)
1	B	0.80	0/2283	0.76	2/3097 (0.1%)
1	C	0.75	0/2283	0.75	1/3097 (0.0%)
1	D	0.79	0/2373	0.80	2/3220 (0.1%)
1	E	0.76	0/2270	0.74	1/3079 (0.0%)
1	F	0.63	0/2277	0.71	2/3089 (0.1%)
1	G	0.73	0/2292	0.74	1/3110 (0.0%)
1	H	0.80	0/2277	0.85	3/3089 (0.1%)
1	I	0.74	0/2281	0.78	3/3094 (0.1%)
1	J	0.77	0/2264	0.77	0/3070
1	K	0.71	0/2285	0.73	3/3100 (0.1%)
1	L	0.73	0/2270	0.74	0/3079
All	All	0.75	0/27424	0.77	22/37202 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	ARG	NE-CZ-NH1	-13.72	113.44	120.30
1	H	207	ARG	NE-CZ-NH1	-8.53	116.03	120.30
1	I	207	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	D	207	ARG	NE-CZ-NH1	-7.27	116.66	120.30
1	B	207	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	207	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	I	139	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	F	34	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	H	118	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	108	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	E	138	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	H	63	ASP	CB-CG-OD1	5.77	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	141	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	196	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	K	118	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	I	34	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	K	207	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	279	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	108	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	63	ASP	CB-CG-OD1	5.08	122.88	118.30
1	G	229	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	F	207	ARG	NE-CZ-NH1	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2102	23	0
1	B	2217	0	2113	21	0
1	C	2217	0	2113	22	0
1	D	2293	0	2187	18	0
1	E	2214	0	2107	23	0
1	F	2216	0	2112	33	0
1	G	2220	0	2118	22	0
1	H	2216	0	2112	22	0
1	I	2219	0	2110	22	0
1	J	2204	0	2098	20	0
1	K	2219	0	2112	21	0
1	L	2214	0	2107	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	F	26	0	19	1	0
3	G	26	0	19	1	0
3	H	26	0	19	1	0
3	I	26	0	19	1	0
3	J	26	0	19	0	0
3	K	26	0	19	1	0
3	L	26	0	19	0	0
4	A	19	0	17	1	0
4	B	19	0	17	2	0
4	C	19	0	17	1	0
4	D	19	0	17	1	0
4	E	19	0	17	0	0
4	F	19	0	17	1	0
4	G	19	0	17	1	0
4	H	19	0	17	0	0
4	I	19	0	17	1	0
4	J	19	0	17	0	0
4	K	19	0	17	1	0
4	L	19	0	17	2	0
5	A	18	0	24	9	0
5	B	6	0	8	0	0
5	C	12	0	16	2	0
5	D	6	0	8	0	0
5	E	18	0	24	5	0
5	F	6	0	8	1	0
5	G	6	0	8	2	0
5	H	6	0	8	1	0
5	I	6	0	7	1	0
5	J	6	0	8	1	0
5	L	6	0	8	0	0
6	E	5	0	0	0	0
7	A	185	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	175	0	0	4	0
7	C	151	0	0	2	0
7	D	182	0	0	1	0
7	E	165	0	0	5	0
7	F	99	0	0	0	0
7	G	157	0	0	0	0
7	H	187	0	0	2	0
7	I	161	0	0	1	0
7	J	157	0	0	0	0
7	K	133	0	0	1	0
7	L	152	0	0	1	0
All	All	29215	0	25950	245	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 5.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:PRO:HG2	1:C:23:GLU:HG2	1.42	1.01
1:B:243:PRO:HD2	1:E:233:LEU:HD23	1.41	1.00
1:E:138:ARG:HD2	7:H:579:HOH:O	1.74	0.86
1:C:17:PRO:CG	1:C:23:GLU:HG2	2.10	0.82
1:F:177:TYR:OH	4:F:303:GST:H101	1.85	0.76
1:F:66:HIS:CD2	1:F:68:GLU:H	2.03	0.76
1:F:66:HIS:HD2	1:F:68:GLU:H	1.31	0.76
1:A:243:PRO:HD2	1:D:233:LEU:HD22	1.68	0.75
1:B:233:LEU:HD23	1:E:243:PRO:HD2	1.69	0.75
1:I:207:ARG:NH1	1:L:194:GLY:O	2.19	0.74
1:E:207:ARG:HD3	7:E:556:HOH:O	1.88	0.72
1:H:230:ARG:HH11	5:H:304:GOL:H11	1.53	0.72
1:J:17:PRO:HG2	1:J:23:GLU:HG2	1.71	0.70
1:I:17:PRO:HG2	1:I:23:GLU:HG2	1.74	0.69
1:L:68:GLU:O	1:L:72:LYS:HG2	1.93	0.68
1:H:17:PRO:CB	1:H:23:GLU:HG2	2.25	0.67
1:F:64:PRO:HA	1:F:69:TYR:CD2	2.30	0.67
1:A:230:ARG:HH11	5:A:306:GOL:H12	1.62	0.65
1:H:17:PRO:HG2	1:H:23:GLU:HG2	1.78	0.65
1:F:61:LEU:O	1:F:72:LYS:HG3	1.99	0.62
1:A:204:TRP:CE2	1:A:228:SER:HB3	2.35	0.62
1:B:31:ASN:ND2	7:B:555:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:PRO:HB2	1:F:265:LEU:HD22	1.81	0.61
1:J:204:TRP:CE2	1:J:228:SER:HB3	2.35	0.61
1:E:101:LEU:HD22	1:E:168:ALA:HB3	1.83	0.61
1:G:213:LYS:HD2	1:L:220:ALA:O	2.01	0.60
1:E:138:ARG:HH21	5:E:305[A]:GOL:C2	2.15	0.59
1:H:17:PRO:CG	1:H:23:GLU:HG2	2.32	0.59
1:B:213:LYS:HB3	1:F:223:GLU:HG2	1.85	0.59
1:H:118:ARG:HD2	1:H:119:PHE:CZ	2.38	0.59
1:L:204:TRP:CE2	1:L:228:SER:HB3	2.38	0.58
1:G:233[B]:LEU:CD2	1:J:243:PRO:HD2	2.34	0.58
1:K:204:TRP:CE2	1:K:228:SER:HB3	2.39	0.58
1:C:17:PRO:CB	1:C:23:GLU:HG2	2.33	0.58
1:I:17:PRO:HB2	1:I:23:GLU:HG3	1.86	0.58
1:B:66:HIS:NE2	1:B:68:GLU:OE1	2.37	0.57
5:E:306:GOL:H11	7:E:420:HOH:O	2.04	0.57
1:L:64:PRO:HA	1:L:69:TYR:CD2	2.39	0.57
7:I:547:HOH:O	1:K:213:LYS:HG3	2.05	0.57
1:B:188[B]:SER:OG	1:B:239:ASN:O	2.17	0.57
1:B:243:PRO:HD2	1:E:233:LEU:CD2	2.28	0.56
1:I:225:ASN:HB2	7:K:421:HOH:O	2.06	0.56
1:A:230:ARG:HH11	5:A:306:GOL:C1	2.17	0.56
5:G:304:GOL:O3	1:L:179:ASP:HB2	2.06	0.55
1:B:207:ARG:NH1	1:E:194:GLY:O	2.37	0.55
1:F:230:ARG:HH11	5:F:304:GOL:H11	1.72	0.54
1:A:230:ARG:NH1	5:A:306:GOL:H12	2.22	0.54
1:H:290:ASP:OD1	1:K:207:ARG:HD2	2.07	0.54
1:H:141:ARG:NH2	7:H:537:HOH:O	2.40	0.54
1:K:118:ARG:HD2	1:K:119:PHE:CZ	2.42	0.54
1:J:17:PRO:CG	1:J:23:GLU:HG2	2.37	0.54
1:J:180:LEU:HB2	5:J:304:GOL:H11	1.89	0.54
1:B:27:ARG:HD3	7:B:563:HOH:O	2.08	0.54
1:A:194:GLY:O	1:D:207:ARG:NH1	2.26	0.53
1:B:204:TRP:CE2	1:B:228:SER:HB3	2.43	0.53
1:I:292:VAL:HG11	1:L:206:PRO:HB2	1.91	0.53
1:A:207:ARG:NH1	1:D:194:GLY:O	2.35	0.53
1:F:41:GLY:HA3	1:F:47:TYR:CD1	2.43	0.53
1:F:35:PRO:HB2	1:F:265:LEU:CD2	2.39	0.53
1:F:259:LEU:HD23	1:F:259:LEU:O	2.09	0.53
1:L:118:ARG:HD2	1:L:119:PHE:CZ	2.44	0.53
1:G:247[A]:VAL:CG1	1:G:286:LEU:HB3	2.38	0.53
1:L:68:GLU:HB3	1:L:72:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:TYR:OH	4:K:303:GST:H101	2.08	0.53
1:C:17:PRO:HB2	1:C:23:GLU:HG3	1.89	0.53
1:B:66:HIS:HE2	1:B:68:GLU:CD	2.12	0.53
1:G:247[A]:VAL:HG13	1:G:286:LEU:HB3	1.91	0.53
1:F:56:VAL:CG1	1:F:259:LEU:HD12	2.39	0.52
1:L:144:ARG:NH2	7:L:533:HOH:O	2.34	0.52
1:K:66:HIS:NE2	1:K:68:GLU:HB2	2.24	0.52
1:B:31:ASN:CG	7:B:555:HOH:O	2.46	0.52
1:D:86:GLU:HG3	1:D:118:ARG:HH21	1.74	0.52
1:A:204:TRP:CZ2	1:A:228:SER:HB3	2.45	0.51
1:I:17:PRO:CG	1:I:23:GLU:HG2	2.41	0.51
1:F:36:VAL:O	1:F:40:LEU:HD13	2.10	0.50
1:I:64:PRO:HA	1:I:69:TYR:CD2	2.47	0.50
1:H:64:PRO:HA	1:H:69:TYR:CD2	2.47	0.50
1:F:113:VAL:O	1:F:117:ARG:HG3	2.11	0.50
1:G:233[A]:LEU:HD13	1:J:243:PRO:HD2	1.94	0.50
1:K:66:HIS:CD2	1:K:68:GLU:H	2.30	0.50
1:L:177:TYR:OH	4:L:303:GST:H101	2.11	0.50
1:B:177:TYR:OH	4:B:303:GST:H101	2.12	0.50
1:I:213:LYS:HB3	1:K:223:GLU:HG2	1.92	0.50
1:E:250:THR:HB	1:E:251:PRO:HD3	1.93	0.50
1:F:42:ASP:O	1:F:43:VAL:C	2.49	0.50
1:E:138:ARG:NH2	5:E:305[A]:GOL:H2	2.27	0.49
1:E:17:PRO:CB	1:E:23:GLU:HG3	2.42	0.49
1:C:17:PRO:CB	1:C:23:GLU:CG	2.90	0.49
1:E:68:GLU:HG2	1:E:68:GLU:O	2.12	0.49
1:H:194:GLY:O	1:K:207:ARG:NH1	2.27	0.49
1:C:17:PRO:HB2	1:C:23:GLU:CG	2.42	0.49
1:I:233:LEU:HD13	1:L:243:PRO:HD2	1.94	0.48
1:I:177:TYR:OH	4:I:303:GST:H101	2.13	0.48
1:G:209:GLY:O	5:G:304:GOL:H31	2.13	0.48
1:I:207:ARG:NH2	1:L:196:ARG:NH2	2.61	0.48
5:A:304:GOL:C1	7:A:421:HOH:O	2.61	0.48
1:G:159:THR:HB	1:G:160:PRO:HD2	1.95	0.48
1:K:210:GLN:HB3	1:K:211:PRO:HD2	1.96	0.48
1:D:167:THR:HA	1:D:192[B]:LYS:HE2	1.94	0.48
1:A:177:TYR:OH	4:A:303:GST:H101	2.13	0.48
1:E:142:GLU:HG2	7:E:503:HOH:O	2.13	0.48
1:C:239:ASN:O	1:C:240:ARG:HB2	2.14	0.47
1:B:68:GLU:HG2	1:B:72:LYS:HE3	1.96	0.47
1:D:167:THR:HA	1:D:192[A]:LYS:HE3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:HG3	1:A:285[A]:VAL:HG13	1.96	0.47
1:B:118:ARG:HD2	1:B:119:PHE:CZ	2.50	0.47
1:F:28:TYR:OH	1:F:34:ARG:NH2	2.39	0.47
1:A:157:LEU:HD12	5:A:304:GOL:H2	1.95	0.47
1:A:283:GLN:HG3	1:A:285[B]:VAL:HG23	1.97	0.47
1:I:66:HIS:CG	1:I:67:SER:N	2.83	0.47
1:A:223:GLU:HG2	1:E:213:LYS:HB3	1.96	0.47
1:F:260:ARG:O	1:F:263:SER:HB3	2.14	0.47
1:E:138:ARG:HH21	5:E:305[A]:GOL:H2	1.80	0.47
1:F:61:LEU:HA	1:F:72:LYS:HB3	1.97	0.47
1:H:17:PRO:HB2	1:H:23:GLU:HG2	1.97	0.47
1:H:49:HIS:HB2	3:H:302:SAH:HB2	1.97	0.46
1:G:243:PRO:HD2	1:J:233:LEU:HD13	1.96	0.46
1:F:259:LEU:O	1:F:262:THR:HB	2.15	0.46
1:D:192[A]:LYS:NZ	7:D:561:HOH:O	2.38	0.46
1:G:204:TRP:CE2	1:G:228:SER:HB3	2.50	0.46
1:C:21:TYR:CD2	1:D:210:GLN:HB2	2.51	0.46
1:H:204:TRP:CE2	1:H:228:SER:HB3	2.51	0.46
1:E:86:GLU:HG3	1:E:118:ARG:HH21	1.80	0.46
3:F:302:SAH:H4'	3:F:302:SAH:HB1	1.98	0.46
1:F:122:ARG:NH1	1:F:122:ARG:HG3	2.30	0.46
1:L:159:THR:HB	1:L:160:PRO:HD2	1.97	0.46
1:J:63:ASP:C	1:J:65:GLU:H	2.19	0.46
1:J:204:TRP:CZ2	1:J:228:SER:HB3	2.51	0.46
5:A:304:GOL:C2	7:A:526:HOH:O	2.64	0.46
3:E:302:SAH:HB1	3:E:302:SAH:H4'	1.98	0.45
1:K:66:HIS:CD2	1:K:68:GLU:HB2	2.52	0.45
1:C:64:PRO:HA	1:C:69:TYR:CD2	2.52	0.45
1:C:93:GLY:HA3	1:C:196:ARG:HD2	1.97	0.45
1:J:213:LYS:HE2	1:J:217:GLN:HE21	1.82	0.45
1:L:204:TRP:CZ2	1:L:228:SER:HB3	2.51	0.45
1:G:223:GLU:CD	1:L:213:LYS:HE2	2.36	0.45
1:B:66:HIS:NE2	1:B:68:GLU:CD	2.70	0.45
1:H:159:THR:HB	1:H:160:PRO:HD2	1.97	0.45
1:G:213:LYS:HZ2	1:L:220:ALA:HB1	1.81	0.45
1:I:260:ARG:HD2	5:I:304:GOL:O2	2.17	0.45
1:H:17:PRO:HB2	1:H:23:GLU:CG	2.47	0.45
1:H:243:PRO:HD2	1:K:233:LEU:HD12	1.99	0.45
1:I:271:LYS:O	1:I:275:GLU:HB2	2.16	0.45
1:B:147:ASP:HB2	7:B:568:HOH:O	2.16	0.45
1:I:250:THR:HB	1:I:251:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:THR:HB	1:J:160:PRO:HD2	1.98	0.45
1:J:41:GLY:HA3	1:J:47:TYR:CD1	2.52	0.45
1:G:127:THR:O	1:G:153:VAL:HA	2.17	0.45
1:J:239:ASN:O	1:J:240:ARG:HB2	2.17	0.45
1:I:206:PRO:HB2	1:L:292:VAL:HG11	1.98	0.45
1:K:64:PRO:HA	1:K:69:TYR:CD2	2.52	0.45
1:A:207:ARG:CG	1:A:207:ARG:NH1	2.75	0.44
1:G:68:GLU:O	1:G:72:LYS:HG2	2.17	0.44
1:E:204:TRP:CE2	1:E:228:SER:HB3	2.52	0.44
1:A:64:PRO:HA	1:A:69:TYR:CD2	2.53	0.44
1:I:45:GLY:O	1:I:139:ARG:HD3	2.18	0.44
1:F:64:PRO:HA	1:F:69:TYR:CG	2.52	0.44
1:A:159:THR:HB	1:A:160:PRO:HD2	1.99	0.44
1:C:243:PRO:HD2	1:F:233:LEU:HD13	2.00	0.44
5:A:304:GOL:H2	7:A:526:HOH:O	2.17	0.44
5:C:305:GOL:H2	7:C:486:HOH:O	2.18	0.44
1:J:64:PRO:HA	1:J:69:TYR:CD2	2.53	0.44
1:A:127:THR:O	1:A:153:VAL:HA	2.18	0.43
1:K:214:TRP:HB2	1:K:276:SER:HB3	1.99	0.43
1:I:41:GLY:HA3	1:I:47:TYR:CD1	2.54	0.43
1:G:233[B]:LEU:HD23	1:J:243:PRO:HD2	2.00	0.43
1:K:177:TYR:CD2	3:K:302:SAH:H8	2.52	0.43
1:J:168:ALA:HA	1:J:196:ARG:O	2.19	0.43
1:G:210:GLN:HB3	1:G:211:PRO:HD2	2.01	0.43
1:F:66:HIS:CD2	1:F:67:SER:N	2.87	0.43
1:J:62:GLY:O	1:J:64:PRO:HD3	2.18	0.43
1:C:66:HIS:CD2	1:C:68:GLU:HB2	2.54	0.43
1:F:56:VAL:HG11	1:F:259:LEU:HD12	2.00	0.43
1:K:17:PRO:HG2	1:K:23:GLU:HG3	2.00	0.43
1:D:269:ILE:HA	1:D:269:ILE:HD12	1.86	0.43
1:A:231:GLU:HB3	5:A:305:GOL:O2	2.18	0.43
1:A:39:ARG:HD3	7:A:556:HOH:O	2.17	0.43
1:K:63:ASP:HA	1:K:64:PRO:HD3	1.83	0.43
1:I:28:TYR:CD2	1:I:28:TYR:C	2.92	0.43
1:F:85:ALA:O	1:F:89:MET:HG3	2.19	0.42
1:C:210:GLN:HB2	1:D:21:TYR:CD2	2.54	0.42
1:G:177:TYR:CD2	3:G:302:SAH:H8	2.54	0.42
1:F:159:THR:HB	1:F:160:PRO:HD2	2.00	0.42
1:K:204:TRP:CZ2	1:K:228:SER:HB3	2.54	0.42
1:H:63:ASP:HA	1:H:64:PRO:HD3	1.91	0.42
1:A:41:GLY:HA3	1:A:47:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:VAL:HA	1:C:265:LEU:HD13	2.01	0.42
1:C:233:LEU:HD12	1:F:243:PRO:HD2	2.00	0.42
1:D:260:ARG:O	1:D:263:SER:HB3	2.19	0.42
1:G:147:ASP:OD1	1:G:147:ASP:N	2.42	0.42
1:K:127:THR:O	1:K:153:VAL:HA	2.20	0.42
1:A:207:ARG:CG	1:A:207:ARG:HH11	2.28	0.42
1:L:66:HIS:ND1	1:L:67:SER:N	2.68	0.42
1:C:54:GLY:HA3	7:C:432:HOH:O	2.19	0.42
1:F:66:HIS:CG	1:F:67:SER:N	2.88	0.42
1:C:28:TYR:CE1	5:C:305:GOL:H31	2.54	0.42
1:B:66:HIS:CG	1:B:67:SER:N	2.87	0.42
1:A:180:LEU:HB2	5:A:305:GOL:H31	2.02	0.42
1:F:28:TYR:CD2	1:F:28:TYR:C	2.93	0.42
1:H:243:PRO:HD2	1:K:233:LEU:CD1	2.50	0.42
1:L:210:GLN:HB3	1:L:211:PRO:CD	2.50	0.42
1:C:214:TRP:HB2	1:C:276:SER:HB3	2.01	0.42
1:E:89:MET:SD	7:E:548:HOH:O	2.62	0.41
1:I:29:TRP:CD1	3:I:302:SAH:H2'	2.55	0.41
1:J:93:GLY:HA3	1:J:196:ARG:HD2	2.01	0.41
1:C:177:TYR:OH	4:C:303:GST:H101	2.19	0.41
1:I:63:ASP:HA	1:I:64:PRO:HD3	1.88	0.41
1:L:88:LEU:C	1:L:88:LEU:HD23	2.41	0.41
1:E:138:ARG:NH2	5:E:305[A]:GOL:C2	2.81	0.41
1:F:41:GLY:HA3	1:F:47:TYR:CE1	2.56	0.41
1:G:41:GLY:HA3	1:G:47:TYR:CD1	2.55	0.41
1:B:291:ARG:NH1	1:B:292:VAL:OXT	2.52	0.41
1:D:250:THR:HG23	1:D:277:TYR:CD1	2.55	0.41
1:E:92:LEU:HD22	1:E:168:ALA:HB1	2.03	0.41
1:E:17:PRO:HB2	1:E:23:GLU:HG3	2.02	0.41
1:G:177:TYR:OH	4:G:303:GST:H101	2.21	0.41
1:H:66:HIS:ND1	1:H:68:GLU:HG2	2.36	0.41
1:G:269:ILE:HA	1:G:269:ILE:HD12	1.99	0.41
4:B:303:GST:H103	4:B:303:GST:H11	1.81	0.41
1:J:58:ARG:HA	1:J:58:ARG:HD3	1.82	0.41
1:H:207:ARG:NH1	1:H:207:ARG:CG	2.82	0.41
1:L:63:ASP:OD2	1:L:64:PRO:HD2	2.20	0.41
1:I:66:HIS:ND1	1:I:67:SER:N	2.68	0.41
1:H:207:ARG:NH1	1:K:194:GLY:O	2.38	0.41
1:D:88:LEU:C	1:D:88:LEU:HD23	2.42	0.41
1:D:214:TRP:HB2	1:D:276:SER:HB3	2.03	0.41
1:G:290:ASP:CG	1:J:207:ARG:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:LYS:CD	1:L:220:ALA:O	2.68	0.41
1:F:239:ASN:O	1:F:240:ARG:HB2	2.20	0.41
1:B:21:TYR:CD2	1:F:210:GLN:HB2	2.56	0.40
1:E:108:ARG:HD2	1:E:108:ARG:HH21	1.70	0.40
1:H:214:TRP:HB2	1:H:276:SER:HB3	2.02	0.40
1:D:282:PHE:HZ	4:D:303:GST:H91	1.85	0.40
1:L:282:PHE:HZ	4:L:303:GST:H91	1.85	0.40
1:C:210:GLN:HB3	1:C:211:PRO:HD2	2.02	0.40
1:D:16:ALA:N	1:D:17:PRO:CD	2.84	0.40
1:E:214:TRP:HB2	1:E:276:SER:HB3	2.02	0.40
1:D:101:LEU:HD22	1:D:168:ALA:HB3	2.02	0.40
1:H:17:PRO:CB	1:H:23:GLU:CG	2.98	0.40
1:B:283:GLN:HG3	1:B:285[B]:VAL:HG13	2.04	0.40
1:C:147:ASP:N	1:C:147:ASP:OD1	2.51	0.40
1:A:225:ASN:HB2	7:E:520:HOH:O	2.21	0.40
1:C:127:THR:O	1:C:153:VAL:HA	2.22	0.40
1:F:69:TYR:O	1:F:73:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	276/312 (88%)	268 (97%)	8 (3%)	0	100 100
1	B	278/312 (89%)	269 (97%)	9 (3%)	0	100 100
1	C	278/312 (89%)	271 (98%)	7 (2%)	0	100 100
1	D	290/312 (93%)	281 (97%)	9 (3%)	0	100 100
1	E	276/312 (88%)	268 (97%)	8 (3%)	0	100 100
1	F	277/312 (89%)	267 (96%)	7 (2%)	3 (1%)	17 5
1	G	279/312 (89%)	270 (97%)	8 (3%)	1 (0%)	39 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	277/312 (89%)	269 (97%)	8 (3%)	0	100	100
1	I	277/312 (89%)	267 (96%)	10 (4%)	0	100	100
1	J	275/312 (88%)	263 (96%)	11 (4%)	1 (0%)	39	23
1	K	278/312 (89%)	270 (97%)	7 (2%)	1 (0%)	39	23
1	L	276/312 (88%)	266 (96%)	10 (4%)	0	100	100
All	All	3337/3744 (89%)	3229 (97%)	102 (3%)	6 (0%)	52	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	66	HIS
1	F	33	ALA
1	F	66	HIS
1	K	33	ALA
1	G	33	ALA
1	F	266	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/260 (89%)	228 (98%)	4 (2%)	68	57
1	B	234/260 (90%)	232 (99%)	2 (1%)	84	79
1	C	234/260 (90%)	229 (98%)	5 (2%)	61	47
1	D	243/260 (94%)	238 (98%)	5 (2%)	61	47
1	E	232/260 (89%)	228 (98%)	4 (2%)	68	57
1	F	233/260 (90%)	231 (99%)	2 (1%)	84	79
1	G	235/260 (90%)	229 (97%)	6 (3%)	54	37
1	H	233/260 (90%)	231 (99%)	2 (1%)	84	79
1	I	233/260 (90%)	229 (98%)	4 (2%)	68	57
1	J	232/260 (89%)	230 (99%)	2 (1%)	84	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	234/260 (90%)	229 (98%)	5 (2%)	61 47
1	L	232/260 (89%)	230 (99%)	2 (1%)	84 79
All	All	2807/3120 (90%)	2764 (98%)	43 (2%)	72 62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ASP
1	A	176	MET
1	A	190	PHE
1	A	207	ARG
1	B	176	MET
1	B	190	PHE
1	C	31	ASN
1	C	138	ARG
1	C	176	MET
1	C	228	SER
1	C	275	GLU
1	D	147	ASP
1	D	176	MET
1	D	190	PHE
1	D	207	ARG
1	D	228	SER
1	E	71	LYS
1	E	138	ARG
1	E	176	MET
1	E	190	PHE
1	F	147	ASP
1	F	190	PHE
1	G	138	ARG
1	G	139	ARG
1	G	147	ASP
1	G	190	PHE
1	G	247[A]	VAL
1	G	247[B]	VAL
1	H	27	ARG
1	H	176	MET
1	I	176	MET
1	I	190	PHE
1	I	228	SER
1	I	275	GLU

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Mol	Chain	Res	Type
1	J	190	PHE
1	J	283	GLN
1	K	147[A]	ASP
1	K	147[B]	ASP
1	K	176	MET
1	K	263	SER
1	K	275	GLU
1	L	98	ASP
1	L	176	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	GLN
1	D	94	GLN
1	E	66	HIS
1	E	94	GLN
1	F	66	HIS
1	F	221	HIS
1	G	31	ASN
1	K	66	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 12 are monoatomic - leaving 41 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	SAH	A	302	-	20,28,28	2.22	3 (15%)	19,40,40	5.22	5 (26%)
4	GST	A	303	2	13,18,18	1.16	1 (7%)	19,25,25	2.73	4 (21%)
5	GOL	A	304	-	5,5,5	0.22	0	5,5,5	0.72	0
5	GOL	A	305	-	5,5,5	0.47	0	5,5,5	0.68	0
5	GOL	A	306	-	5,5,5	0.37	0	5,5,5	0.44	0
3	SAH	B	302	-	20,28,28	2.45	4 (20%)	19,40,40	5.00	3 (15%)
4	GST	B	303	2	13,18,18	0.81	1 (7%)	19,25,25	2.59	5 (26%)
5	GOL	B	304	-	5,5,5	0.30	0	5,5,5	1.15	0
3	SAH	C	302	-	20,28,28	2.44	4 (20%)	19,40,40	4.81	4 (21%)
4	GST	C	303	2	13,18,18	1.19	1 (7%)	19,25,25	2.22	7 (36%)
5	GOL	C	304	-	5,5,5	0.50	0	5,5,5	1.54	1 (20%)
5	GOL	C	305	-	5,5,5	0.39	0	5,5,5	0.68	0
3	SAH	D	302	-	20,28,28	2.33	5 (25%)	19,40,40	4.31	5 (26%)
4	GST	D	303	2	13,18,18	0.91	1 (7%)	19,25,25	1.91	4 (21%)
5	GOL	D	304	-	5,5,5	0.42	0	5,5,5	0.61	0
3	SAH	E	302	-	20,28,28	2.68	4 (20%)	19,40,40	4.76	5 (26%)
4	GST	E	303	2	13,18,18	1.08	1 (7%)	19,25,25	2.09	5 (26%)
6	SO4	E	304	-	4,4,4	0.29	0	6,6,6	0.67	0
5	GOL	E	305[A]	-	5,5,5	0.77	0	5,5,5	0.69	0
5	GOL	E	305[B]	-	5,5,5	0.36	0	5,5,5	0.79	0
5	GOL	E	306	-	5,5,5	0.40	0	5,5,5	0.68	0
3	SAH	F	302	-	20,28,28	2.48	4 (20%)	19,40,40	4.44	5 (26%)
4	GST	F	303	2	13,18,18	0.82	1 (7%)	19,25,25	2.55	6 (31%)
5	GOL	F	304	-	5,5,5	0.53	0	5,5,5	0.18	0
3	SAH	G	302	-	20,28,28	2.44	4 (20%)	19,40,40	4.72	5 (26%)
4	GST	G	303	2	13,18,18	1.05	1 (7%)	19,25,25	1.66	4 (21%)
5	GOL	G	304	-	5,5,5	0.49	0	5,5,5	0.87	0
3	SAH	H	302	-	20,28,28	2.50	4 (20%)	19,40,40	5.06	5 (26%)
4	GST	H	303	2	13,18,18	1.14	1 (7%)	19,25,25	2.71	3 (15%)
5	GOL	H	304	-	5,5,5	0.56	0	5,5,5	0.63	0
3	SAH	I	302	-	20,28,28	2.45	4 (20%)	19,40,40	4.81	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GST	I	303	2	13,18,18	1.01	1 (7%)	19,25,25	2.26	5 (26%)
5	GOL	I	304	2	5,5,5	0.34	0	5,5,5	0.10	0
3	SAH	J	302	-	20,28,28	2.30	4 (20%)	19,40,40	5.14	4 (21%)
4	GST	J	303	2	13,18,18	0.93	1 (7%)	19,25,25	1.93	2 (10%)
5	GOL	J	304	-	5,5,5	0.43	0	5,5,5	0.89	0
3	SAH	K	302	-	20,28,28	2.40	3 (15%)	19,40,40	4.81	7 (36%)
4	GST	K	303	2	13,18,18	1.04	1 (7%)	19,25,25	2.10	4 (21%)
3	SAH	L	302	-	20,28,28	2.29	3 (15%)	19,40,40	4.86	4 (21%)
4	GST	L	303	2	13,18,18	0.81	0	19,25,25	2.80	4 (21%)
5	GOL	L	304	-	5,5,5	0.28	0	5,5,5	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	302	-	-	0/7/31/31	0/3/3/3
4	GST	A	303	2	-	0/13/19/19	0/0/0/0
5	GOL	A	304	-	-	0/4/4/4	0/0/0/0
5	GOL	A	305	-	-	0/4/4/4	0/0/0/0
5	GOL	A	306	-	-	0/4/4/4	0/0/0/0
3	SAH	B	302	-	-	0/7/31/31	0/3/3/3
4	GST	B	303	2	-	0/13/19/19	0/0/0/0
5	GOL	B	304	-	-	0/4/4/4	0/0/0/0
3	SAH	C	302	-	-	0/7/31/31	0/3/3/3
4	GST	C	303	2	-	0/13/19/19	0/0/0/0
5	GOL	C	304	-	-	0/4/4/4	0/0/0/0
5	GOL	C	305	-	-	0/4/4/4	0/0/0/0
3	SAH	D	302	-	-	0/7/31/31	0/3/3/3
4	GST	D	303	2	-	0/13/19/19	0/0/0/0
5	GOL	D	304	-	-	0/4/4/4	0/0/0/0
3	SAH	E	302	-	-	0/7/31/31	0/3/3/3
4	GST	E	303	2	-	0/13/19/19	0/0/0/0
6	SO4	E	304	-	-	0/0/0/0	0/0/0/0
5	GOL	E	305[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	E	305[B]	-	-	0/4/4/4	0/0/0/0
5	GOL	E	306	-	-	0/4/4/4	0/0/0/0
3	SAH	F	302	-	-	0/7/31/31	0/3/3/3
4	GST	F	303	2	-	0/13/19/19	0/0/0/0
5	GOL	F	304	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	G	302	-	-	0/7/31/31	0/3/3/3
4	GST	G	303	2	-	0/13/19/19	0/0/0/0
5	GOL	G	304	-	-	0/4/4/4	0/0/0/0
3	SAH	H	302	-	-	0/7/31/31	0/3/3/3
4	GST	H	303	2	-	0/13/19/19	0/0/0/0
5	GOL	H	304	-	-	0/4/4/4	0/0/0/0
3	SAH	I	302	-	-	0/7/31/31	0/3/3/3
4	GST	I	303	2	-	0/13/19/19	0/0/0/0
5	GOL	I	304	2	-	0/4/4/4	0/0/0/0
3	SAH	J	302	-	-	0/7/31/31	0/3/3/3
4	GST	J	303	2	-	0/13/19/19	0/0/0/0
5	GOL	J	304	-	-	0/4/4/4	0/0/0/0
3	SAH	K	302	-	-	0/7/31/31	0/3/3/3
4	GST	K	303	2	-	0/13/19/19	0/0/0/0
3	SAH	L	302	-	-	0/7/31/31	0/3/3/3
4	GST	L	303	2	-	0/13/19/19	0/0/0/0
5	GOL	L	304	-	-	0/4/4/4	0/0/0/0

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	GST	PB-O3B	-3.44	1.47	1.56
4	C	303	GST	PB-O3B	-3.42	1.47	1.56
4	H	303	GST	PB-O3B	-3.13	1.48	1.56
4	K	303	GST	PB-O3B	-3.01	1.48	1.56
4	E	303	GST	PB-O3B	-2.75	1.49	1.56
4	G	303	GST	PB-O3B	-2.62	1.49	1.56
4	J	303	GST	PB-O3B	-2.48	1.50	1.56
4	I	303	GST	PB-O3B	-2.40	1.50	1.56
4	D	303	GST	PB-O3B	-2.23	1.50	1.56
4	F	303	GST	PB-O3B	-2.15	1.51	1.56
3	D	302	SAH	C5'-SD	-2.15	1.77	1.81
4	B	303	GST	PB-O3B	-2.02	1.51	1.56
3	D	302	SAH	C5-C4	2.02	1.45	1.40
3	H	302	SAH	C5-C4	2.03	1.45	1.40
3	B	302	SAH	O4'-C1'	2.09	1.43	1.41
3	G	302	SAH	C5-C4	2.37	1.45	1.40
3	C	302	SAH	C5-C4	2.79	1.46	1.40
3	D	302	SAH	C6-N6	2.94	1.44	1.34
3	J	302	SAH	C5-C4	2.94	1.47	1.40
3	E	302	SAH	C5-C4	2.98	1.47	1.40
3	F	302	SAH	C5-C4	3.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	SAH	C6-N6	3.12	1.44	1.34
3	I	302	SAH	C5-C4	3.15	1.47	1.40
3	B	302	SAH	C6-N6	3.41	1.45	1.34
3	A	302	SAH	C6-N6	3.58	1.46	1.34
3	K	302	SAH	C6-N6	3.69	1.46	1.34
3	J	302	SAH	C6-N6	3.70	1.46	1.34
3	G	302	SAH	C6-N6	3.75	1.46	1.34
3	C	302	SAH	C6-N6	3.87	1.46	1.34
3	F	302	SAH	C6-N6	3.92	1.47	1.34
3	H	302	SAH	C6-N6	3.96	1.47	1.34
3	I	302	SAH	C6-N6	4.17	1.47	1.34
3	E	302	SAH	C6-N6	4.51	1.48	1.34
3	L	302	SAH	C2-N1	5.34	1.44	1.33
3	G	302	SAH	C2-N1	5.34	1.44	1.33
3	C	302	SAH	C2-N1	5.46	1.44	1.33
3	D	302	SAH	C2-N1	5.62	1.44	1.33
3	H	302	SAH	C2-N1	5.66	1.44	1.33
3	B	302	SAH	C2-N1	5.82	1.45	1.33
3	J	302	SAH	C2-N1	5.93	1.45	1.33
3	A	302	SAH	C2-N1	5.95	1.45	1.33
3	I	302	SAH	C2-N1	6.03	1.45	1.33
3	E	302	SAH	C2-N1	6.09	1.45	1.33
3	A	302	SAH	C2-N3	6.23	1.43	1.32
3	F	302	SAH	C2-N1	6.27	1.45	1.33
3	K	302	SAH	C2-N1	6.27	1.45	1.33
3	J	302	SAH	C2-N3	6.34	1.43	1.32
3	C	302	SAH	C2-N3	6.99	1.44	1.32
3	K	302	SAH	C2-N3	7.05	1.44	1.32
3	I	302	SAH	C2-N3	7.05	1.44	1.32
3	D	302	SAH	C2-N3	7.06	1.44	1.32
3	F	302	SAH	C2-N3	7.33	1.45	1.32
3	L	302	SAH	C2-N3	7.36	1.45	1.32
3	B	302	SAH	C2-N3	7.47	1.45	1.32
3	G	302	SAH	C2-N3	7.64	1.45	1.32
3	H	302	SAH	C2-N3	7.94	1.46	1.32
3	E	302	SAH	C2-N3	8.29	1.46	1.32

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	SAH	N3-C2-N1	-21.57	112.38	128.89
3	J	302	SAH	N3-C2-N1	-21.12	112.72	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	SAH	N3-C2-N1	-20.89	112.90	128.89
3	H	302	SAH	N3-C2-N1	-20.15	113.47	128.89
3	L	302	SAH	N3-C2-N1	-19.95	113.62	128.89
3	I	302	SAH	N3-C2-N1	-19.87	113.68	128.89
3	E	302	SAH	N3-C2-N1	-19.78	113.75	128.89
3	C	302	SAH	N3-C2-N1	-19.67	113.83	128.89
3	K	302	SAH	N3-C2-N1	-19.58	113.90	128.89
3	G	302	SAH	N3-C2-N1	-19.44	114.01	128.89
3	F	302	SAH	N3-C2-N1	-18.06	115.07	128.89
3	D	302	SAH	N3-C2-N1	-17.65	115.38	128.89
4	L	303	GST	C1-C2-C3	-10.15	114.20	127.83
4	H	303	GST	C1-C2-C3	-9.98	114.42	127.83
4	A	303	GST	C1-C2-C3	-9.34	115.28	127.83
4	B	303	GST	C1-C2-C3	-9.10	115.61	127.83
4	F	303	GST	C1-C2-C3	-7.75	117.42	127.83
4	K	303	GST	C1-C2-C3	-7.13	118.26	127.83
4	I	303	GST	C1-C2-C3	-6.78	118.72	127.83
4	C	303	GST	C1-C2-C3	-6.74	118.77	127.83
4	J	303	GST	C1-C2-C3	-6.66	118.88	127.83
4	D	303	GST	C1-C2-C3	-6.31	119.36	127.83
4	E	303	GST	C1-C2-C3	-5.76	120.09	127.83
4	G	303	GST	C1-C2-C3	-5.12	120.96	127.83
3	H	302	SAH	CB-CG-SD	-4.91	104.10	113.57
3	K	302	SAH	C1'-N9-C4	-4.34	120.39	126.94
3	B	302	SAH	C1'-N9-C4	-4.13	120.72	126.94
3	J	302	SAH	C1'-N9-C4	-3.88	121.09	126.94
4	A	303	GST	C10-C3-C2	-3.83	115.98	123.50
3	C	302	SAH	C1'-N9-C4	-3.83	121.17	126.94
3	H	302	SAH	C1'-N9-C4	-3.77	121.26	126.94
3	L	302	SAH	C1'-N9-C4	-3.74	121.29	126.94
3	I	302	SAH	C1'-N9-C4	-3.72	121.33	126.94
4	L	303	GST	C10-C3-C2	-3.71	116.22	123.50
3	A	302	SAH	CB-CG-SD	-3.68	106.48	113.57
3	D	302	SAH	C1'-N9-C4	-3.55	121.58	126.94
3	A	302	SAH	C1'-N9-C4	-3.53	121.62	126.94
3	G	302	SAH	C1'-N9-C4	-3.46	121.72	126.94
3	F	302	SAH	CB-CG-SD	-3.41	107.00	113.57
4	C	303	GST	C10-C3-C2	-3.39	116.84	123.50
4	B	303	GST	C10-C3-C2	-3.38	116.86	123.50
3	E	302	SAH	C1'-N9-C4	-3.22	122.08	126.94
5	C	304	GOL	C3-C2-C1	-3.21	98.53	111.12
4	F	303	GST	C10-C3-C2	-3.17	117.29	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	302	SAH	C1'-N9-C4	-3.14	122.21	126.94
3	J	302	SAH	CB-CG-SD	-3.13	107.53	113.57
3	I	302	SAH	C4'-O4'-C1'	-2.98	106.45	109.72
4	H	303	GST	C10-C3-C2	-2.88	117.84	123.50
3	H	302	SAH	C4'-O4'-C1'	-2.81	106.63	109.72
4	L	303	GST	C5-C6-C7	-2.70	117.35	127.73
3	L	302	SAH	CB-CG-SD	-2.66	108.45	113.57
3	E	302	SAH	C4-C5-N7	-2.62	107.07	109.48
3	C	302	SAH	CB-CG-SD	-2.56	108.64	113.57
3	K	302	SAH	CB-CG-SD	-2.55	108.66	113.57
4	E	303	GST	C10-C3-C2	-2.41	118.76	123.50
3	F	302	SAH	C4-C5-N7	-2.37	107.30	109.48
4	K	303	GST	C10-C3-C2	-2.31	118.97	123.50
3	G	302	SAH	C4-C5-N7	-2.25	107.41	109.48
3	D	302	SAH	CB-CG-SD	-2.21	109.32	113.57
3	A	302	SAH	O3'-C3'-C2'	-2.17	104.78	111.83
4	C	303	GST	C5-C6-C7	-2.10	119.64	127.73
3	G	302	SAH	CB-CG-SD	-2.10	109.52	113.57
3	D	302	SAH	C4'-O4'-C1'	-2.08	107.43	109.72
3	K	302	SAH	C4'-O4'-C1'	-2.05	107.47	109.72
3	K	302	SAH	O3'-C3'-C2'	-2.05	105.17	111.83
4	K	303	GST	O3B-PB-O2B	2.07	115.21	110.05
3	E	302	SAH	C5'-SD-CG	2.09	108.67	102.41
4	G	303	GST	O3B-PB-O1B	2.10	114.55	104.88
4	I	303	GST	C4-C3-C2	2.12	125.07	121.05
4	C	303	GST	O3B-PB-O1B	2.15	114.80	104.88
4	E	303	GST	O3A-PA-O1A	2.15	115.58	107.38
4	I	303	GST	O3A-PA-O2A	2.16	117.53	110.58
4	J	303	GST	O3B-PB-O2B	2.16	115.44	110.05
4	G	303	GST	O1A-PA-O2A	2.24	117.79	110.58
4	D	303	GST	O3B-PB-O2B	2.24	115.65	110.05
4	D	303	GST	C8-C7-C9	2.28	120.24	114.64
4	G	303	GST	O3B-PB-O2B	2.30	115.79	110.05
4	C	303	GST	C4-C3-C2	2.31	125.43	121.05
4	F	303	GST	O3A-PA-O1A	2.33	116.26	107.38
4	K	303	GST	C10-C3-C4	2.34	118.98	115.41
4	D	303	GST	O3A-PA-O1A	2.35	116.33	107.38
4	C	303	GST	C8-C7-C9	2.41	120.56	114.64
4	B	303	GST	O3B-PB-O2B	2.43	116.11	110.05
4	B	303	GST	C10-C3-C4	2.43	119.12	115.41
4	B	303	GST	O3B-PB-O1B	2.46	116.23	104.88
3	K	302	SAH	C5'-SD-CG	2.57	110.11	102.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	302	SAH	C2-N1-C6	2.57	123.36	118.77
4	E	303	GST	O3B-PB-O1B	2.58	116.77	104.88
4	C	303	GST	O3B-PB-O2B	2.69	116.76	110.05
3	F	302	SAH	C2-N1-C6	2.70	123.59	118.77
4	I	303	GST	O3A-PA-O1A	2.79	118.02	107.38
4	H	303	GST	O3B-PB-O1B	2.81	117.86	104.88
4	A	303	GST	C10-C3-C4	2.86	119.78	115.41
4	L	303	GST	C4-C3-C2	2.88	126.51	121.05
3	E	302	SAH	C2-N1-C6	3.02	124.17	118.77
3	B	302	SAH	C2-N1-C6	3.26	124.58	118.77
3	A	302	SAH	C2-N1-C6	3.27	124.61	118.77
4	F	303	GST	O1A-PA-O2A	3.27	121.12	110.58
3	D	302	SAH	C2-N1-C6	3.41	124.85	118.77
3	L	302	SAH	C2-N1-C6	3.41	124.87	118.77
4	F	303	GST	O3B-PB-O2B	3.44	118.62	110.05
4	A	303	GST	O3B-PB-O2B	3.61	119.05	110.05
4	F	303	GST	C10-C3-C4	3.65	120.98	115.41
3	C	302	SAH	C2-N1-C6	3.81	125.57	118.77
3	I	302	SAH	C2-N1-C6	3.86	125.66	118.77
4	I	303	GST	O3B-PB-O2B	4.09	120.26	110.05
3	G	302	SAH	C2-N1-C6	4.28	126.42	118.77
3	J	302	SAH	C2-N1-C6	4.43	126.68	118.77
3	H	302	SAH	C2-N1-C6	4.53	126.85	118.77
4	E	303	GST	O3B-PB-O2B	4.62	121.59	110.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GST	1	0
5	A	304	GOL	4	0
5	A	305	GOL	2	0
5	A	306	GOL	3	0
4	B	303	GST	2	0
4	C	303	GST	1	0
5	C	305	GOL	2	0
4	D	303	GST	1	0
3	E	302	SAH	1	0
5	E	305[A]	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	306	GOL	1	0
3	F	302	SAH	1	0
4	F	303	GST	1	0
5	F	304	GOL	1	0
3	G	302	SAH	1	0
4	G	303	GST	1	0
5	G	304	GOL	2	0
3	H	302	SAH	1	0
5	H	304	GOL	1	0
3	I	302	SAH	1	0
4	I	303	GST	1	0
5	I	304	GOL	1	0
5	J	304	GOL	1	0
3	K	302	SAH	1	0
4	K	303	GST	1	0
4	L	303	GST	2	0

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	277/312 (88%)	-0.41	6 (2%)	65	60	15, 21, 37, 55	1 (0%)
1	B	278/312 (89%)	-0.60	1 (0%)	93	91	17, 22, 37, 56	1 (0%)
1	C	278/312 (89%)	-0.44	4 (1%)	78	74	17, 22, 35, 56	1 (0%)
1	D	288/312 (92%)	-0.51	9 (3%)	52	47	16, 21, 43, 61	1 (0%)
1	E	278/312 (89%)	-0.33	5 (1%)	71	67	16, 23, 43, 63	1 (0%)
1	F	278/312 (89%)	0.14	24 (8%)	13	10	19, 31, 59, 92	1 (0%)
1	G	278/312 (89%)	-0.21	12 (4%)	39	32	17, 23, 43, 73	2 (0%)
1	H	278/312 (89%)	-0.66	3 (1%)	82	80	16, 21, 31, 57	2 (0%)
1	I	278/312 (89%)	-0.32	8 (2%)	55	49	17, 22, 45, 71	1 (0%)
1	J	276/312 (88%)	-0.27	8 (2%)	55	49	16, 22, 48, 76	1 (0%)
1	K	278/312 (89%)	-0.27	13 (4%)	35	29	17, 24, 47, 72	1 (0%)
1	L	278/312 (89%)	-0.48	5 (1%)	71	67	17, 24, 43, 69	2 (0%)
All	All	3343/3744 (89%)	-0.36	98 (2%)	55	49	15, 22, 44, 92	15 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	66	HIS	6.9
1	F	62	GLY	6.7
1	J	63	ASP	5.9
1	F	65	GLU	5.9
1	F	63	ASP	5.4
1	F	64	PRO	5.3
1	J	17	PRO	5.1
1	G	65	GLU	5.0
1	G	63	ASP	4.9
1	F	61	LEU	4.8
1	D	14	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	62	GLY	4.4
1	K	65	GLU	4.4
1	D	7	THR	4.4
1	F	15	PRO	4.4
1	J	66	HIS	4.4
1	F	69	TYR	4.1
1	J	62	GLY	4.1
1	F	68	GLU	4.0
1	H	15	PRO	4.0
1	D	12	ALA	4.0
1	F	60	ALA	4.0
1	K	66	HIS	4.0
1	F	72	LYS	3.8
1	G	67	SER	3.8
1	K	67	SER	3.7
1	G	66	HIS	3.7
1	K	63	ASP	3.6
1	K	62	GLY	3.5
1	F	59	ALA	3.5
1	K	68	GLU	3.5
1	F	144	ARG	3.5
1	J	67	SER	3.4
1	K	15	PRO	3.4
1	K	16	ALA	3.3
1	A	16	ALA	3.3
1	A	65	GLU	3.3
1	D	5	THR	3.3
1	C	15	PRO	3.2
1	A	66	HIS	3.1
1	D	6	THR	3.1
1	F	16	ALA	3.1
1	H	17	PRO	3.0
1	F	67	SER	3.0
1	K	59	ALA	3.0
1	F	56	VAL	3.0
1	L	15	PRO	3.0
1	G	61	LEU	3.0
1	C	16	ALA	2.9
1	K	17	PRO	2.9
1	G	64	PRO	2.9
1	J	59	ALA	2.9
1	A	17	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	16	ALA	2.8
1	E	67	SER	2.7
1	F	58	ARG	2.7
1	G	17	PRO	2.7
1	I	64	PRO	2.6
1	F	17	PRO	2.5
1	I	15	PRO	2.5
1	L	16	ALA	2.5
1	B	65	GLU	2.5
1	F	57	ASP	2.5
1	G	15	PRO	2.5
1	K	69	TYR	2.5
1	F	259	LEU	2.5
1	E	68	GLU	2.5
1	G	68	GLU	2.5
1	E	15	PRO	2.5
1	I	66	HIS	2.4
1	K	64	PRO	2.4
1	J	60	ALA	2.4
1	G	59	ALA	2.3
1	D	8	ALA	2.3
1	I	16	ALA	2.3
1	D	11	THR	2.3
1	E	66	HIS	2.3
1	L	58	ARG	2.3
1	A	67	SER	2.2
1	D	13	LYS	2.2
1	F	140	ALA	2.2
1	A	63	ASP	2.2
1	I	67	SER	2.2
1	I	62	GLY	2.2
1	I	181[A]	HIS	2.2
1	D	10	ALA	2.2
1	L	17	PRO	2.2
1	G	69	TYR	2.2
1	J	65	GLU	2.2
1	F	73	VAL	2.2
1	E	65	GLU	2.1
1	I	63	ASP	2.1
1	C	66	HIS	2.1
1	K	70	GLU	2.1
1	L	39	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	GLU	2.0
1	F	261	ALA	2.0
1	F	70	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	GOL	C	304	6/6	0.87	0.18	11.11	29,31,36,37	0
5	GOL	A	304	6/6	0.96	0.21	8.16	28,32,34,40	0
5	GOL	I	304	6/6	0.95	0.16	4.68	20,27,28,31	0
5	GOL	C	305	6/6	0.96	0.13	4.36	25,36,38,39	0
5	GOL	E	306	6/6	0.88	0.13	3.68	31,34,38,43	0
2	MG	G	301	1/1	0.98	0.09	3.03	23,23,23,23	0
2	MG	D	301	1/1	0.99	0.07	2.77	16,16,16,16	0
5	GOL	B	304	6/6	0.92	0.14	2.71	34,36,38,41	0
5	GOL	G	304	6/6	0.85	0.15	2.32	27,40,41,42	0
5	GOL	H	304	6/6	0.94	0.11	2.12	32,34,36,37	0
5	GOL	J	304	6/6	0.89	0.15	1.98	24,29,33,40	0
5	GOL	A	305	6/6	0.91	0.14	1.40	23,28,34,42	0
5	GOL	D	304	6/6	0.91	0.11	1.37	30,33,34,39	0
5	GOL	E	305[A]	6/6	0.89	0.15	1.31	23,29,30,30	6
5	GOL	E	305[B]	6/6	0.89	0.15	1.26	27,28,30,32	6
5	GOL	F	304	6/6	0.88	0.12	1.02	34,35,36,40	0
3	SAH	J	302	26/26	0.98	0.11	0.92	15,17,19,21	0
2	MG	H	301	1/1	0.99	0.07	0.88	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	I	301	1/1	0.98	0.10	0.64	22,22,22,22	0
3	SAH	G	302	26/26	0.98	0.08	0.49	15,20,22,22	0
3	SAH	I	302	26/26	0.98	0.10	0.31	16,18,20,21	0
4	GST	E	303	19/19	0.99	0.08	0.28	18,22,25,29	0
2	MG	F	301	1/1	0.94	0.09	0.23	35,35,35,35	0
3	SAH	C	302	26/26	0.97	0.09	0.23	16,18,20,21	0
3	SAH	L	302	26/26	0.98	0.07	0.17	17,20,21,23	0
4	GST	C	303	19/19	0.98	0.08	0.06	20,26,30,30	0
4	GST	G	303	19/19	0.99	0.09	0.02	20,24,27,29	0
4	GST	J	303	19/19	0.99	0.08	0.02	18,22,26,28	0
3	SAH	E	302	26/26	0.98	0.09	-0.09	17,19,21,22	0
5	GOL	A	306	6/6	0.94	0.10	-0.10	32,34,35,36	0
3	SAH	B	302	26/26	0.97	0.06	-0.12	16,19,21,22	0
4	GST	A	303	19/19	0.99	0.07	-0.13	17,22,27,29	0
3	SAH	A	302	26/26	0.98	0.06	-0.17	16,18,20,20	0
4	GST	B	303	19/19	0.98	0.07	-0.24	18,24,28,32	0
4	GST	I	303	19/19	0.99	0.08	-0.24	18,23,27,27	0
5	GOL	L	304	6/6	0.95	0.09	-0.39	25,29,34,38	0
4	GST	F	303	19/19	0.97	0.08	-0.52	24,32,35,37	0
4	GST	D	303	19/19	0.99	0.06	-0.53	18,21,26,28	0
4	GST	H	303	19/19	0.99	0.06	-0.53	18,21,29,29	0
6	SO4	E	304	5/5	0.99	0.07	-0.68	24,26,28,28	0
4	GST	K	303	19/19	0.98	0.06	-0.70	24,27,30,34	0
2	MG	A	301	1/1	0.99	0.06	-0.70	19,19,19,19	0
3	SAH	F	302	26/26	0.96	0.07	-0.71	24,27,29,31	0
3	SAH	K	302	26/26	0.98	0.06	-0.84	19,22,23,25	0
4	GST	L	303	19/19	0.98	0.06	-0.88	21,24,28,31	0
3	SAH	D	302	26/26	0.98	0.05	-0.92	14,17,19,19	0
2	MG	E	301	1/1	0.98	0.06	-1.20	20,20,20,20	0
3	SAH	H	302	26/26	0.98	0.06	-1.20	15,17,19,20	0
2	MG	B	301	1/1	0.98	0.04	-1.27	21,21,21,21	0
2	MG	C	301	1/1	0.96	0.05	-1.48	26,26,26,26	0
2	MG	K	301	1/1	0.97	0.03	-1.94	26,26,26,26	0
2	MG	L	301	1/1	1.00	0.05	-2.96	20,20,20,20	0
2	MG	J	301	1/1	0.98	0.04	-3.20	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.