Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:57 PM GMT

PDB ID	:	3VC2
Title	:	Crystal structure of geranyl diphosphate C-methyltransferase from Streptomyces coelicolor A3(2) in complex with Mg2+, geranyl diphosphate, and S-adenosyl-L-homocysteine
Authors	:	Koksal, M.; Christianson, D.W.
Deposited on	:	2012-01-03
Resolution	:	2.05 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:

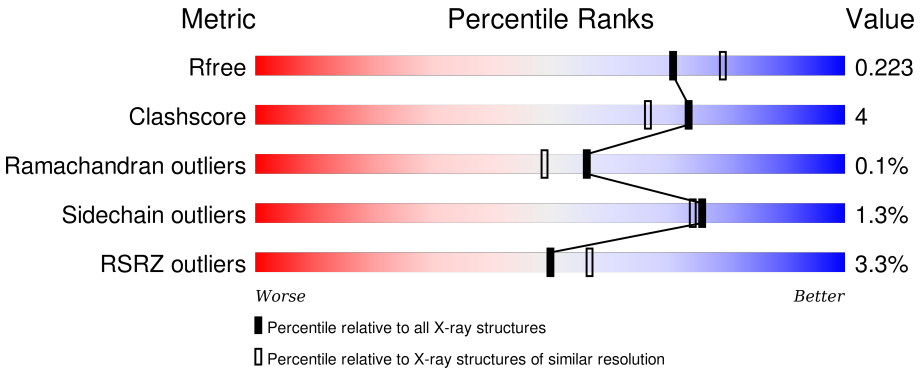
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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% 83% 5% 11%
1	B	312	2% 79% 6% 14%
1	C	312	% 79% 6% 14%
1	D	312	2% 85% 7% 8%
1	E	312	% 79% 10% 11%

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Mol	Chain	Length	Quality of chain
1	F	312	7% 75% 12% 13%
1	G	312	4% 80% 9% 11%
1	H	312	% 77% 12% 11%
1	I	312	2% 75% 13% 12%
1	J	312	2% 83% 5% 12%
1	K	312	7% 75% 9% 16%
1	L	312	4% 75% 11% 14%

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
4	GPP	A	303	-	-	X	X
4	GPP	D	303	-	-	-	X
4	GPP	H	303	-	-	X	X
5	SO4	E	302	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27843 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
			2212	1379	409	414	10			
1	B	267	Total	C	N	O	S	0	2	0
			2135	1332	392	401	10			
1	C	267	Total	C	N	O	S	0	2	0
			2135	1332	392	401	10			
1	D	288	Total	C	N	O	S	0	3	0
			2288	1427	421	430	10			
1	E	277	Total	C	N	O	S	0	3	0
			2217	1381	412	414	10			
1	F	273	Total	C	N	O	S	0	3	0
			2180	1360	401	409	10			
1	G	278	Total	C	N	O	S	0	4	0
			2222	1386	410	416	10			
1	H	277	Total	C	N	O	S	0	3	0
			2214	1381	409	414	10			
1	I	276	Total	C	N	O	S	0	2	0
			2207	1376	408	413	10			
1	J	275	Total	C	N	O	S	0	3	0
			2202	1373	407	412	10			
1	K	263	Total	C	N	O	S	0	4	0
			2114	1320	388	396	10			
1	L	269	Total	C	N	O	S	0	4	0
			2155	1343	394	408	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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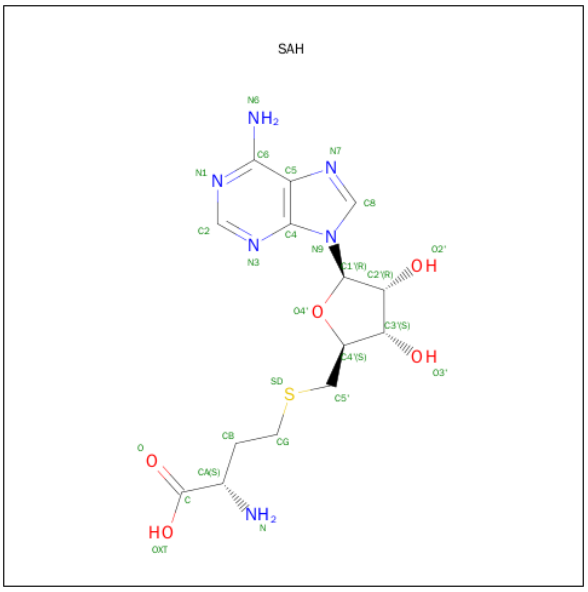
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	EXPRESSION TAG	UNP Q9F1Y5
K	-3	ARG	-	EXPRESSION TAG	UNP Q9F1Y5
K	-2	GLY	-	EXPRESSION TAG	UNP Q9F1Y5
K	-1	SER	-	EXPRESSION TAG	UNP Q9F1Y5
K	0	HIS	-	EXPRESSION TAG	UNP Q9F1Y5
L	-19	MET	-	EXPRESSION TAG	UNP Q9F1Y5
L	-18	GLY	-	EXPRESSION TAG	UNP 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).

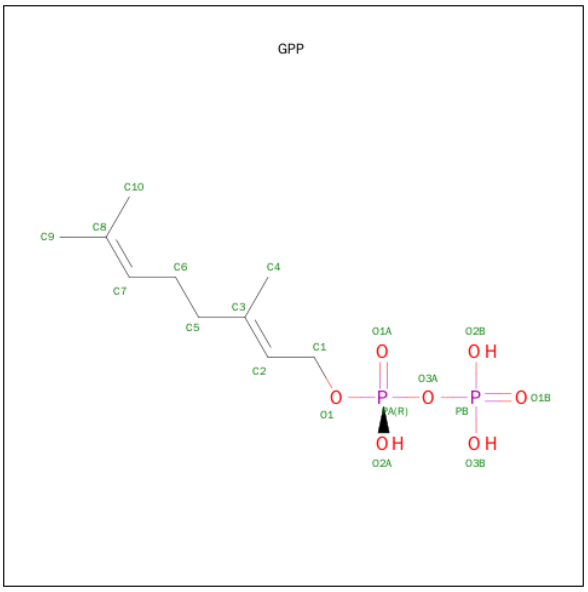
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

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



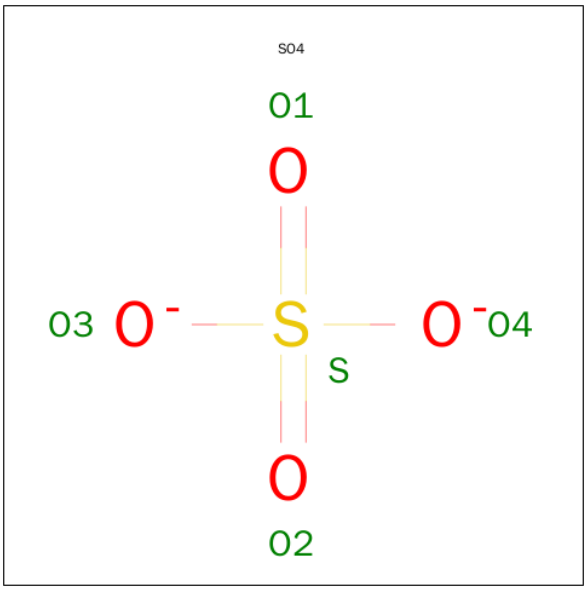
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	G	1	Total	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 DIPHOSPHATE (three-letter code: GPP) (formula: $C_{10}H_{20}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			19	10	7	2		
4	D	1	Total	C	O	P	0	0
			19	10	7	2		
4	H	1	Total	C	O	P	0	0
			19	10	7	2		
4	J	1	Total	C	O	P	0	0
			19	10	7	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

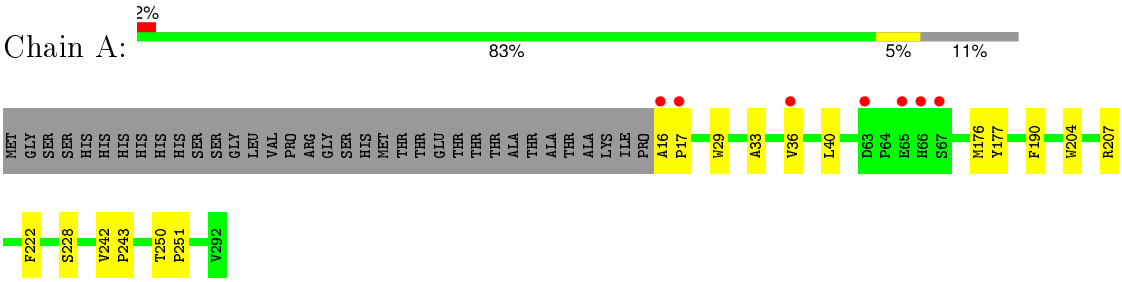
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	125	Total O 125 125	0	0
6	B	92	Total O 92 92	0	0
6	C	62	Total O 62 62	0	0
6	D	117	Total O 117 117	0	0
6	E	124	Total O 124 124	0	0
6	F	65	Total O 65 65	0	0
6	G	101	Total O 101 101	0	0
6	H	121	Total O 121 121	0	0
6	I	92	Total O 92 92	0	0
6	J	122	Total O 122 122	0	0
6	K	71	Total O 71 71	0	0
6	L	73	Total O 73 73	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.

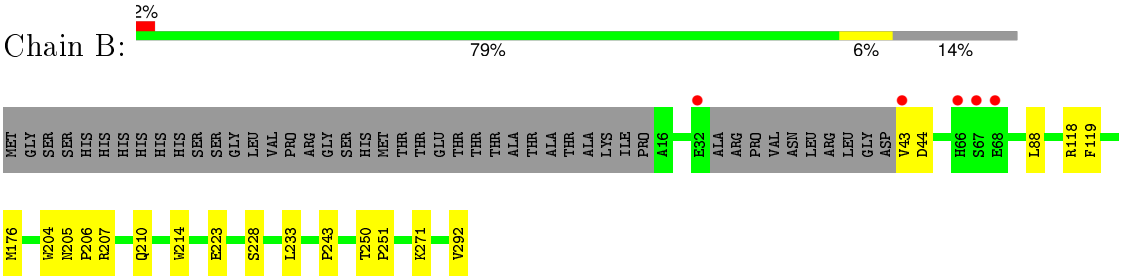
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain A:



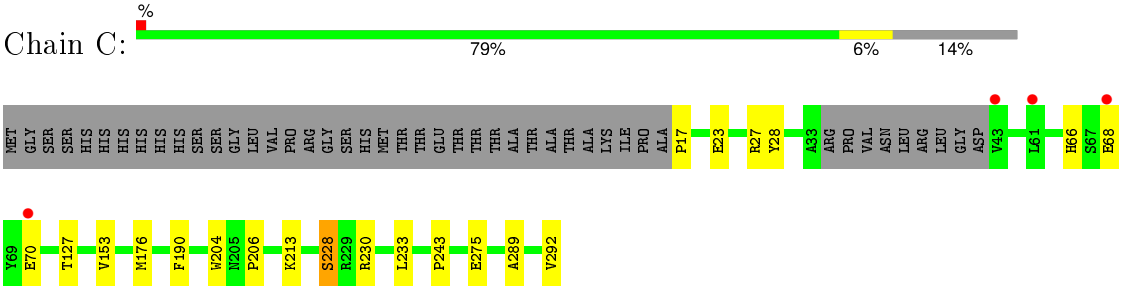
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain B:



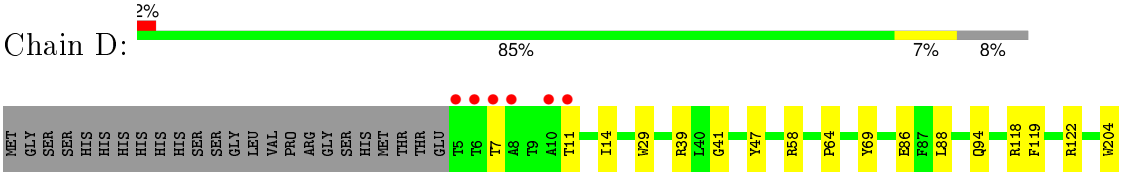
- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

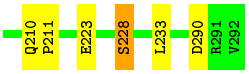
Chain C:



- Molecule 1: Geranyl diphosphate 2-C-methyltransferase

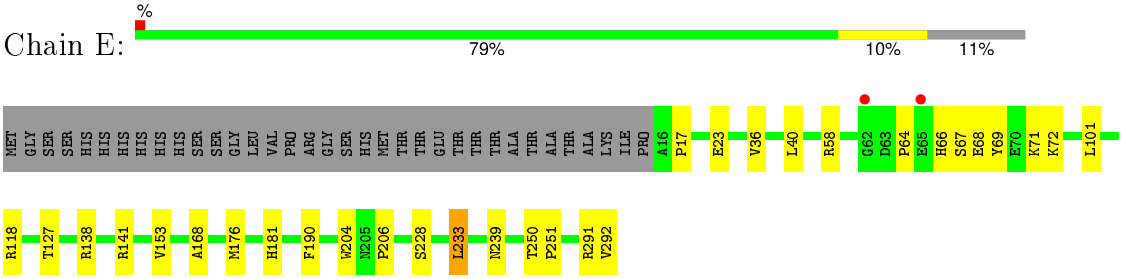
Chain D:





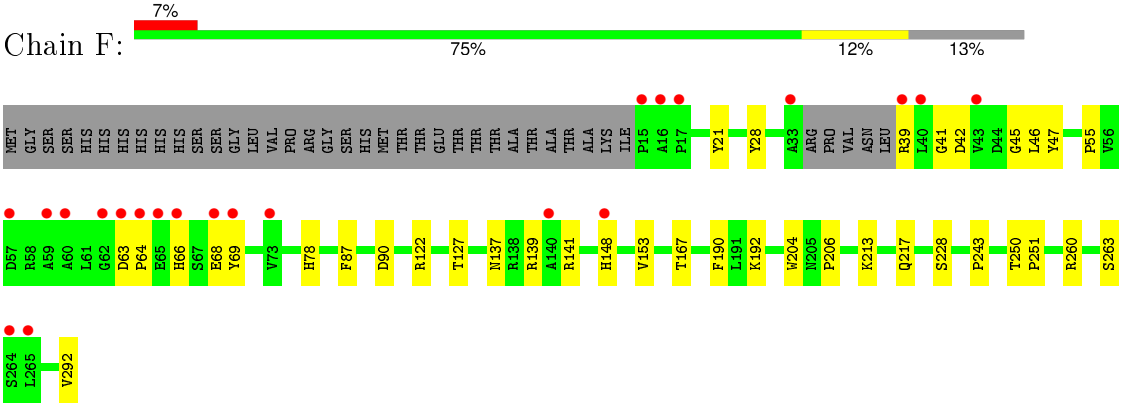
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain E:



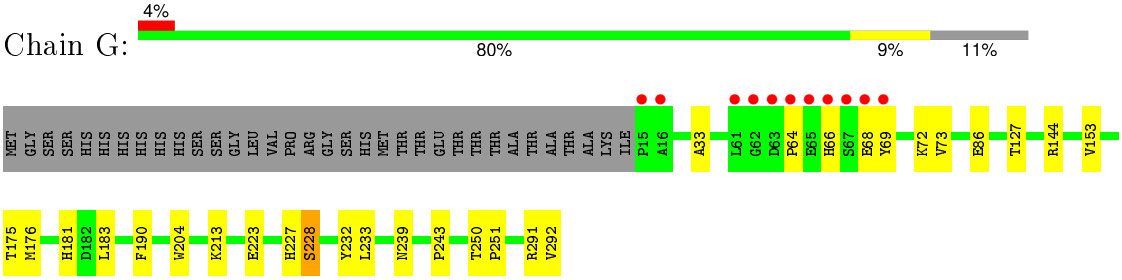
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain F:



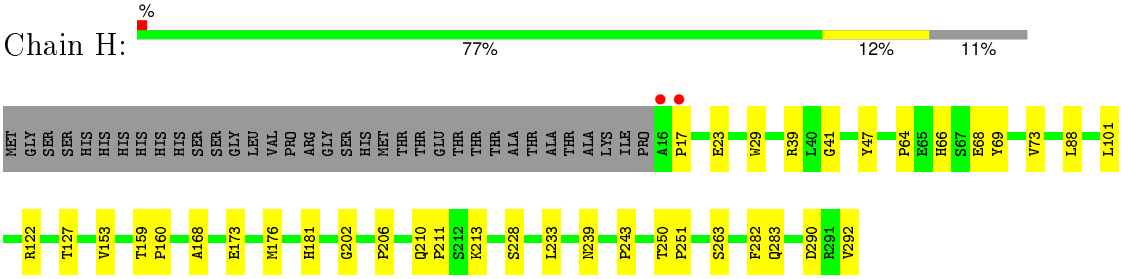
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain G:



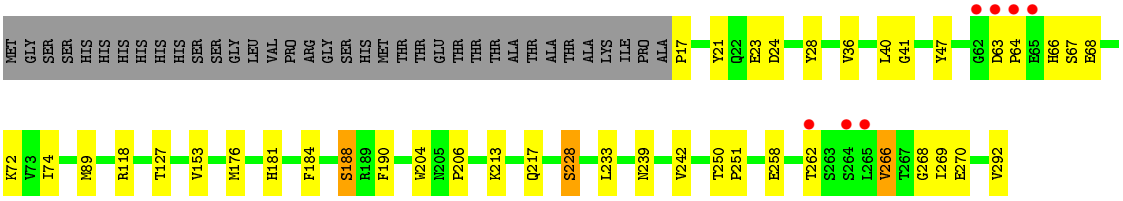
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain H:

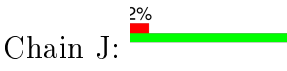


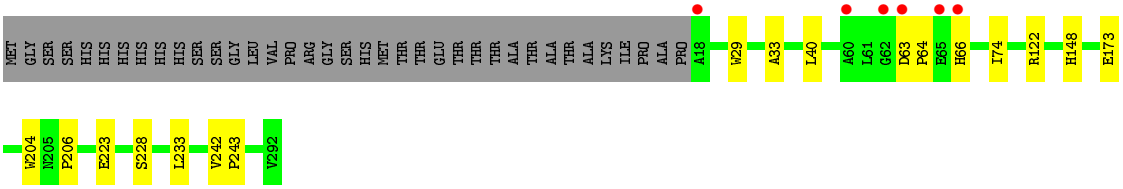
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase

Chain I:

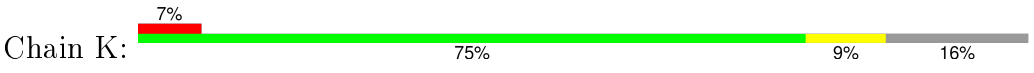


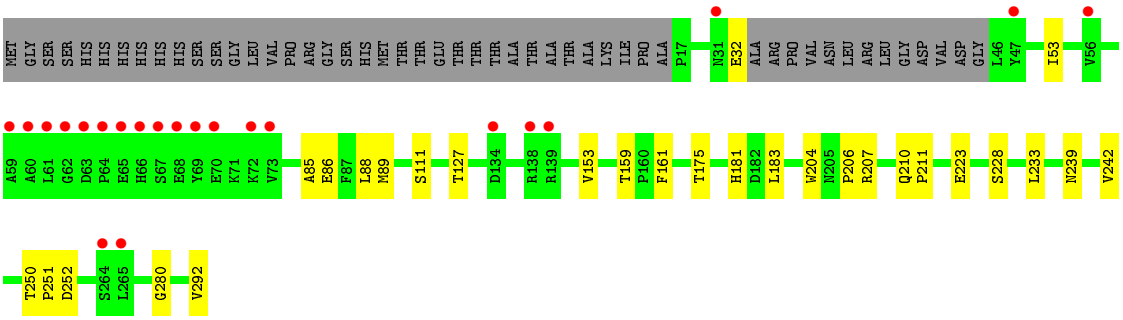
• Molecule 1: Geranyl diphosphate 2-C-methyltransferase



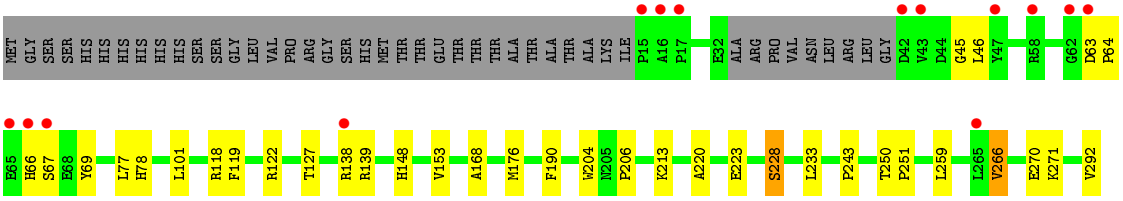


• Molecule 1: Geranyl diphosphate 2-C-methyltransferase





• 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	98.13Å 103.25Å 204.13Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	48.89 – 2.05 48.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.4 (48.89-2.05) 90.4 (48.89-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.181 , 0.222 0.182 , 0.223	Depositor DCC
R_{free} test set	2001 reflections (0.88%)	DCC
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 246176 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27843	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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: MG, SAH, GPP, 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	0.40	0/2273	0.51	0/3083
1	B	0.38	0/2194	0.50	0/2974
1	C	0.36	0/2194	0.50	0/2973
1	D	0.40	0/2355	0.50	0/3198
1	E	0.39	0/2284	0.50	0/3097
1	F	0.34	0/2245	0.49	0/3043
1	G	0.38	0/2294	0.50	0/3112
1	H	0.41	0/2280	0.52	0/3093
1	I	0.38	0/2268	0.49	0/3075
1	J	0.39	0/2267	0.52	0/3074
1	K	0.37	0/2183	0.50	0/2958
1	L	0.38	0/2225	0.50	0/3016
All	All	0.38	0/27062	0.50	0/36696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2212	0	2100	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2135	0	2017	14	0
1	C	2135	0	2018	17	0
1	D	2288	0	2186	19	0
1	E	2217	0	2105	17	0
1	F	2180	0	2068	26	0
1	G	2222	0	2116	22	0
1	H	2214	0	2107	32	0
1	I	2207	0	2098	27	0
1	J	2202	0	2095	16	0
1	K	2114	0	2005	21	0
1	L	2155	0	2034	21	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	1	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	0	0
3	F	26	0	19	0	0
3	G	26	0	19	0	0
3	H	26	0	19	0	0
3	I	26	0	19	0	0
3	J	26	0	19	0	0
3	K	26	0	19	0	0
3	L	26	0	19	0	0
4	A	19	0	17	8	0
4	D	19	0	17	1	0
4	H	19	0	17	10	0
4	J	19	0	17	3	0
5	E	5	0	0	0	0
6	A	125	0	0	0	0
6	B	92	0	0	0	0
6	C	62	0	0	1	0
6	D	117	0	0	0	0
6	E	124	0	0	0	0
6	F	65	0	0	1	0
6	G	101	0	0	1	0
6	H	121	0	0	0	0
6	I	92	0	0	2	0
6	J	122	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	71	0	0	1	0
6	L	73	0	0	0	0
All	All	27843	0	25245	215	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 4.

All (215) 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:H:202:GLY:HA3	4:H:303:GPP:H91	1.61	0.83
1:D:11:THR:HA	1:D:14:ILE:HD12	1.69	0.75
1:I:36:VAL:HG23	6:I:490:HOH:O	1.87	0.74
1:I:292:VAL:HG11	1:L:206:PRO:HB2	1.71	0.73
1:B:43:VAL:HG12	1:B:44:ASP:N	2.03	0.71
1:G:144:ARG:HG3	6:G:497:HOH:O	1.91	0.71
1:I:206:PRO:HB2	1:L:292:VAL:HG11	1.71	0.70
1:H:173:GLU:HB3	4:H:303:GPP:H41	1.73	0.69
1:G:292:VAL:HG11	1:J:206:PRO:HB2	1.75	0.69
1:G:233:LEU:HD13	1:J:243:PRO:HD2	1.74	0.69
1:H:206:PRO:HB2	1:K:292:VAL:HG11	1.75	0.68
1:A:243:PRO:HD2	1:D:233:LEU:HD13	1.78	0.66
1:B:243:PRO:HD2	1:E:233:LEU:HD23	1.78	0.65
1:B:206:PRO:HB2	1:E:292:VAL:HG11	1.79	0.64
1:C:233:LEU:HD12	1:F:243:PRO:HD2	1.79	0.64
1:H:66:HIS:ND1	1:H:68:GLU:HG2	2.13	0.64
1:J:63:ASP:HB3	1:J:66:HIS:HB2	1.80	0.64
1:I:233:LEU:HD13	1:L:243:PRO:HD2	1.80	0.63
1:G:181[B]:HIS:CD2	1:G:239:ASN:HD21	2.16	0.63
1:D:11:THR:HA	1:D:14:ILE:CD1	2.29	0.61
1:H:66:HIS:CE1	1:H:68:GLU:HG2	2.34	0.61
1:C:66:HIS:CD2	1:C:68:GLU:H	2.19	0.61
1:I:181[B]:HIS:CD2	1:I:239:ASN:HD21	2.19	0.61
1:G:213:LYS:HD2	1:L:220:ALA:O	2.01	0.60
1:G:233:LEU:HD12	1:J:242:VAL:HG13	1.83	0.60
1:H:17:PRO:CB	1:H:23:GLU:HG2	2.33	0.59
1:E:101:LEU:HD22	1:E:168:ALA:HB3	1.86	0.58
1:J:204:TRP:CE2	1:J:228:SER:HB3	2.39	0.58
1:F:66:HIS:CD2	1:F:68:GLU:H	2.22	0.57
1:E:36:VAL:O	1:E:40:LEU:HD13	2.03	0.57
4:A:303:GPP:H2	4:A:303:GPP:H7	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:GLU:O	1:G:72:LYS:HG2	2.04	0.57
1:C:292:VAL:HG11	1:F:206:PRO:HB2	1.86	0.56
1:H:17:PRO:HB3	1:H:23:GLU:HG2	1.88	0.56
1:E:138:ARG:HG2	1:E:141:ARG:NH1	2.21	0.56
1:I:66:HIS:ND1	1:I:67:SER:N	2.55	0.55
1:B:204:TRP:CE2	1:B:228:SER:HB2	2.41	0.55
1:K:204:TRP:CZ2	1:K:228:SER:HB2	2.42	0.54
1:B:223:GLU:HG2	1:F:213:LYS:HB2	1.90	0.54
1:L:204:TRP:CE2	1:L:228:SER:HB3	2.43	0.54
1:F:204:TRP:CE2	1:F:228:SER:HB2	2.43	0.54
1:I:266:VAL:HG13	1:I:268:GLY:H	1.73	0.54
1:E:204:TRP:CE2	1:E:228:SER:HB2	2.43	0.53
1:L:66:HIS:ND1	1:L:67:SER:N	2.56	0.53
1:A:29:TRP:HZ2	4:A:303:GPP:H42	1.73	0.53
1:A:204:TRP:CE2	1:A:228:SER:HB2	2.44	0.53
1:A:177:TYR:OH	4:A:303:GPP:H41	2.09	0.52
1:E:127:THR:O	1:E:153:VAL:HA	2.09	0.52
1:I:204:TRP:CE2	1:I:228:SER:HB2	2.45	0.52
1:C:204:TRP:CE2	1:C:228:SER:HB2	2.44	0.52
1:D:94:GLN:HA	1:D:94:GLN:NE2	2.23	0.52
1:G:213:LYS:HB2	1:L:223:GLU:HG2	1.92	0.52
1:I:258:GLU:O	1:I:262:THR:HG23	2.10	0.52
1:G:69:TYR:O	1:G:73:VAL:HG23	2.10	0.51
1:C:230:ARG:HD2	1:F:292:VAL:HG21	1.92	0.51
1:K:85:ALA:O	1:K:89:MET:HG3	2.09	0.51
1:C:27:ARG:HD2	1:C:28:TYR:N	2.25	0.51
1:I:68:GLU:O	1:I:72:LYS:HG2	2.10	0.51
1:H:213:LYS:HB3	1:J:223:GLU:HG2	1.92	0.51
1:L:127:THR:O	1:L:153:VAL:HA	2.10	0.51
1:G:86:GLU:HA	1:G:86:GLU:OE1	2.08	0.51
1:I:204:TRP:CZ2	1:I:228:SER:HB2	2.46	0.51
1:C:17:PRO:HB3	1:C:23:GLU:CG	2.41	0.51
1:B:204:TRP:CZ2	1:B:228:SER:HB2	2.46	0.51
1:I:184:PHE:O	1:I:188:SER:HB2	2.10	0.51
1:I:213:LYS:O	1:I:217:GLN:HG3	2.11	0.50
1:J:173:GLU:HG2	4:J:303:GPP:H103	1.93	0.50
1:F:260:ARG:O	1:F:263:SER:HB3	2.12	0.50
1:L:250:THR:HB	1:L:251:PRO:HD3	1.93	0.50
1:H:282:PHE:HZ	4:H:303:GPP:C9	2.24	0.50
1:H:282:PHE:HZ	4:H:303:GPP:H93	1.75	0.50
1:A:242:VAL:HG13	1:D:233:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:GLY:HA3	1:F:139:ARG:HH21	1.77	0.50
1:G:66:HIS:CD2	1:G:68:GLU:H	2.30	0.50
1:A:207:ARG:HD2	1:D:290:ASP:CG	2.32	0.50
1:E:204:TRP:CZ2	1:E:228:SER:HB2	2.47	0.49
1:K:89:MET:HE1	1:K:111:SER:O	2.12	0.49
1:L:118:ARG:HD2	1:L:119:PHE:CZ	2.48	0.49
1:G:66:HIS:CD2	1:G:68:GLU:HB2	2.47	0.49
1:F:64:PRO:HA	1:F:69:TYR:CE2	2.47	0.49
1:E:68:GLU:O	1:E:72:LYS:HG2	2.12	0.49
1:L:101:LEU:HD22	1:L:168:ALA:HB3	1.94	0.49
1:I:17:PRO:HB3	1:I:23:GLU:HG2	1.94	0.49
1:K:250:THR:HB	1:K:251:PRO:HD3	1.94	0.49
1:G:233:LEU:CD1	1:J:243:PRO:HD2	2.40	0.49
1:C:213:LYS:HB3	1:D:223:GLU:HG2	1.94	0.49
1:I:40:LEU:HD23	1:I:74:ILE:HG23	1.95	0.48
1:A:222:PHE:CD1	4:A:303:GPP:H43	2.48	0.48
1:A:204:TRP:CZ2	1:A:228:SER:HB2	2.48	0.48
1:H:181[B]:HIS:CD2	1:H:239:ASN:HD21	2.31	0.48
1:L:204:TRP:CZ2	1:L:228:SER:HB3	2.48	0.48
1:K:280:GLY:HA2	6:K:454:HOH:O	2.13	0.48
1:F:87:PHE:O	1:F:90:ASP:HB2	2.13	0.48
1:E:64:PRO:HA	1:E:69:TYR:CD2	2.49	0.48
1:E:17:PRO:CB	1:E:23:GLU:HG2	2.43	0.48
1:K:86:GLU:OE2	1:K:86:GLU:HA	2.13	0.48
1:C:204:TRP:CZ2	1:C:228:SER:HB2	2.49	0.48
1:K:204:TRP:CE2	1:K:228:SER:HB2	2.49	0.47
1:C:27:ARG:C	1:C:27:ARG:HD2	2.34	0.47
1:G:243:PRO:HD2	1:J:233:LEU:CD1	2.44	0.47
1:D:64:PRO:HA	1:D:69:TYR:CD2	2.50	0.47
1:H:29:TRP:HH2	4:H:303:GPP:H12	1.80	0.47
1:F:46:LEU:O	1:F:78:HIS:HE1	1.97	0.47
1:I:242:VAL:HG13	1:L:233:LEU:HD12	1.97	0.47
1:E:250:THR:HB	1:E:251:PRO:HD3	1.96	0.47
1:I:21:TYR:O	1:I:24:ASP:HB2	2.14	0.47
1:C:66:HIS:CD2	1:C:68:GLU:HB2	2.50	0.46
1:L:138:ARG:HE	1:L:138:ARG:HB2	1.60	0.46
1:H:41:GLY:HA3	1:H:47:TYR:CD1	2.50	0.46
1:F:64:PRO:HA	1:F:69:TYR:CD2	2.51	0.46
1:H:202:GLY:CA	4:H:303:GPP:H91	2.39	0.46
1:C:70:GLU:HG2	6:C:458:HOH:O	2.15	0.46
1:L:122:ARG:HD3	1:L:148:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:HIS:ND1	1:E:67:SER:N	2.64	0.46
1:F:137:ASN:O	1:F:141:ARG:HG3	2.16	0.46
1:L:45:GLY:HA3	1:L:139:ARG:NH1	2.31	0.46
1:H:173:GLU:CB	4:H:303:GPP:H41	2.45	0.46
1:K:159:THR:HG1	1:K:161:PHE:HD2	1.63	0.46
1:E:66:HIS:CE1	1:E:68:GLU:HG2	2.51	0.45
1:D:88:LEU:C	1:D:88:LEU:HD23	2.37	0.45
1:D:118:ARG:HD2	1:D:119:PHE:CZ	2.52	0.45
1:A:177:TYR:OH	4:A:303:GPP:C4	2.65	0.45
1:J:29:TRP:HH2	4:J:303:GPP:O2A	2.00	0.45
1:G:243:PRO:HD2	1:J:233:LEU:HD12	1.98	0.45
1:F:28:TYR:CD2	1:F:28:TYR:C	2.90	0.45
1:A:29:TRP:CZ2	4:A:303:GPP:H42	2.51	0.45
1:F:213:LYS:HG2	1:F:217:GLN:HE21	1.81	0.45
1:K:210:GLN:HB3	1:K:211:PRO:HD2	1.99	0.45
1:G:223:GLU:HG2	1:L:213:LYS:HB3	1.99	0.45
1:C:127:THR:O	1:C:153:VAL:HA	2.17	0.45
1:D:29:TRP:HH2	4:D:303:GPP:O2A	1.99	0.45
1:F:122:ARG:HD2	1:F:148:HIS:HA	1.99	0.44
1:K:181[B]:HIS:CD2	1:K:239:ASN:HD21	2.35	0.44
1:A:36:VAL:O	1:A:40:LEU:HD13	2.17	0.44
1:D:7:THR:O	1:D:11:THR:HG23	2.17	0.44
1:G:250:THR:HB	1:G:251:PRO:HD3	1.99	0.44
1:H:250:THR:HB	1:H:251:PRO:HD3	2.00	0.44
1:I:266:VAL:HG13	1:I:270:GLU:OE2	2.18	0.44
1:I:250:THR:HB	1:I:251:PRO:HD3	1.98	0.44
1:J:29:TRP:HH2	4:J:303:GPP:H12	1.82	0.44
1:G:127:THR:O	1:G:153:VAL:HA	2.17	0.44
1:L:64:PRO:HA	1:L:69:TYR:CD2	2.51	0.44
1:H:64:PRO:HA	1:H:69:TYR:CD2	2.53	0.44
1:H:101:LEU:HD22	1:H:168:ALA:HB3	1.99	0.44
1:B:118:ARG:HD2	1:B:119:PHE:CZ	2.53	0.44
1:C:17:PRO:HB3	1:C:23:GLU:HG3	2.00	0.44
1:I:213:LYS:HB3	1:K:223:GLU:HG2	2.00	0.44
1:E:181[B]:HIS:CD2	1:E:239:ASN:HD21	2.35	0.44
1:H:39:ARG:HA	1:H:39:ARG:HD2	1.71	0.44
1:I:269:ILE:HD12	1:I:269:ILE:HA	1.88	0.44
1:I:66:HIS:CG	1:I:67:SER:N	2.86	0.43
1:I:127:THR:O	1:I:153:VAL:HA	2.18	0.43
1:H:29:TRP:HH2	4:H:303:GPP:C1	2.32	0.43
1:G:227:HIS:HB2	1:G:232:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TRP:HH2	4:A:303:GPP:O2A	2.01	0.43
4:A:303:GPP:C2	4:A:303:GPP:H7	2.47	0.43
1:K:127:THR:O	1:K:153:VAL:HA	2.17	0.43
1:F:39:ARG:O	1:F:42:ASP:HB2	2.18	0.43
1:B:214:TRP:HH2	1:B:271:LYS:HE3	1.83	0.43
1:F:55:PRO:HD2	6:F:445:HOH:O	2.19	0.43
1:L:77:LEU:CD2	1:L:259:LEU:HD23	2.49	0.43
1:H:88:LEU:HD23	1:H:88:LEU:C	2.39	0.43
1:F:250:THR:HB	1:F:251:PRO:HD3	1.99	0.43
1:H:29:TRP:CH2	4:H:303:GPP:H12	2.53	0.43
1:H:243:PRO:HD2	1:K:233:LEU:HD13	2.01	0.43
1:D:58:ARG:HA	1:D:58:ARG:HD3	1.86	0.43
1:B:214:TRP:CH2	1:B:271:LYS:HE3	2.54	0.42
1:D:41:GLY:HA3	1:D:47:TYR:CD1	2.53	0.42
1:K:53:ILE:HA	1:K:252:ASP:O	2.18	0.42
1:B:210:GLN:HB2	1:F:21:TYR:CD2	2.53	0.42
1:I:89:MET:SD	6:I:467:HOH:O	2.62	0.42
1:F:41:GLY:HA3	1:F:47:TYR:CD1	2.54	0.42
1:I:63:ASP:HA	1:I:64:PRO:HD3	1.87	0.42
1:J:204:TRP:CZ2	1:J:228:SER:HB3	2.53	0.42
1:J:40:LEU:HD12	1:J:74:ILE:HG23	2.01	0.42
1:C:243:PRO:HA	1:C:289:ALA:HA	2.01	0.42
1:B:250:THR:HB	1:B:251:PRO:HD3	2.02	0.42
1:G:64:PRO:HA	1:G:69:TYR:CD2	2.55	0.42
1:H:210:GLN:HB3	1:H:211:PRO:HD2	2.02	0.42
1:A:16:ALA:HA	1:A:17:PRO:HD3	1.86	0.42
1:J:122:ARG:HD2	1:J:148:HIS:O	2.20	0.42
1:B:205:ASN:OD1	1:B:207:ARG:HB2	2.20	0.42
1:D:210:GLN:HB3	1:D:211:PRO:HD2	2.00	0.42
1:L:266:VAL:HA	1:L:270:GLU:OE1	2.20	0.42
1:B:88:LEU:HD23	1:B:88:LEU:C	2.39	0.41
1:H:206:PRO:HB2	1:K:292:VAL:CG1	2.49	0.41
1:F:204:TRP:CZ2	1:F:228:SER:HB2	2.55	0.41
1:C:17:PRO:HB3	1:C:23:GLU:HG2	2.02	0.41
1:H:29:TRP:CH2	4:H:303:GPP:C1	3.03	0.41
1:B:292:VAL:HG11	1:E:206:PRO:HB2	2.02	0.41
3:B:301:SAH:H4'	3:B:301:SAH:HB1	2.02	0.41
1:I:41:GLY:HA3	1:I:47:TYR:CD1	2.56	0.41
1:H:127:THR:O	1:H:153:VAL:HA	2.21	0.41
1:H:292:VAL:HG11	1:K:206:PRO:HB2	2.01	0.41
1:J:63:ASP:HA	1:J:64:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:THR:HG22	1:G:183:LEU:CD2	2.50	0.41
1:C:206:PRO:HB2	1:F:292:VAL:HG11	2.03	0.41
1:K:88:LEU:C	1:K:88:LEU:HD23	2.41	0.41
1:D:39:ARG:HA	1:D:39:ARG:NE	2.36	0.41
1:F:167:THR:HA	1:F:192:LYS:HE3	2.02	0.41
1:L:46:LEU:O	1:L:78:HIS:HE1	2.04	0.41
1:F:127:THR:O	1:F:153:VAL:HA	2.20	0.41
1:H:73:VAL:HG11	1:H:263:SER:HB3	2.02	0.41
1:D:86:GLU:HG3	1:D:118:ARG:HH21	1.86	0.41
1:D:204:TRP:CE2	1:D:228:SER:HB3	2.56	0.40
1:H:233:LEU:HD12	1:K:242:VAL:HG13	2.02	0.40
1:I:28:TYR:CD2	1:I:28:TYR:C	2.94	0.40
1:D:86:GLU:HG3	1:D:118:ARG:NH2	2.36	0.40
1:K:175:THR:HG22	1:K:183:LEU:HD21	2.03	0.40
1:H:159:THR:HB	1:H:160:PRO:CD	2.51	0.40
1:H:290:ASP:CG	1:K:207:ARG:HD2	2.42	0.40
1:F:63:ASP:HA	1:F:64:PRO:HD3	1.81	0.40
1:E:58:ARG:HA	1:E:58:ARG:HD3	1.95	0.40
1:G:204:TRP:CE2	1:G:228:SER:HB3	2.56	0.40
1:A:250:THR:HB	1:A:251:PRO:HD3	2.02	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%)	7 (2%)	1 (0%)	39 28
1	B	264/312 (85%)	257 (97%)	7 (3%)	0	100 100
1	C	264/312 (85%)	255 (97%)	9 (3%)	0	100 100
1	D	288/312 (92%)	280 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	277/312 (89%)	267 (96%)	10 (4%)	0	100	100
1	F	271/312 (87%)	262 (97%)	9 (3%)	0	100	100
1	G	279/312 (89%)	273 (98%)	5 (2%)	1 (0%)	39	28
1	H	277/312 (89%)	268 (97%)	9 (3%)	0	100	100
1	I	275/312 (88%)	262 (95%)	12 (4%)	1 (0%)	39	28
1	J	275/312 (88%)	265 (96%)	9 (3%)	1 (0%)	39	28
1	K	262/312 (84%)	256 (98%)	6 (2%)	0	100	100
1	L	268/312 (86%)	259 (97%)	9 (3%)	0	100	100
All	All	3276/3744 (88%)	3172 (97%)	100 (3%)	4 (0%)	56	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	33	ALA
1	A	33	ALA
1	J	33	ALA
1	I	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%)	230 (99%)	2 (1%)	84	84
1	B	224/260 (86%)	222 (99%)	2 (1%)	84	84
1	C	224/260 (86%)	220 (98%)	4 (2%)	66	62
1	D	241/260 (93%)	239 (99%)	2 (1%)	86	86
1	E	233/260 (90%)	227 (97%)	6 (3%)	54	47
1	F	229/260 (88%)	228 (100%)	1 (0%)	93	94
1	G	235/260 (90%)	231 (98%)	4 (2%)	68	65
1	H	233/260 (90%)	229 (98%)	4 (2%)	68	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	232/260 (89%)	227 (98%)	5 (2%)	60 53
1	J	232/260 (89%)	232 (100%)	0	100 100
1	K	224/260 (86%)	223 (100%)	1 (0%)	93 94
1	L	228/260 (88%)	222 (97%)	6 (3%)	54 47
All	All	2767/3120 (89%)	2730 (99%)	37 (1%)	76 74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	MET
1	A	190	PHE
1	B	176	MET
1	B	233	LEU
1	C	176	MET
1	C	190	PHE
1	C	228	SER
1	C	275	GLU
1	D	122	ARG
1	D	228	SER
1	E	71	LYS
1	E	118	ARG
1	E	176	MET
1	E	190	PHE
1	E	233	LEU
1	E	291	ARG
1	F	190	PHE
1	G	176	MET
1	G	190	PHE
1	G	228	SER
1	G	291	ARG
1	H	122	ARG
1	H	176	MET
1	H	228	SER
1	H	283	GLN
1	I	118	ARG
1	I	176	MET
1	I	188	SER
1	I	190	PHE
1	I	228	SER
1	K	32	GLU
1	L	63	ASP

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Mol	Chain	Res	Type
1	L	176	MET
1	L	190	PHE
1	L	228	SER
1	L	266	VAL
1	L	271	LYS

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

Mol	Chain	Res	Type
1	A	37	ASN
1	B	132	GLN
1	C	66	HIS
1	D	94	GLN
1	F	66	HIS
1	F	217	GLN
1	H	94	GLN
1	K	78	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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	2.63	4 (20%)	19,40,40	4.63	6 (31%)
4	GPP	A	303	2	16,18,18	3.39	3 (18%)	21,25,25	1.51	4 (19%)
3	SAH	B	301	-	20,28,28	2.78	5 (25%)	19,40,40	4.71	5 (26%)
3	SAH	C	301	-	20,28,28	2.71	5 (25%)	19,40,40	4.62	5 (26%)
3	SAH	D	302	-	20,28,28	2.61	5 (25%)	19,40,40	4.57	5 (26%)
4	GPP	D	303	2	16,18,18	3.32	4 (25%)	21,25,25	1.58	5 (23%)
3	SAH	E	301	-	20,28,28	2.72	4 (20%)	19,40,40	4.65	6 (31%)
5	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.27	0
3	SAH	F	301	-	20,28,28	2.88	6 (30%)	19,40,40	4.44	5 (26%)
3	SAH	G	301	-	20,28,28	2.71	4 (20%)	19,40,40	4.70	5 (26%)
3	SAH	H	302	-	20,28,28	2.73	4 (20%)	19,40,40	4.75	6 (31%)
4	GPP	H	303	2	16,18,18	3.37	4 (25%)	21,25,25	1.68	7 (33%)
3	SAH	I	301	-	20,28,28	2.73	4 (20%)	19,40,40	4.56	6 (31%)
3	SAH	J	302	-	20,28,28	2.70	5 (25%)	19,40,40	4.81	6 (31%)
4	GPP	J	303	2	16,18,18	3.32	3 (18%)	21,25,25	1.37	4 (19%)
3	SAH	K	301	-	20,28,28	2.78	5 (25%)	19,40,40	4.55	8 (42%)
3	SAH	L	301	-	20,28,28	2.78	5 (25%)	19,40,40	4.31	5 (26%)

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	GPP	A	303	2	-	0/19/19/19	0/0/0/0
3	SAH	B	301	-	-	0/7/31/31	0/3/3/3
3	SAH	C	301	-	-	0/7/31/31	0/3/3/3
3	SAH	D	302	-	-	0/7/31/31	0/3/3/3
4	GPP	D	303	2	-	0/19/19/19	0/0/0/0
3	SAH	E	301	-	-	0/7/31/31	0/3/3/3
5	SO4	E	302	-	-	0/0/0/0	0/0/0/0
3	SAH	F	301	-	-	0/7/31/31	0/3/3/3
3	SAH	G	301	-	-	0/7/31/31	0/3/3/3
3	SAH	H	302	-	-	0/7/31/31	0/3/3/3
4	GPP	H	303	2	-	0/19/19/19	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	I	301	-	-	0/7/31/31	0/3/3/3
3	SAH	J	302	-	-	0/7/31/31	0/3/3/3
4	GPP	J	303	2	-	0/19/19/19	0/0/0/0
3	SAH	K	301	-	-	0/7/31/31	0/3/3/3
3	SAH	L	301	-	-	0/7/31/31	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	SAH	C5'-SD	-2.24	1.76	1.81
3	J	302	SAH	C5'-SD	-2.20	1.76	1.81
3	B	301	SAH	C5'-SD	-2.19	1.76	1.81
3	F	301	SAH	C5'-SD	-2.13	1.77	1.81
3	D	302	SAH	C5'-SD	-2.10	1.77	1.81
3	L	301	SAH	C5'-SD	-2.03	1.77	1.81
3	K	301	SAH	C5'-SD	-2.03	1.77	1.81
3	F	301	SAH	O4'-C1'	2.02	1.43	1.41
4	D	303	GPP	PB-O3B	2.15	1.62	1.54
4	D	303	GPP	PB-O2B	2.21	1.62	1.54
4	J	303	GPP	PB-O3B	2.25	1.62	1.54
4	A	303	GPP	PB-O2B	2.43	1.63	1.54
3	E	301	SAH	C5-C4	2.73	1.46	1.40
3	D	302	SAH	C5-C4	2.75	1.46	1.40
3	A	302	SAH	C5-C4	2.76	1.46	1.40
3	G	301	SAH	C5-C4	2.78	1.46	1.40
3	K	301	SAH	C5-C4	2.82	1.46	1.40
3	J	302	SAH	C5-C4	2.83	1.46	1.40
3	H	302	SAH	C5-C4	2.84	1.46	1.40
3	B	301	SAH	C5-C4	2.89	1.47	1.40
3	L	301	SAH	C5-C4	2.95	1.47	1.40
3	I	301	SAH	C5-C4	3.01	1.47	1.40
4	H	303	GPP	PB-O1B	3.10	1.61	1.51
3	C	301	SAH	C5-C4	3.12	1.47	1.40
3	F	301	SAH	C5-C4	3.30	1.47	1.40
4	H	303	GPP	PA-O1A	3.59	1.64	1.51
3	A	302	SAH	C6-N6	4.37	1.48	1.34
3	D	302	SAH	C6-N6	4.38	1.48	1.34
3	J	302	SAH	C6-N6	4.40	1.48	1.34
3	L	301	SAH	C6-N6	4.40	1.48	1.34
3	E	301	SAH	C6-N6	4.40	1.48	1.34
3	I	301	SAH	C6-N6	4.43	1.48	1.34
3	F	301	SAH	C6-N6	4.43	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	SAH	C6-N6	4.48	1.48	1.34
3	K	301	SAH	C6-N6	4.48	1.48	1.34
3	C	301	SAH	C6-N6	4.56	1.49	1.34
3	B	301	SAH	C6-N6	4.59	1.49	1.34
3	H	302	SAH	C6-N6	4.95	1.50	1.34
3	D	302	SAH	C2-N1	6.24	1.45	1.33
3	C	301	SAH	C2-N1	6.47	1.46	1.33
3	H	302	SAH	C2-N1	6.61	1.46	1.33
3	A	302	SAH	C2-N1	6.66	1.46	1.33
3	L	301	SAH	C2-N1	6.74	1.46	1.33
3	I	301	SAH	C2-N1	6.74	1.46	1.33
3	E	301	SAH	C2-N1	6.75	1.46	1.33
3	G	301	SAH	C2-N1	6.76	1.46	1.33
3	J	302	SAH	C2-N1	6.93	1.47	1.33
4	H	303	GPP	C7-C8	7.01	1.53	1.32
4	J	303	GPP	C7-C8	7.03	1.53	1.32
3	B	301	SAH	C2-N1	7.04	1.47	1.33
4	D	303	GPP	C7-C8	7.04	1.53	1.32
3	K	301	SAH	C2-N1	7.10	1.47	1.33
4	A	303	GPP	C7-C8	7.10	1.54	1.32
3	F	301	SAH	C2-N1	7.13	1.47	1.33
3	A	302	SAH	C2-N3	7.61	1.45	1.32
3	J	302	SAH	C2-N3	7.72	1.45	1.32
3	D	302	SAH	C2-N3	7.78	1.45	1.32
3	G	301	SAH	C2-N3	7.86	1.46	1.32
3	C	301	SAH	C2-N3	7.90	1.46	1.32
3	H	302	SAH	C2-N3	7.90	1.46	1.32
3	K	301	SAH	C2-N3	8.02	1.46	1.32
3	I	301	SAH	C2-N3	8.06	1.46	1.32
3	B	301	SAH	C2-N3	8.07	1.46	1.32
3	E	301	SAH	C2-N3	8.12	1.46	1.32
3	F	301	SAH	C2-N3	8.43	1.47	1.32
3	L	301	SAH	C2-N3	8.53	1.47	1.32
4	H	303	GPP	C2-C3	9.70	1.52	1.33
4	J	303	GPP	C2-C3	10.27	1.53	1.33
4	D	303	GPP	C2-C3	10.34	1.53	1.33
4	A	303	GPP	C2-C3	10.63	1.53	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	302	SAH	N3-C2-N1	-19.51	113.95	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	SAH	N3-C2-N1	-19.28	114.14	128.89
3	B	301	SAH	N3-C2-N1	-19.21	114.19	128.89
3	G	301	SAH	N3-C2-N1	-19.18	114.21	128.89
3	E	301	SAH	N3-C2-N1	-18.98	114.36	128.89
3	A	302	SAH	N3-C2-N1	-18.92	114.41	128.89
3	C	301	SAH	N3-C2-N1	-18.78	114.52	128.89
3	D	302	SAH	N3-C2-N1	-18.58	114.67	128.89
3	I	301	SAH	N3-C2-N1	-18.33	114.86	128.89
3	K	301	SAH	N3-C2-N1	-18.30	114.88	128.89
3	F	301	SAH	N3-C2-N1	-18.23	114.94	128.89
3	L	301	SAH	N3-C2-N1	-17.51	115.49	128.89
4	A	303	GPP	C6-C7-C8	-4.31	111.12	127.73
4	D	303	GPP	C6-C7-C8	-3.77	113.20	127.73
3	I	301	SAH	C4-C5-N7	-3.61	106.16	109.48
3	C	301	SAH	C4-C5-N7	-3.49	106.27	109.48
3	B	301	SAH	C1'-N9-C4	-3.39	121.82	126.94
3	H	302	SAH	C1'-N9-C4	-3.39	121.83	126.94
4	H	303	GPP	C6-C7-C8	-3.30	115.03	127.73
3	L	301	SAH	C4-C5-N7	-3.28	106.46	109.48
3	G	301	SAH	C4-C5-N7	-3.28	106.46	109.48
3	E	301	SAH	C4-C5-N7	-3.27	106.47	109.48
3	J	302	SAH	C4-C5-N7	-3.12	106.61	109.48
3	I	301	SAH	CB-CG-SD	-3.12	107.56	113.57
3	K	301	SAH	CB-CG-SD	-3.11	107.57	113.57
3	B	301	SAH	C4-C5-N7	-3.11	106.62	109.48
3	K	301	SAH	C4-C5-N7	-3.11	106.62	109.48
3	D	302	SAH	C1'-N9-C4	-3.03	122.37	126.94
3	I	301	SAH	C1'-N9-C4	-3.02	122.39	126.94
3	H	302	SAH	C4-C5-N7	-3.01	106.71	109.48
3	J	302	SAH	C1'-N9-C4	-2.99	122.44	126.94
4	A	303	GPP	C4-C3-C2	-2.96	117.69	123.50
3	A	302	SAH	C4-C5-N7	-2.94	106.78	109.48
4	J	303	GPP	C6-C7-C8	-2.82	116.89	127.73
3	C	301	SAH	C1'-N9-C4	-2.80	122.71	126.94
3	G	301	SAH	C1'-N9-C4	-2.76	122.78	126.94
3	K	301	SAH	C1'-N9-C4	-2.75	122.79	126.94
4	D	303	GPP	PA-O3A-PB	-2.71	123.58	132.67
3	A	302	SAH	CB-CG-SD	-2.69	108.39	113.57
3	J	302	SAH	CB-CG-SD	-2.68	108.40	113.57
3	E	301	SAH	C1'-N9-C4	-2.58	123.04	126.94
3	F	301	SAH	CB-CG-SD	-2.57	108.62	113.57
3	C	301	SAH	CB-CG-SD	-2.57	108.62	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	SAH	C4-C5-N7	-2.55	107.13	109.48
3	L	301	SAH	CB-CG-SD	-2.52	108.70	113.57
3	E	301	SAH	CB-CG-SD	-2.46	108.82	113.57
3	L	301	SAH	C1'-N9-C4	-2.46	123.23	126.94
3	D	302	SAH	C4-C5-N7	-2.43	107.24	109.48
3	A	302	SAH	C1'-N9-C4	-2.28	123.50	126.94
3	J	302	SAH	C4'-C5'-SD	-2.17	106.83	113.53
3	B	301	SAH	CB-CG-SD	-2.17	109.39	113.57
3	H	302	SAH	CB-CG-SD	-2.15	109.44	113.57
4	H	303	GPP	C6-C5-C3	-2.10	105.88	112.71
4	D	303	GPP	C4-C3-C2	-2.09	119.39	123.50
4	J	303	GPP	PA-O3A-PB	-2.08	125.69	132.67
4	H	303	GPP	C4-C3-C2	-2.07	119.44	123.50
3	K	301	SAH	C4'-C5'-SD	-2.06	107.17	113.53
3	F	301	SAH	C4'-C5'-SD	-2.04	107.23	113.53
3	H	302	SAH	C4'-O4'-C1'	-2.04	107.48	109.72
4	H	303	GPP	O2A-PA-O3A	2.01	114.22	105.09
4	A	303	GPP	C10-C8-C9	2.02	119.61	114.64
4	A	303	GPP	C5-C3-C2	2.03	124.91	121.05
4	H	303	GPP	C10-C8-C9	2.15	119.92	114.64
4	J	303	GPP	C10-C8-C9	2.16	119.94	114.64
3	K	301	SAH	O4'-C1'-N9	2.23	112.76	108.10
3	I	301	SAH	C5'-SD-CG	2.27	109.22	102.41
4	D	303	GPP	C10-C8-C9	2.30	120.29	114.64
3	D	302	SAH	O4'-C1'-N9	2.42	113.16	108.10
3	E	301	SAH	C5'-SD-CG	2.43	109.69	102.41
3	A	302	SAH	O4'-C1'-N9	2.47	113.26	108.10
3	G	301	SAH	O4'-C1'-N9	2.48	113.28	108.10
3	K	301	SAH	C5'-SD-CG	2.69	110.48	102.41
4	H	303	GPP	O3B-PB-O3A	2.75	117.58	105.09
3	L	301	SAH	C2-N1-C6	2.80	123.77	118.77
4	J	303	GPP	C4-C3-C5	3.02	120.02	115.41
3	K	301	SAH	C2-N1-C6	3.03	124.18	118.77
3	E	301	SAH	C2-N1-C6	3.15	124.39	118.77
3	F	301	SAH	C2-N1-C6	3.21	124.50	118.77
3	G	301	SAH	C2-N1-C6	3.23	124.55	118.77
4	D	303	GPP	C4-C3-C5	3.26	120.38	115.41
3	I	301	SAH	C2-N1-C6	3.37	124.79	118.77
3	B	301	SAH	C2-N1-C6	3.40	124.84	118.77
4	H	303	GPP	C4-C3-C5	3.58	120.87	115.41
3	A	302	SAH	C2-N1-C6	3.60	125.20	118.77
3	C	301	SAH	C2-N1-C6	3.64	125.28	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	SAH	C2-N1-C6	3.68	125.35	118.77
3	J	302	SAH	C2-N1-C6	3.69	125.36	118.77
3	H	302	SAH	C2-N1-C6	4.03	125.98	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GPP	8	0
3	B	301	SAH	1	0
4	D	303	GPP	1	0
4	H	303	GPP	10	0
4	J	303	GPP	3	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%)	-0.23	7 (2%)	61	67	15, 22, 43, 61	1 (0%)
1	B	267/312 (85%)	-0.29	5 (1%)	70	75	17, 25, 47, 68	1 (0%)
1	C	267/312 (85%)	-0.20	4 (1%)	76	81	18, 27, 47, 61	1 (0%)
1	D	288/312 (92%)	-0.38	6 (2%)	67	72	14, 22, 47, 71	1 (0%)
1	E	277/312 (88%)	-0.28	2 (0%)	89	91	15, 24, 44, 66	1 (0%)
1	F	273/312 (87%)	0.09	22 (8%)	15	17	18, 31, 58, 84	1 (0%)
1	G	278/312 (89%)	-0.16	11 (3%)	42	48	15, 25, 47, 75	1 (0%)
1	H	277/312 (88%)	-0.49	2 (0%)	89	91	15, 22, 36, 58	2 (0%)
1	I	276/312 (88%)	-0.11	7 (2%)	61	67	17, 26, 53, 83	1 (0%)
1	J	275/312 (88%)	-0.17	6 (2%)	65	71	14, 23, 47, 74	1 (0%)
1	K	263/312 (84%)	0.12	22 (8%)	14	15	18, 31, 59, 82	1 (0%)
1	L	269/312 (86%)	-0.16	14 (5%)	31	36	17, 27, 57, 84	1 (0%)
All	All	3287/3744 (87%)	-0.19	108 (3%)	50	57	14, 25, 52, 84	13 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	THR	5.7
1	H	16	ALA	4.4
1	F	265	LEU	4.3
1	F	65	GLU	4.2
1	L	15	PRO	4.2
1	K	64	PRO	4.2
1	F	62	GLY	4.0
1	L	65	GLU	4.0
1	F	15	PRO	3.9
1	F	63	ASP	3.9
1	K	69	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	264	SER	3.8
1	C	43	VAL	3.8
1	L	42	ASP	3.8
1	A	16	ALA	3.8
1	K	68	GLU	3.8
1	K	62	GLY	3.8
1	F	66	HIS	3.7
1	G	15	PRO	3.7
1	D	11	THR	3.7
1	K	61	LEU	3.6
1	D	8	ALA	3.6
1	G	63	ASP	3.6
1	G	65	GLU	3.5
1	L	67	SER	3.4
1	G	66	HIS	3.4
1	G	64	PRO	3.3
1	G	67	SER	3.3
1	K	65	GLU	3.3
1	I	262	THR	3.2
1	F	40	LEU	3.2
1	D	10	ALA	3.1
1	G	62	GLY	3.1
1	D	5	THR	3.1
1	K	66	HIS	3.1
1	L	62	GLY	3.1
1	L	63	ASP	3.1
1	D	6	THR	3.1
1	F	264	SER	3.1
1	K	63	ASP	3.0
1	L	16	ALA	3.0
1	K	265	LEU	3.0
1	F	17	PRO	2.9
1	K	67	SER	2.8
1	A	63	ASP	2.8
1	F	16	ALA	2.8
1	K	70	GLU	2.8
1	A	66	HIS	2.7
1	F	73	VAL	2.7
1	A	17	PRO	2.7
1	J	62	GLY	2.7
1	I	265	LEU	2.6
1	B	43	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLU	2.6
1	I	62	GLY	2.6
1	I	65	GLU	2.6
1	L	43	VAL	2.6
1	J	65	GLU	2.6
1	B	67	SER	2.5
1	G	69	TYR	2.5
1	J	18	ALA	2.5
1	F	69	TYR	2.5
1	B	66	HIS	2.4
1	K	56	VAL	2.4
1	F	140	ALA	2.4
1	K	59	ALA	2.4
1	J	63	ASP	2.4
1	L	47	TYR	2.4
1	L	66	HIS	2.4
1	C	70	GLU	2.4
1	G	61	LEU	2.4
1	F	60	ALA	2.3
1	A	36	VAL	2.3
1	F	64	PRO	2.3
1	L	58	ARG	2.3
1	I	63	ASP	2.3
1	F	59	ALA	2.3
1	F	57	ASP	2.3
1	C	68	GLU	2.3
1	K	72	LYS	2.3
1	F	68	GLU	2.3
1	F	33	ALA	2.3
1	K	47	TYR	2.2
1	B	68	GLU	2.2
1	G	68	GLU	2.2
1	K	31	ASN	2.2
1	F	148	HIS	2.2
1	H	17	PRO	2.2
1	E	65	GLU	2.2
1	G	16	ALA	2.2
1	L	265	LEU	2.2
1	K	264	SER	2.2
1	K	134	ASP	2.2
1	L	17	PRO	2.2
1	E	62	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	138	ARG	2.2
1	J	60	ALA	2.2
1	L	138	ARG	2.1
1	K	73	VAL	2.1
1	F	39	ARG	2.1
1	K	60	ALA	2.1
1	A	67	SER	2.1
1	F	43	VAL	2.1
1	J	66	HIS	2.0
1	I	64	PRO	2.0
1	C	61	LEU	2.0
1	K	139	ARG	2.0
1	B	32	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
4	GPP	H	303	19/19	0.90	0.23	16.33	28,36,44,47	0
5	SO4	E	302	5/5	0.89	0.18	6.56	32,32,36,40	5
4	GPP	A	303	19/19	0.87	0.26	5.01	25,40,52,52	0
4	GPP	D	303	19/19	0.93	0.17	4.72	29,35,44,47	0
3	SAH	J	302	26/26	0.98	0.12	1.10	14,19,23,24	0
3	SAH	G	301	26/26	0.97	0.10	0.88	17,21,24,29	0
3	SAH	D	302	26/26	0.97	0.09	0.52	14,18,20,20	0
3	SAH	I	301	26/26	0.98	0.12	0.37	16,20,23,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GPP	J	303	19/19	0.96	0.11	0.15	26,31,39,39	0
3	SAH	A	302	26/26	0.98	0.09	0.12	14,17,21,22	0
3	SAH	K	301	26/26	0.95	0.11	0.11	21,27,32,35	0
3	SAH	E	301	26/26	0.98	0.11	0.06	17,19,21,22	0
3	SAH	L	301	26/26	0.98	0.09	-0.20	19,23,25,26	0
3	SAH	B	301	26/26	0.97	0.08	-0.28	19,22,25,27	0
3	SAH	F	301	26/26	0.96	0.08	-0.68	22,27,32,35	0
3	SAH	H	302	26/26	0.98	0.07	-0.74	16,18,20,21	0
3	SAH	C	301	26/26	0.98	0.09	-0.85	18,22,26,27	0
2	MG	A	301	1/1	0.88	0.07	-1.18	41,41,41,41	0
2	MG	D	301	1/1	0.79	0.05	-1.90	39,39,39,39	0
2	MG	H	301	1/1	0.92	0.06	-2.09	36,36,36,36	0
2	MG	J	301	1/1	0.91	0.04	-5.72	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.