



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EIL
Title : Crystal Structure of the loop truncated Toxoplasma gondii TS-DHFR
Authors : Sharma, H.
Deposited on : 2012-04-05
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

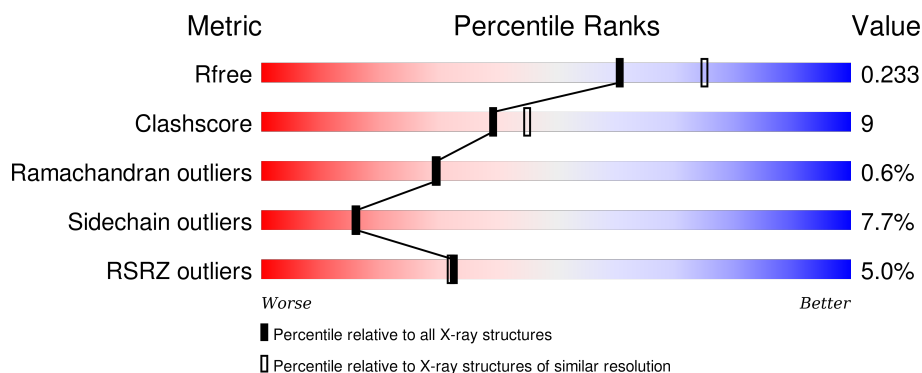
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>3%</div> <div>70% 17% • 10%</div> </div>
1	B	566	<div> <div>5%</div> <div>67% 18% • 13%</div> </div>
1	C	566	<div> <div>4%</div> <div>71% 17% • 10%</div> </div>
1	D	566	<div> <div>5%</div> <div>66% 17% • 13%</div> </div>
1	E	566	<div> <div>4%</div> <div>73% 16% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	566	
1	G	566	
1	H	566	

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	UMP	B	701	-	-	X	-
4	FOL	A	703	-	-	-	X
4	FOL	C	703	-	-	-	X
4	FOL	E	703	-	-	-	X
4	FOL	G	703	-	-	-	X
4	FOL	H	703	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35087 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	F	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	G	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	H	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP Q07422
A	?	-	LEU	DELETION	UNP Q07422
A	?	-	ASN	DELETION	UNP Q07422
A	?	-	GLY	DELETION	UNP Q07422
A	?	-	TRP	DELETION	UNP Q07422
A	?	-	LEU	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	ARG	DELETION	UNP Q07422
A	?	-	LYS	DELETION	UNP Q07422
A	?	-	PHE	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	LYS	DELETION	UNP Q07422
A	?	-	THR	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	DELETION	UNP Q07422
A	?	-	ASP	DELETION	UNP Q07422
A	?	-	SER	DELETION	UNP Q07422
A	?	-	GLY	DELETION	UNP Q07422
A	?	-	LEU	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	SER	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	SER	DELETION	UNP Q07422
A	?	-	VAL	DELETION	UNP Q07422
A	?	-	GLY	DELETION	UNP Q07422
A	?	-	LYS	DELETION	UNP Q07422
A	?	-	GLN	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	ALA	DELETION	UNP Q07422
A	?	-	GLU	DELETION	UNP Q07422
A	?	-	SER	DELETION	UNP Q07422
A	?	-	VAL	DELETION	UNP Q07422
A	?	-	PHE	DELETION	UNP Q07422
A	?	-	VAL	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	PHE	DELETION	UNP Q07422
A	?	-	CYS	DELETION	UNP Q07422
A	?	-	PRO	DELETION	UNP Q07422
A	?	-	GLU	DELETION	UNP Q07422
A	?	-	LEU	DELETION	UNP Q07422
A	?	-	GLY	DELETION	UNP Q07422
A	?	-	ARG	DELETION	UNP Q07422
B	?	-	ARG	DELETION	UNP Q07422
B	?	-	LEU	DELETION	UNP Q07422
B	?	-	ASN	DELETION	UNP Q07422
B	?	-	GLY	DELETION	UNP Q07422
B	?	-	TRP	DELETION	UNP Q07422
B	?	-	LEU	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	ARG	DELETION	UNP Q07422
B	?	-	LYS	DELETION	UNP Q07422
B	?	-	PHE	DELETION	UNP Q07422
B	?	-	ALA	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q07422
B	?	-	THR	DELETION	UNP Q07422
B	?	-	GLY	DELETION	UNP Q07422
B	?	-	ASP	DELETION	UNP Q07422
B	?	-	SER	DELETION	UNP Q07422
B	?	-	GLY	DELETION	UNP Q07422
B	?	-	LEU	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	SER	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	SER	DELETION	UNP Q07422
B	?	-	VAL	DELETION	UNP Q07422
B	?	-	GLY	DELETION	UNP Q07422
B	?	-	LYS	DELETION	UNP Q07422
B	?	-	GLN	DELETION	UNP Q07422
B	?	-	ALA	DELETION	UNP Q07422
B	?	-	ALA	DELETION	UNP Q07422
B	?	-	ALA	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	ALA	DELETION	UNP Q07422
B	?	-	GLU	DELETION	UNP Q07422
B	?	-	SER	DELETION	UNP Q07422
B	?	-	VAL	DELETION	UNP Q07422
B	?	-	PHE	DELETION	UNP Q07422
B	?	-	VAL	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	PHE	DELETION	UNP Q07422
B	?	-	CYS	DELETION	UNP Q07422
B	?	-	PRO	DELETION	UNP Q07422
B	?	-	GLU	DELETION	UNP Q07422
B	?	-	LEU	DELETION	UNP Q07422
B	?	-	GLY	DELETION	UNP Q07422
B	?	-	ARG	DELETION	UNP Q07422
C	?	-	ARG	DELETION	UNP Q07422
C	?	-	LEU	DELETION	UNP Q07422
C	?	-	ASN	DELETION	UNP Q07422
C	?	-	GLY	DELETION	UNP Q07422
C	?	-	TRP	DELETION	UNP Q07422
C	?	-	LEU	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	ARG	DELETION	UNP Q07422
C	?	-	LYS	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	DELETION	UNP Q07422
C	?	-	ALA	DELETION	UNP Q07422
C	?	-	LYS	DELETION	UNP Q07422
C	?	-	THR	DELETION	UNP Q07422
C	?	-	GLY	DELETION	UNP Q07422
C	?	-	ASP	DELETION	UNP Q07422
C	?	-	SER	DELETION	UNP Q07422
C	?	-	GLY	DELETION	UNP Q07422
C	?	-	LEU	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	SER	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	SER	DELETION	UNP Q07422
C	?	-	VAL	DELETION	UNP Q07422
C	?	-	GLY	DELETION	UNP Q07422
C	?	-	LYS	DELETION	UNP Q07422
C	?	-	GLN	DELETION	UNP Q07422
C	?	-	ALA	DELETION	UNP Q07422
C	?	-	ALA	DELETION	UNP Q07422
C	?	-	ALA	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	ALA	DELETION	UNP Q07422
C	?	-	GLU	DELETION	UNP Q07422
C	?	-	SER	DELETION	UNP Q07422
C	?	-	VAL	DELETION	UNP Q07422
C	?	-	PHE	DELETION	UNP Q07422
C	?	-	VAL	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	PHE	DELETION	UNP Q07422
C	?	-	CYS	DELETION	UNP Q07422
C	?	-	PRO	DELETION	UNP Q07422
C	?	-	GLU	DELETION	UNP Q07422
C	?	-	LEU	DELETION	UNP Q07422
C	?	-	GLY	DELETION	UNP Q07422
C	?	-	ARG	DELETION	UNP Q07422
D	?	-	ARG	DELETION	UNP Q07422
D	?	-	LEU	DELETION	UNP Q07422
D	?	-	ASN	DELETION	UNP Q07422
D	?	-	GLY	DELETION	UNP Q07422
D	?	-	TRP	DELETION	UNP Q07422
D	?	-	LEU	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ARG	DELETION	UNP Q07422
D	?	-	LYS	DELETION	UNP Q07422
D	?	-	PHE	DELETION	UNP Q07422
D	?	-	ALA	DELETION	UNP Q07422
D	?	-	LYS	DELETION	UNP Q07422
D	?	-	THR	DELETION	UNP Q07422
D	?	-	GLY	DELETION	UNP Q07422
D	?	-	ASP	DELETION	UNP Q07422
D	?	-	SER	DELETION	UNP Q07422
D	?	-	GLY	DELETION	UNP Q07422
D	?	-	LEU	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422
D	?	-	SER	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422
D	?	-	SER	DELETION	UNP Q07422
D	?	-	VAL	DELETION	UNP Q07422
D	?	-	GLY	DELETION	UNP Q07422
D	?	-	LYS	DELETION	UNP Q07422
D	?	-	GLN	DELETION	UNP Q07422
D	?	-	ALA	DELETION	UNP Q07422
D	?	-	ALA	DELETION	UNP Q07422
D	?	-	ALA	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422
D	?	-	ALA	DELETION	UNP Q07422
D	?	-	GLU	DELETION	UNP Q07422
D	?	-	SER	DELETION	UNP Q07422
D	?	-	VAL	DELETION	UNP Q07422
D	?	-	PHE	DELETION	UNP Q07422
D	?	-	VAL	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422
D	?	-	PHE	DELETION	UNP Q07422
D	?	-	CYS	DELETION	UNP Q07422
D	?	-	PRO	DELETION	UNP Q07422
D	?	-	GLU	DELETION	UNP Q07422
D	?	-	LEU	DELETION	UNP Q07422
D	?	-	GLY	DELETION	UNP Q07422
D	?	-	ARG	DELETION	UNP Q07422
E	?	-	ARG	DELETION	UNP Q07422
E	?	-	LEU	DELETION	UNP Q07422
E	?	-	ASN	DELETION	UNP Q07422
E	?	-	GLY	DELETION	UNP Q07422
E	?	-	TRP	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	ARG	DELETION	UNP Q07422
E	?	-	LYS	DELETION	UNP Q07422
E	?	-	PHE	DELETION	UNP Q07422
E	?	-	ALA	DELETION	UNP Q07422
E	?	-	LYS	DELETION	UNP Q07422
E	?	-	THR	DELETION	UNP Q07422
E	?	-	GLY	DELETION	UNP Q07422
E	?	-	ASP	DELETION	UNP Q07422
E	?	-	SER	DELETION	UNP Q07422
E	?	-	GLY	DELETION	UNP Q07422
E	?	-	LEU	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	SER	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	SER	DELETION	UNP Q07422
E	?	-	VAL	DELETION	UNP Q07422
E	?	-	GLY	DELETION	UNP Q07422
E	?	-	LYS	DELETION	UNP Q07422
E	?	-	GLN	DELETION	UNP Q07422
E	?	-	ALA	DELETION	UNP Q07422
E	?	-	ALA	DELETION	UNP Q07422
E	?	-	ALA	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	ALA	DELETION	UNP Q07422
E	?	-	GLU	DELETION	UNP Q07422
E	?	-	SER	DELETION	UNP Q07422
E	?	-	VAL	DELETION	UNP Q07422
E	?	-	PHE	DELETION	UNP Q07422
E	?	-	VAL	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	PHE	DELETION	UNP Q07422
E	?	-	CYS	DELETION	UNP Q07422
E	?	-	PRO	DELETION	UNP Q07422
E	?	-	GLU	DELETION	UNP Q07422
E	?	-	LEU	DELETION	UNP Q07422
E	?	-	GLY	DELETION	UNP Q07422
E	?	-	ARG	DELETION	UNP Q07422
F	?	-	ARG	DELETION	UNP Q07422
F	?	-	LEU	DELETION	UNP Q07422
F	?	-	ASN	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLY	DELETION	UNP Q07422
F	?	-	TRP	DELETION	UNP Q07422
F	?	-	LEU	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	ARG	DELETION	UNP Q07422
F	?	-	LYS	DELETION	UNP Q07422
F	?	-	PHE	DELETION	UNP Q07422
F	?	-	ALA	DELETION	UNP Q07422
F	?	-	LYS	DELETION	UNP Q07422
F	?	-	THR	DELETION	UNP Q07422
F	?	-	GLY	DELETION	UNP Q07422
F	?	-	ASP	DELETION	UNP Q07422
F	?	-	SER	DELETION	UNP Q07422
F	?	-	GLY	DELETION	UNP Q07422
F	?	-	LEU	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	SER	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	SER	DELETION	UNP Q07422
F	?	-	VAL	DELETION	UNP Q07422
F	?	-	GLY	DELETION	UNP Q07422
F	?	-	LYS	DELETION	UNP Q07422
F	?	-	GLN	DELETION	UNP Q07422
F	?	-	ALA	DELETION	UNP Q07422
F	?	-	ALA	DELETION	UNP Q07422
F	?	-	ALA	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	ALA	DELETION	UNP Q07422
F	?	-	GLU	DELETION	UNP Q07422
F	?	-	SER	DELETION	UNP Q07422
F	?	-	VAL	DELETION	UNP Q07422
F	?	-	PHE	DELETION	UNP Q07422
F	?	-	VAL	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	PHE	DELETION	UNP Q07422
F	?	-	CYS	DELETION	UNP Q07422
F	?	-	PRO	DELETION	UNP Q07422
F	?	-	GLU	DELETION	UNP Q07422
F	?	-	LEU	DELETION	UNP Q07422
F	?	-	GLY	DELETION	UNP Q07422
F	?	-	ARG	DELETION	UNP Q07422
G	?	-	ARG	DELETION	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LEU	DELETION	UNP Q07422
G	?	-	ASN	DELETION	UNP Q07422
G	?	-	GLY	DELETION	UNP Q07422
G	?	-	TRP	DELETION	UNP Q07422
G	?	-	LEU	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	ARG	DELETION	UNP Q07422
G	?	-	LYS	DELETION	UNP Q07422
G	?	-	PHE	DELETION	UNP Q07422
G	?	-	ALA	DELETION	UNP Q07422
G	?	-	LYS	DELETION	UNP Q07422
G	?	-	THR	DELETION	UNP Q07422
G	?	-	GLY	DELETION	UNP Q07422
G	?	-	ASP	DELETION	UNP Q07422
G	?	-	SER	DELETION	UNP Q07422
G	?	-	GLY	DELETION	UNP Q07422
G	?	-	LEU	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	SER	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	SER	DELETION	UNP Q07422
G	?	-	VAL	DELETION	UNP Q07422
G	?	-	GLY	DELETION	UNP Q07422
G	?	-	LYS	DELETION	UNP Q07422
G	?	-	GLN	DELETION	UNP Q07422
G	?	-	ALA	DELETION	UNP Q07422
G	?	-	ALA	DELETION	UNP Q07422
G	?	-	ALA	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	ALA	DELETION	UNP Q07422
G	?	-	GLU	DELETION	UNP Q07422
G	?	-	SER	DELETION	UNP Q07422
G	?	-	VAL	DELETION	UNP Q07422
G	?	-	PHE	DELETION	UNP Q07422
G	?	-	VAL	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	PHE	DELETION	UNP Q07422
G	?	-	CYS	DELETION	UNP Q07422
G	?	-	PRO	DELETION	UNP Q07422
G	?	-	GLU	DELETION	UNP Q07422
G	?	-	LEU	DELETION	UNP Q07422
G	?	-	GLY	DELETION	UNP Q07422

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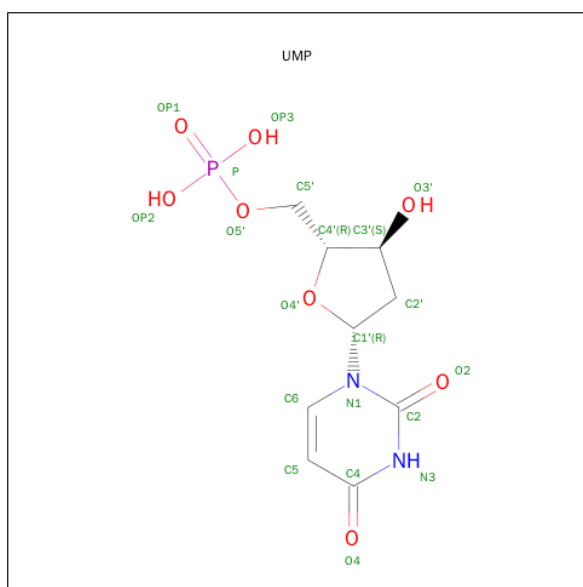
Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ARG	DELETION	UNP Q07422
H	?	-	ARG	DELETION	UNP Q07422
H	?	-	LEU	DELETION	UNP Q07422
H	?	-	ASN	DELETION	UNP Q07422
H	?	-	GLY	DELETION	UNP Q07422
H	?	-	TRP	DELETION	UNP Q07422
H	?	-	LEU	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	ARG	DELETION	UNP Q07422
H	?	-	LYS	DELETION	UNP Q07422
H	?	-	PHE	DELETION	UNP Q07422
H	?	-	ALA	DELETION	UNP Q07422
H	?	-	LYS	DELETION	UNP Q07422
H	?	-	THR	DELETION	UNP Q07422
H	?	-	GLY	DELETION	UNP Q07422
H	?	-	ASP	DELETION	UNP Q07422
H	?	-	SER	DELETION	UNP Q07422
H	?	-	GLY	DELETION	UNP Q07422
H	?	-	LEU	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	SER	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	SER	DELETION	UNP Q07422
H	?	-	VAL	DELETION	UNP Q07422
H	?	-	GLY	DELETION	UNP Q07422
H	?	-	LYS	DELETION	UNP Q07422
H	?	-	GLN	DELETION	UNP Q07422
H	?	-	ALA	DELETION	UNP Q07422
H	?	-	ALA	DELETION	UNP Q07422
H	?	-	ALA	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	ALA	DELETION	UNP Q07422
H	?	-	GLU	DELETION	UNP Q07422
H	?	-	SER	DELETION	UNP Q07422
H	?	-	VAL	DELETION	UNP Q07422
H	?	-	PHE	DELETION	UNP Q07422
H	?	-	VAL	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	PHE	DELETION	UNP Q07422
H	?	-	CYS	DELETION	UNP Q07422
H	?	-	PRO	DELETION	UNP Q07422
H	?	-	GLU	DELETION	UNP Q07422

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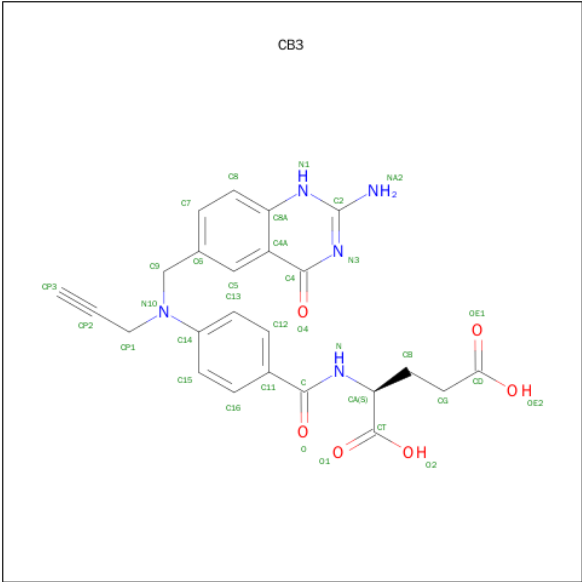
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	DELETION	UNP Q07422
H	?	-	GLY	DELETION	UNP Q07422
H	?	-	ARG	DELETION	UNP Q07422

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



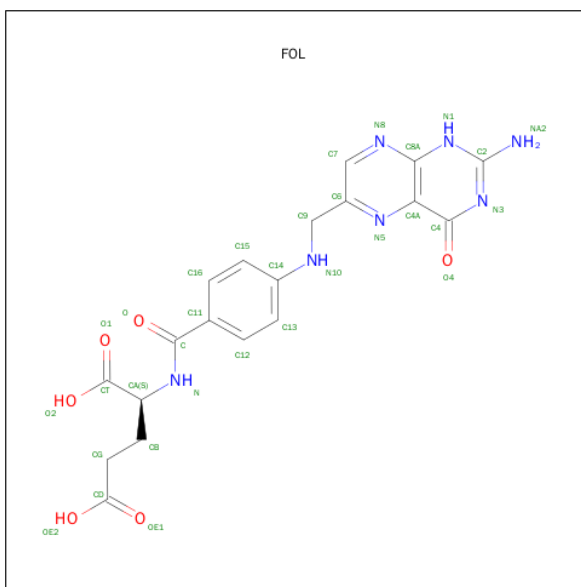
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	G	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	H	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

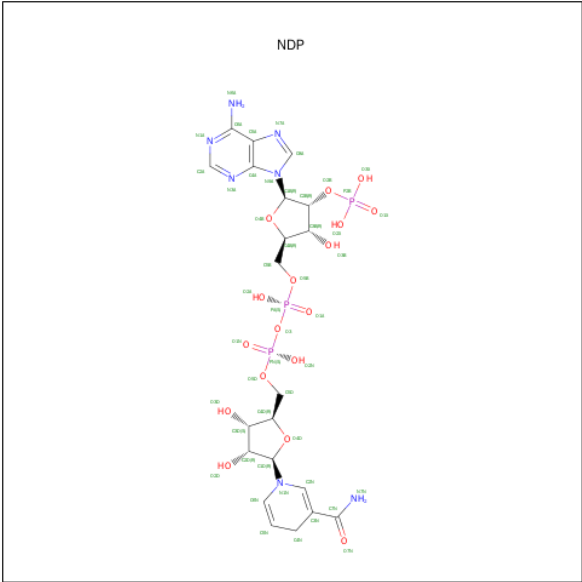
- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		
3	F	1	Total	C	N	O	0	0
			35	24	5	6		
3	G	1	Total	C	N	O	0	0
			35	24	5	6		
3	H	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	248	Total	O	0	0
			248	248		
6	B	229	Total	O	0	0
			229	229		
6	C	224	Total	O	0	0
			224	224		
6	D	232	Total	O	0	0
			232	232		

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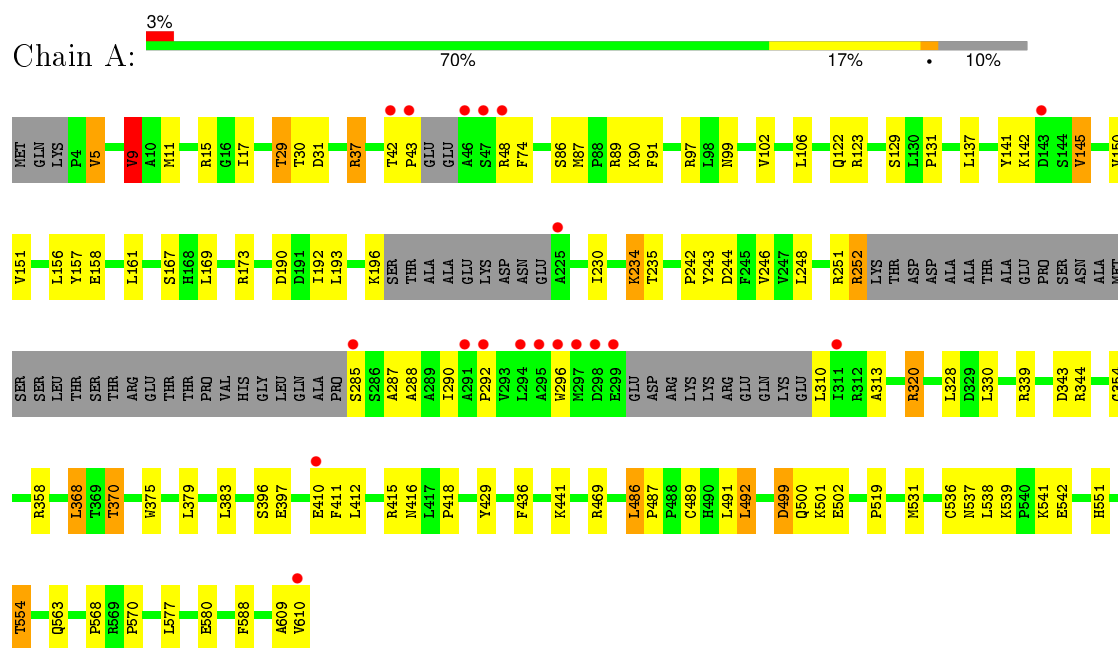
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	220	Total 220	O 220	0	0
6	F	242	Total 242	O 242	0	0
6	G	221	Total 221	O 221	0	0
6	H	215	Total 215	O 215	0	0

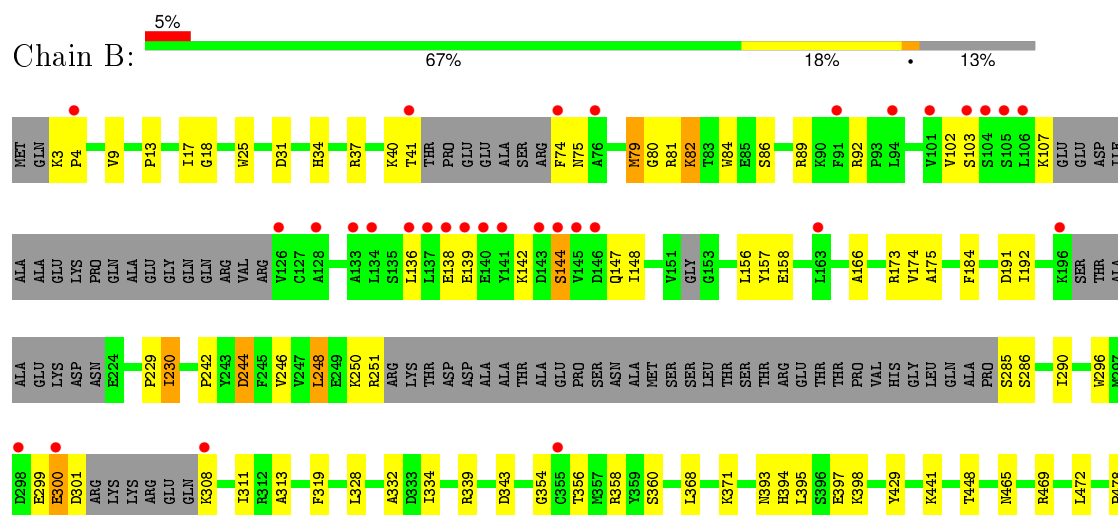
3 Residue-property plots [i](#)

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: Bifunctional dihydrofolate reductase-thymidylate synthase

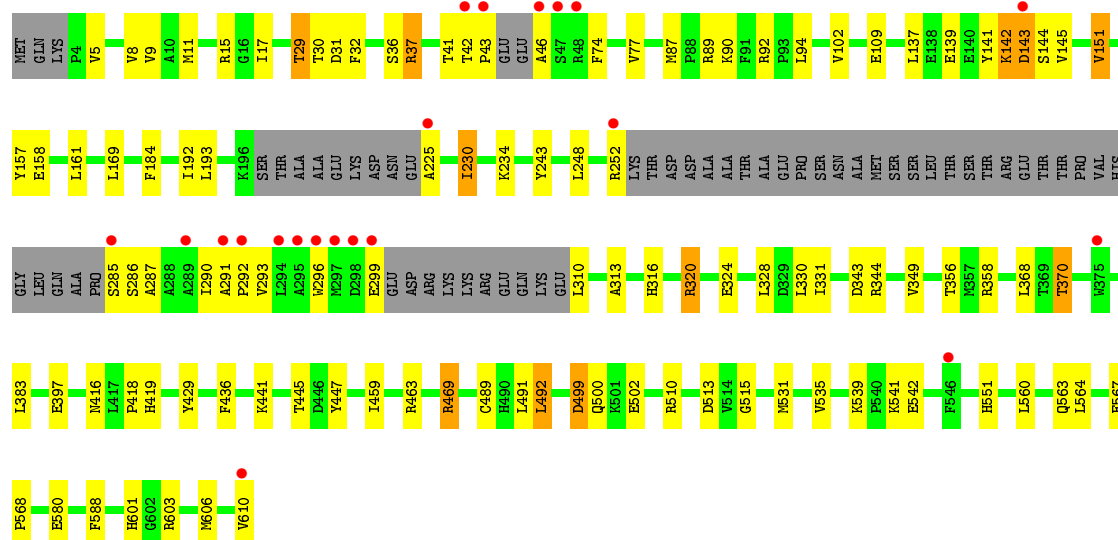


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

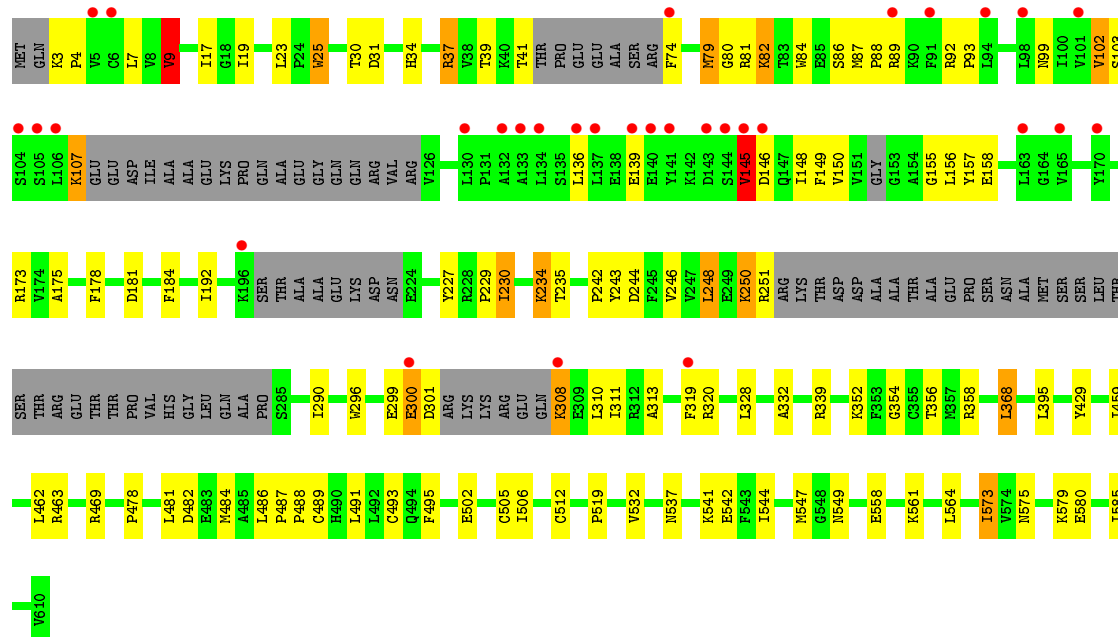




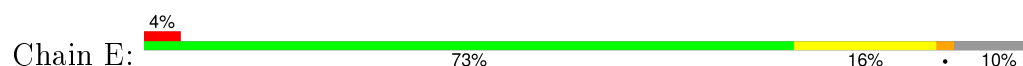
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

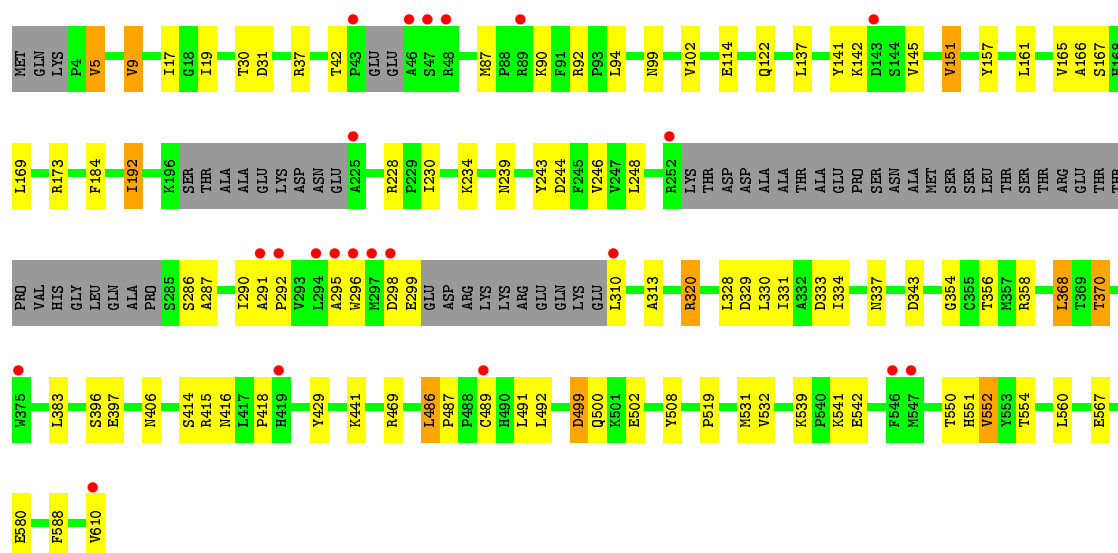


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

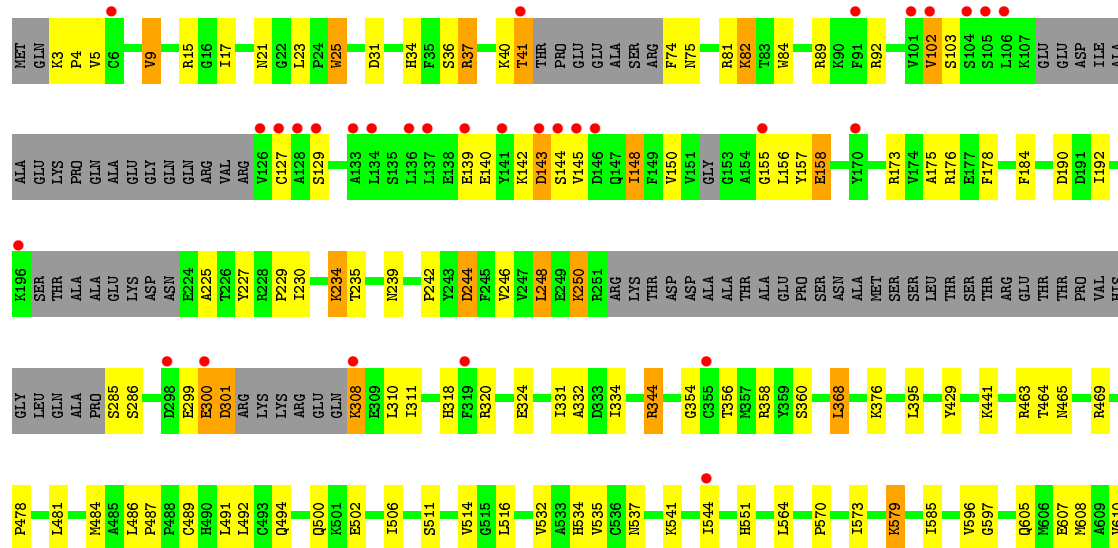


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

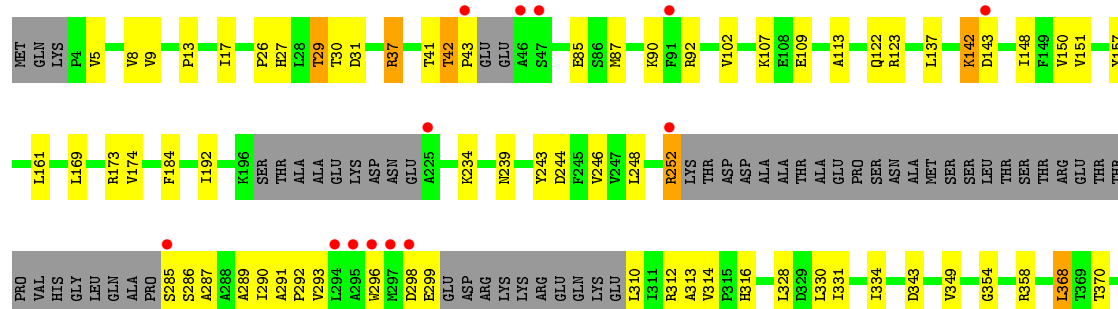


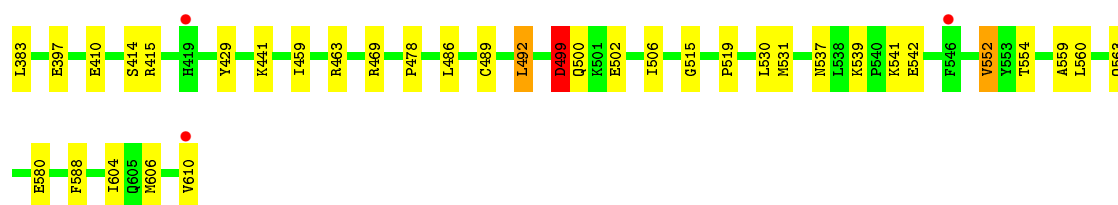


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

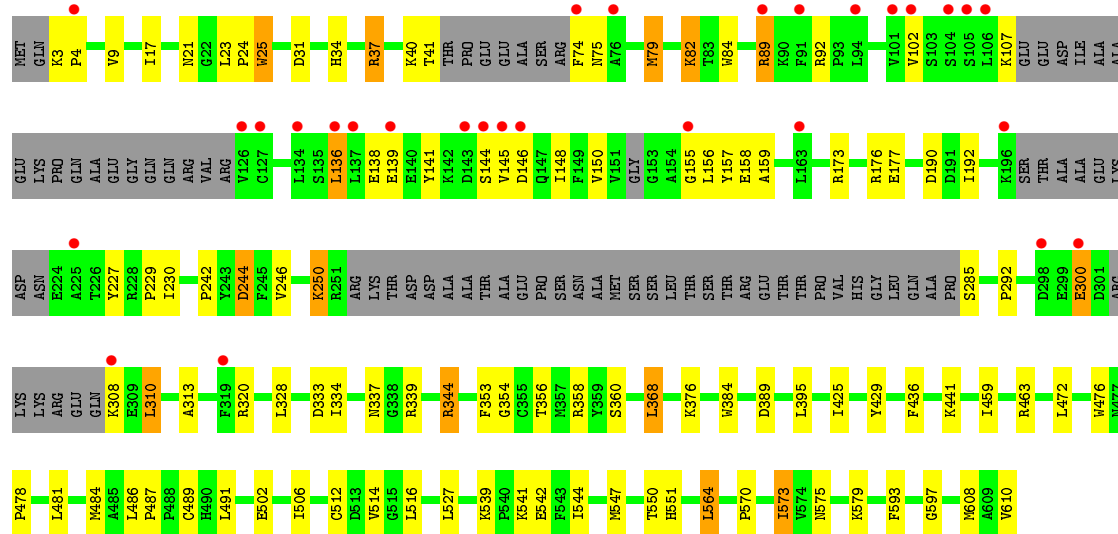


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.79 Å 144.40 Å 177.60 Å 90.01° 89.93° 90.38°	Depositor
Resolution (Å)	48.40 – 2.20 48.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.40-2.20) 97.3 (48.60-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.183 , 0.233 0.182 , 0.233	Depositor DCC
R_{free} test set	13380 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.7	EDS
Estimated twinning fraction	0.417 for h,-k,-l 0.410 for -h,k,-l 0.447 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 265051 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35087	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FOL, CB3, UMP, NDP

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	0.37	0/4196	0.58	1/5683 (0.0%)
1	B	0.36	0/4043	0.59	0/5473
1	C	0.37	0/4196	0.58	0/5683
1	D	0.37	0/4043	0.58	1/5473 (0.0%)
1	E	0.36	0/4196	0.57	1/5683 (0.0%)
1	F	0.35	0/4043	0.58	1/5473 (0.0%)
1	G	0.36	0/4196	0.57	0/5683
1	H	0.35	0/4043	0.59	0/5473
All	All	0.36	0/32956	0.58	4/44624 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	VAL	CB-CA-C	-6.13	99.75	111.40
1	A	9	VAL	CB-CA-C	-6.06	99.88	111.40
1	F	9	VAL	CB-CA-C	-5.23	101.46	111.40
1	E	9	VAL	CB-CA-C	-5.02	101.86	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	609	ALA	Peptide

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	4096	0	4058	88	0
1	B	3948	0	3910	77	0
1	C	4096	0	4058	65	0
1	D	3948	0	3910	82	0
1	E	4096	0	4058	60	0
1	F	3948	0	3910	85	0
1	G	4096	0	4058	60	0
1	H	3948	0	3910	76	0
2	A	20	0	11	3	0
2	B	20	0	11	7	0
2	C	20	0	11	4	0
2	D	20	0	11	4	0
2	E	20	0	11	3	0
2	F	20	0	11	4	0
2	G	20	0	11	2	0
2	H	20	0	11	5	0
3	A	35	0	21	2	0
3	B	35	0	21	4	0
3	C	35	0	21	4	0
3	D	35	0	21	3	0
3	E	35	0	21	1	0
3	F	35	0	21	4	0
3	G	35	0	21	1	0
3	H	35	0	21	4	0
4	A	32	0	17	4	0
4	B	32	0	17	2	0
4	C	32	0	17	5	0
4	D	32	0	17	2	0
4	E	32	0	17	4	0
4	F	32	0	17	3	0
4	G	32	0	17	4	0
4	H	32	0	17	2	0
5	A	48	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	48	0	25	7	0
5	C	48	0	24	5	0
5	D	48	0	24	7	0
5	E	48	0	24	4	0
5	F	48	0	25	8	0
5	G	48	0	24	3	0
5	H	48	0	25	7	0
6	A	248	0	0	28	0
6	B	229	0	0	11	0
6	C	224	0	0	10	0
6	D	232	0	0	23	0
6	E	220	0	0	16	0
6	F	242	0	0	29	0
6	G	221	0	0	13	0
6	H	215	0	0	20	0
All	All	35087	0	32459	584	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 9.

All (584) 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:G:287:ALA:HA	1:G:290:ILE:HD12	1.54	0.89
1:G:370:THR:HG23	1:G:563:GLN:HE21	1.41	0.82
1:F:484:MET:SD	6:F:872:HOH:O	2.38	0.82
1:G:499:ASP:HB3	1:G:500:GLN:HG2	1.62	0.81
1:F:481:LEU:HA	1:F:484:MET:HE2	1.65	0.79
1:B:484:MET:SD	6:B:842:HOH:O	2.42	0.77
1:D:484:MET:SD	6:D:844:HOH:O	2.43	0.76
1:C:328:LEU:HD21	1:C:370:THR:HG21	1.66	0.76
1:E:358:ARG:NH2	1:F:354:GLY:O	2.20	0.75
1:D:558:GLU:HA	6:D:968:HOH:O	1.87	0.75
1:A:328:LEU:HD21	1:A:370:THR:HG21	1.67	0.74
1:F:234:LYS:HB3	6:F:948:HOH:O	1.88	0.73
1:H:481:LEU:HA	1:H:484:MET:HE2	1.69	0.73
1:H:344:ARG:NH2	1:H:610:VAL:O	2.23	0.72
1:A:287:ALA:HA	1:A:290:ILE:HD12	1.70	0.72
1:H:484:MET:HE3	1:H:487:PRO:HA	1.70	0.72
1:D:495:PHE:HB2	6:D:920:HOH:O	1.90	0.71
1:B:244:ASP:HB2	1:B:570:PRO:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LEU:HA	1:B:484:MET:HE2	1.73	0.71
1:E:354:GLY:O	1:F:358:ARG:NH2	2.24	0.71
1:E:328:LEU:HD21	1:E:370:THR:HG21	1.73	0.70
6:E:886:HOH:O	1:F:494:GLN:HB3	1.90	0.70
1:D:505:CYS:SG	6:D:990:HOH:O	2.49	0.70
1:A:538:LEU:HA	6:A:954:HOH:O	1.91	0.70
1:D:192:ILE:HD12	1:D:248:LEU:HD11	1.72	0.69
1:E:313:ALA:O	1:E:320:ARG:NH2	2.23	0.69
1:D:505:CYS:SG	6:D:1015:HOH:O	2.50	0.69
1:A:296:TRP:HB3	1:B:37:ARG:HG3	1.75	0.68
1:G:328:LEU:HD21	1:G:370:THR:HG21	1.76	0.68
1:A:102:VAL:O	5:A:704:NDP:H1B	1.94	0.68
1:E:499:ASP:HB3	1:E:500:GLN:HG2	1.76	0.68
1:D:481:LEU:HA	1:D:484:MET:HE2	1.73	0.67
1:E:287:ALA:HA	1:E:290:ILE:HD12	1.76	0.67
1:H:141:TYR:O	1:H:145:VAL:HG12	1.94	0.67
1:A:536:CYS:SG	6:A:950:HOH:O	2.51	0.67
1:B:82:LYS:HD3	5:B:704:NDP:H51A	1.75	0.67
1:A:537:ASN:O	6:A:954:HOH:O	2.12	0.67
1:F:244:ASP:HB2	1:F:570:PRO:HG3	1.77	0.66
1:A:313:ALA:O	1:A:320:ARG:NH2	2.19	0.66
1:A:501:LYS:HB3	6:A:954:HOH:O	1.96	0.66
1:F:532:VAL:HA	6:F:930:HOH:O	1.95	0.66
1:F:484:MET:HE3	1:F:487:PRO:HA	1.76	0.66
1:C:102:VAL:O	5:C:704:NDP:H1B	1.96	0.66
1:A:343:ASP:OD1	1:B:469:ARG:NH1	2.29	0.66
1:E:102:VAL:O	5:E:704:NDP:H1B	1.96	0.66
1:A:491:LEU:HD11	1:B:492:LEU:HD11	1.78	0.65
1:A:42:THR:HG22	1:A:43:PRO:HD2	1.78	0.65
1:C:568:PRO:HA	6:C:883:HOH:O	1.96	0.65
1:C:358:ARG:NH2	1:D:354:GLY:O	2.30	0.65
1:G:370:THR:CG2	1:G:563:GLN:HE21	2.10	0.65
1:A:344:ARG:NH2	6:A:862:HOH:O	2.28	0.65
1:G:9:VAL:HG12	1:G:157:TYR:CZ	2.31	0.65
1:D:234:LYS:HB3	6:D:935:HOH:O	1.97	0.65
1:H:176:ARG:HG3	6:H:975:HOH:O	1.96	0.65
1:H:102:VAL:O	5:H:704:NDP:H1B	1.97	0.65
1:H:313:ALA:O	1:H:320:ARG:NH1	2.30	0.64
1:B:484:MET:HE3	1:B:487:PRO:HA	1.79	0.64
1:H:244:ASP:HB2	1:H:570:PRO:HG3	1.79	0.64
1:G:17:ILE:O	5:G:704:NDP:H2N	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ILE:HD13	6:G:981:HOH:O	1.96	0.64
1:H:79:MET:HE2	1:H:84:TRP:HA	1.80	0.63
1:H:82:LYS:HD3	5:H:704:NDP:H51A	1.80	0.63
1:H:313:ALA:HB2	1:H:564:LEU:HD13	1.78	0.63
1:A:368:LEU:HD23	1:A:519:PRO:HB3	1.78	0.63
1:C:225:ALA:HA	1:C:252:ARG:HA	1.80	0.63
1:F:585:ILE:HD13	6:F:930:HOH:O	1.97	0.63
1:G:102:VAL:O	5:G:704:NDP:H1B	1.99	0.63
1:B:313:ALA:HB2	1:B:564:LEU:HD13	1.80	0.62
1:A:469:ARG:NH1	2:B:701:UMP:OP3	2.31	0.62
1:A:554:THR:N	6:A:927:HOH:O	2.31	0.62
1:F:465:ASN:N	6:F:855:HOH:O	2.31	0.62
1:A:141:TYR:HB3	1:A:145:VAL:HG13	1.82	0.62
1:D:478:PRO:HA	1:D:481:LEU:HG	1.81	0.62
1:G:42:THR:HG22	1:G:43:PRO:HD2	1.81	0.62
1:D:17:ILE:O	5:D:704:NDP:H2N	2.00	0.62
1:B:568:PRO:HA	6:B:925:HOH:O	1.99	0.62
1:A:570:PRO:HB2	6:A:999:HOH:O	1.99	0.61
1:G:239:ASN:HB2	6:G:979:HOH:O	2.00	0.61
1:B:393:ASN:HB2	6:B:946:HOH:O	2.00	0.61
1:E:508:TYR:OH	6:E:886:HOH:O	2.10	0.61
1:F:311:ILE:HD11	1:F:332:ALA:HA	1.83	0.61
1:F:234:LYS:NZ	6:F:948:HOH:O	2.32	0.60
1:A:173:ARG:HD3	1:A:244:ASP:OD1	2.01	0.60
1:B:465:ASN:N	6:B:843:HOH:O	2.34	0.60
1:D:484:MET:HE3	1:D:487:PRO:HA	1.81	0.60
1:E:17:ILE:O	5:E:704:NDP:H2N	2.01	0.60
1:C:143:ASP:HB3	6:C:865:HOH:O	2.00	0.60
1:H:3:LYS:N	6:H:853:HOH:O	2.35	0.60
4:F:703:FOL:C7	5:F:704:NDP:H42N	2.32	0.59
1:B:568:PRO:HG3	6:B:972:HOH:O	2.03	0.59
1:E:406:ASN:ND2	6:E:871:HOH:O	2.35	0.59
1:H:40:LYS:HA	1:H:75:ASN:HD22	1.67	0.59
4:D:703:FOL:C7	5:D:704:NDP:H42N	2.33	0.58
1:E:296:TRP:HB3	1:F:37:ARG:HG3	1.86	0.58
1:F:579:LYS:H	1:F:579:LYS:HE2	1.68	0.58
1:F:368:LEU:HD23	6:F:1029:HOH:O	2.03	0.58
1:C:17:ILE:O	5:C:704:NDP:H2N	2.03	0.57
1:A:29:THR:HG22	6:A:851:HOH:O	2.04	0.57
1:A:501:LYS:HE3	6:A:954:HOH:O	2.04	0.57
1:A:48:ARG:NH1	6:A:937:HOH:O	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PRO:HA	6:A:912:HOH:O	2.05	0.57
1:C:368:LEU:HD22	1:C:368:LEU:H	1.69	0.57
1:G:29:THR:HG22	6:G:845:HOH:O	2.05	0.57
1:H:9:VAL:HG12	1:H:157:TYR:CZ	2.39	0.57
1:F:84:TRP:CE2	1:F:92:ARG:HD2	2.39	0.57
1:B:17:ILE:O	5:B:704:NDP:H2N	2.05	0.57
1:E:239:ASN:HB2	6:E:866:HOH:O	2.04	0.57
1:F:84:TRP:HB3	6:F:894:HOH:O	2.04	0.57
1:H:155:GLY:O	1:H:159:ALA:N	2.32	0.57
1:D:561:LYS:HB2	6:D:968:HOH:O	2.05	0.56
1:A:169:LEU:HD12	1:A:248:LEU:HD12	1.86	0.56
1:B:192:ILE:HD11	1:B:229:PRO:HD3	1.87	0.56
1:F:82:LYS:HD3	5:F:704:NDP:H51A	1.88	0.56
1:C:313:ALA:O	1:C:320:ARG:NH2	2.23	0.56
1:G:298:ASP:OD1	1:G:299:GLU:N	2.38	0.56
1:A:411:PHE:HB3	6:A:1012:HOH:O	2.05	0.56
1:D:573:ILE:HD11	1:D:575:ASN:OD1	2.05	0.56
1:H:31:ASP:OD2	4:H:703:FOL:N3	2.39	0.56
1:D:175:ALA:HB3	1:D:242:PRO:HG2	1.88	0.56
1:F:15:ARG:NH2	1:F:184:PHE:O	2.35	0.56
1:F:506:ILE:HG12	1:F:544:ILE:HB	1.88	0.55
4:A:703:FOL:C7	5:A:704:NDP:H42N	2.36	0.55
1:C:31:ASP:OD2	4:C:703:FOL:N3	2.39	0.55
1:D:84:TRP:CZ2	1:D:92:ARG:HD2	2.41	0.55
1:H:310:LEU:N	6:H:979:HOH:O	2.38	0.55
1:D:506:ILE:HG12	1:D:544:ILE:HB	1.88	0.55
1:D:561:LYS:HD3	6:D:968:HOH:O	2.06	0.55
1:B:9:VAL:HG12	1:B:157:TYR:CZ	2.42	0.55
1:D:537:ASN:HB3	6:D:807:HOH:O	2.06	0.55
1:B:74:PHE:N	1:B:144:SER:O	2.40	0.55
1:D:93:PRO:HA	6:D:884:HOH:O	2.06	0.55
1:A:285:SER:HA	1:A:288:ALA:HB3	1.88	0.55
1:H:597:GLY:HA3	6:H:975:HOH:O	2.05	0.55
1:H:17:ILE:O	5:H:704:NDP:H2N	2.07	0.55
1:G:354:GLY:O	1:H:358:ARG:NH2	2.39	0.55
1:G:5:VAL:HG21	1:G:150:VAL:HG23	1.89	0.55
1:F:176:ARG:HG3	6:F:952:HOH:O	2.06	0.55
1:A:551:HIS:NE2	2:A:701:UMP:O3'	2.31	0.55
1:G:492:LEU:HD11	1:H:491:LEU:HD11	1.89	0.55
1:G:9:VAL:HG11	1:G:184:PHE:CE1	2.42	0.54
1:H:368:LEU:HD23	6:H:1004:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HG21	1:B:319:PHE:CD2	2.42	0.54
1:F:3:LYS:HG3	6:F:810:HOH:O	2.07	0.54
1:B:3:LYS:N	1:B:4:PRO:HD3	2.21	0.54
1:C:499:ASP:HB3	1:C:500:GLN:HG2	1.88	0.54
1:B:13:PRO:HD3	1:B:174:VAL:O	2.07	0.54
1:A:354:GLY:O	1:B:358:ARG:NH2	2.39	0.54
1:B:102:VAL:HG21	1:B:156:LEU:HD11	1.89	0.54
1:F:597:GLY:HA3	6:F:952:HOH:O	2.06	0.54
1:B:173:ARG:HD2	1:B:246:VAL:HG13	1.88	0.54
1:D:313:ALA:O	1:D:320:ARG:NH1	2.40	0.54
1:C:169:LEU:HD12	1:C:248:LEU:HD12	1.90	0.54
1:H:551:HIS:NE2	2:H:701:UMP:O3'	2.33	0.54
1:F:5:VAL:HG13	1:F:148:ILE:HG12	1.90	0.53
1:G:370:THR:HG23	1:G:563:GLN:NE2	2.19	0.53
1:D:192:ILE:CD1	1:D:246:VAL:HG21	2.37	0.53
1:C:601:HIS:ND1	6:C:894:HOH:O	2.33	0.53
1:G:368:LEU:HD23	1:G:519:PRO:HB3	1.89	0.53
1:F:484:MET:CE	1:F:487:PRO:HA	2.39	0.53
5:C:704:NDP:N6A	6:C:886:HOH:O	2.34	0.53
1:G:285:SER:HB2	1:G:289:ALA:HB2	1.90	0.53
1:A:339:ARG:HB2	6:B:994:HOH:O	2.08	0.53
1:G:358:ARG:NH2	1:H:354:GLY:O	2.40	0.53
1:A:190:ASP:OD1	1:A:196:LYS:HE3	2.09	0.53
1:A:358:ARG:HD3	1:A:542:GLU:OE1	2.09	0.53
1:G:107:LYS:HB2	1:G:109:GLU:HG2	1.91	0.52
6:E:886:HOH:O	1:F:506:ILE:HB	2.09	0.52
1:E:298:ASP:OD1	1:E:299:GLU:N	2.39	0.52
1:D:585:ILE:HD13	6:D:914:HOH:O	2.08	0.52
1:A:11:MET:HG2	1:A:15:ARG:HA	1.91	0.52
1:H:155:GLY:N	6:H:973:HOH:O	2.30	0.52
1:A:412:LEU:HG	6:A:1012:HOH:O	2.09	0.52
1:H:376:LYS:NZ	6:H:884:HOH:O	2.41	0.52
1:B:40:LYS:HA	1:B:75:ASN:HD22	1.73	0.52
1:H:344:ARG:O	1:H:344:ARG:HG2	2.10	0.52
1:B:551:HIS:NE2	2:B:701:UMP:O3'	2.34	0.52
1:C:469:ARG:HD3	1:D:549:ASN:CG	2.30	0.52
1:A:230:ILE:HG23	1:B:290:ILE:HD11	1.91	0.52
1:A:296:TRP:CZ2	1:B:34:HIS:HB2	2.45	0.52
1:H:74:PHE:O	1:H:145:VAL:HA	2.10	0.52
1:H:242:PRO:HG3	1:H:573:ILE:HG23	1.91	0.52
1:F:324:GLU:HA	6:F:914:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:HG12	1:E:157:TYR:CZ	2.45	0.52
1:F:31:ASP:OD2	4:F:703:FOL:N3	2.42	0.52
1:E:167:SER:HB3	6:E:997:HOH:O	2.10	0.52
1:H:4:PRO:HA	6:H:820:HOH:O	2.09	0.52
1:D:82:LYS:HD3	5:D:704:NDP:H51A	1.92	0.52
1:E:291:ALA:N	1:E:292:PRO:HD2	2.25	0.52
1:E:368:LEU:HD22	6:E:1007:HOH:O	2.10	0.52
1:H:192:ILE:HD11	1:H:229:PRO:HD3	1.91	0.52
1:A:296:TRP:CB	1:B:37:ARG:HG3	2.38	0.52
1:B:102:VAL:O	5:B:704:NDP:H1B	2.10	0.52
1:C:141:TYR:HB3	1:C:145:VAL:HG13	1.92	0.52
1:D:368:LEU:HD23	1:D:519:PRO:HB3	1.92	0.52
1:F:535:VAL:HA	6:F:957:HOH:O	2.09	0.52
1:D:102:VAL:O	5:D:704:NDP:H1B	2.09	0.51
1:D:84:TRP:CE2	1:D:92:ARG:HD2	2.45	0.51
1:E:358:ARG:HD3	1:E:542:GLU:OE1	2.10	0.51
2:A:701:UMP:H1'	3:A:702:CB3:N3	2.26	0.51
4:E:703:FOL:C7	5:E:704:NDP:H42N	2.40	0.51
1:F:21:ASN:HA	5:F:704:NDP:H3D	1.93	0.51
1:C:87:MET:HE2	1:C:92:ARG:HB3	1.92	0.51
1:E:9:VAL:HG11	1:E:184:PHE:CE1	2.45	0.51
1:F:607:GLU:CD	1:F:607:GLU:H	2.14	0.51
1:G:252:ARG:NH2	6:G:952:HOH:O	2.43	0.51
1:E:486:LEU:HD23	1:E:487:PRO:HD2	1.93	0.51
1:F:129:SER:HA	6:F:844:HOH:O	2.10	0.51
1:A:17:ILE:O	5:A:704:NDP:H2N	2.10	0.51
1:F:103:SER:OG	5:F:704:NDP:O1X	2.29	0.51
1:H:333:ASP:OD1	1:H:337:ASN:ND2	2.40	0.51
1:H:506:ILE:HG12	1:H:544:ILE:HB	1.92	0.51
1:C:296:TRP:CZ2	1:D:34:HIS:HB2	2.46	0.51
1:H:484:MET:CE	1:H:487:PRO:HA	2.39	0.51
1:D:87:MET:HE2	6:D:987:HOH:O	2.11	0.51
4:G:703:FOL:H15	6:G:867:HOH:O	2.11	0.50
1:A:31:ASP:OD2	4:A:703:FOL:N3	2.44	0.50
1:H:136:LEU:HB3	6:H:905:HOH:O	2.11	0.50
1:F:150:VAL:HG13	1:F:156:LEU:HD23	1.93	0.50
1:B:484:MET:CE	1:B:487:PRO:HA	2.41	0.50
1:B:31:ASP:OD2	4:B:703:FOL:N3	2.44	0.50
4:G:703:FOL:C7	5:G:704:NDP:H42N	2.41	0.50
1:E:416:ASN:C	1:E:418:PRO:HD3	2.32	0.50
1:F:464:THR:N	6:F:855:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ILE:O	5:F:704:NDP:H2N	2.11	0.50
1:C:29:THR:HG22	6:C:957:HOH:O	2.11	0.50
1:G:173:ARG:HD2	1:G:246:VAL:HG13	1.92	0.50
1:D:512:CYS:SG	1:D:547:MET:HB3	2.52	0.50
1:G:31:ASP:OD2	4:G:703:FOL:N3	2.44	0.50
2:B:701:UMP:H1'	3:B:702:CB3:N3	2.27	0.50
3:A:702:CB3:HB1	6:A:899:HOH:O	2.11	0.50
1:B:175:ALA:HB3	1:B:242:PRO:HG2	1.92	0.50
1:C:531:MET:HE3	1:C:588:PHE:CD2	2.47	0.50
1:G:358:ARG:HD3	1:G:542:GLU:OE1	2.11	0.50
1:E:531:MET:HE3	1:E:588:PHE:CD2	2.46	0.50
2:F:701:UMP:H1'	3:F:702:CB3:N3	2.27	0.50
1:C:9:VAL:HG12	1:C:157:TYR:CZ	2.47	0.50
1:B:9:VAL:HG11	1:B:184:PHE:CE2	2.47	0.49
1:E:19:ILE:HB	6:E:967:HOH:O	2.12	0.49
1:F:344:ARG:NH2	1:F:610:VAL:O	2.46	0.49
1:B:79:MET:HE2	1:B:84:TRP:HA	1.95	0.49
1:G:109:GLU:CD	1:G:109:GLU:H	2.16	0.49
1:H:300:GLU:HG2	1:H:300:GLU:O	2.12	0.49
1:D:234:LYS:HG2	1:D:235:THR:N	2.27	0.49
1:B:358:ARG:HD3	1:B:542:GLU:OE1	2.12	0.49
1:G:368:LEU:HD22	6:G:802:HOH:O	2.11	0.49
1:E:5:VAL:HG12	1:E:166:ALA:HA	1.94	0.49
1:E:165:VAL:HG21	6:E:986:HOH:O	2.11	0.49
1:D:39:THR:HA	1:D:149:PHE:CE2	2.47	0.49
2:H:701:UMP:H1'	3:H:702:CB3:N3	2.28	0.49
1:C:515:GLY:O	1:C:606:MET:HE1	2.13	0.49
1:A:531:MET:HE3	1:A:588:PHE:CD2	2.47	0.49
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.48	0.49
1:G:478:PRO:HD2	1:H:436:PHE:CE1	2.47	0.49
1:A:358:ARG:NH2	1:B:354:GLY:O	2.46	0.48
2:D:701:UMP:H1'	3:D:702:CB3:N3	2.28	0.48
1:D:103:SER:OG	5:D:704:NDP:O1X	2.30	0.48
1:E:492:LEU:HD11	1:F:491:LEU:HD11	1.95	0.48
1:A:368:LEU:HD22	6:A:1041:HOH:O	2.12	0.48
1:E:230:ILE:HB	6:E:953:HOH:O	2.13	0.48
1:E:169:LEU:HD12	1:E:248:LEU:HD12	1.95	0.48
4:C:703:FOL:C7	5:C:704:NDP:H42N	2.42	0.48
5:H:704:NDP:C8A	5:H:704:NDP:C3B	2.91	0.48
1:D:9:VAL:HG13	1:D:157:TYR:CZ	2.49	0.48
1:E:141:TYR:HB3	1:E:145:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:ILE:HG21	1:E:552:VAL:HG13	1.96	0.48
1:G:316:HIS:HB2	6:G:922:HOH:O	2.13	0.48
1:B:394:HIS:CD2	6:B:946:HOH:O	2.66	0.48
1:A:492:LEU:HD11	1:B:491:LEU:HD11	1.94	0.48
1:D:484:MET:CE	1:D:487:PRO:HA	2.44	0.48
1:H:84:TRP:CE2	1:H:92:ARG:HD2	2.47	0.48
1:A:235:THR:HG23	6:A:999:HOH:O	2.13	0.48
1:H:502:GLU:HB3	1:H:541:LYS:HB2	1.96	0.48
1:G:296:TRP:CZ2	1:H:34:HIS:HB2	2.49	0.48
1:D:469:ARG:HD3	6:D:815:HOH:O	2.13	0.48
1:E:296:TRP:CZ2	1:F:34:HIS:HB2	2.49	0.48
1:D:155:GLY:HA2	1:D:158:GLU:CD	2.34	0.48
1:B:81:ARG:HE	5:B:704:NDP:P2B	2.36	0.48
1:A:469:ARG:NH1	2:B:701:UMP:P	2.87	0.48
1:E:502:GLU:HB3	1:E:541:LYS:HB2	1.96	0.48
1:F:300:GLU:HA	1:F:301:ASP:HA	1.66	0.47
1:D:173:ARG:HD2	1:D:246:VAL:HG13	1.95	0.47
1:G:173:ARG:HD3	1:G:244:ASP:OD1	2.14	0.47
4:E:703:FOL:H15	6:E:895:HOH:O	2.13	0.47
1:A:491:LEU:HD11	1:B:492:LEU:CD1	2.43	0.47
1:H:476:TRP:HB2	1:H:491:LEU:HD13	1.96	0.47
1:C:296:TRP:HB3	1:D:37:ARG:HG2	1.97	0.47
1:D:300:GLU:HA	1:D:301:ASP:HA	1.66	0.47
1:A:415:ARG:HB2	6:A:940:HOH:O	2.13	0.47
1:H:3:LYS:HG3	6:H:863:HOH:O	2.13	0.47
1:D:488:PRO:HD2	6:D:895:HOH:O	2.13	0.47
1:F:74:PHE:N	1:F:144:SER:O	2.47	0.47
1:A:86:SER:HB3	6:A:920:HOH:O	2.14	0.47
1:E:230:ILE:HD13	1:F:286:SER:HB2	1.94	0.47
1:D:493:CYS:HB2	6:D:1015:HOH:O	2.13	0.47
1:D:74:PHE:O	1:D:145:VAL:HA	2.13	0.47
1:A:173:ARG:HD2	1:A:246:VAL:HG13	1.96	0.47
1:F:175:ALA:HB3	1:F:242:PRO:HG2	1.96	0.47
1:E:334:ILE:HD11	1:E:550:THR:HG22	1.96	0.47
1:G:291:ALA:N	1:G:292:PRO:HD2	2.28	0.47
1:H:138:GLU:HA	6:H:821:HOH:O	2.15	0.47
1:C:151:VAL:HG13	4:C:703:FOL:H7	1.97	0.47
5:D:704:NDP:C3B	5:D:704:NDP:C8A	2.93	0.47
1:D:84:TRP:HA	6:D:901:HOH:O	2.14	0.47
1:C:9:VAL:HG11	1:C:184:PHE:CE1	2.50	0.47
1:F:173:ARG:HD2	1:F:246:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:539:LYS:HD3	6:H:972:HOH:O	2.15	0.47
1:B:229:PRO:HA	1:B:248:LEU:HD12	1.97	0.47
1:C:287:ALA:HA	1:C:290:ILE:HD13	1.96	0.47
1:G:26:PRO:HG2	6:G:979:HOH:O	2.15	0.46
2:E:701:UMP:H1'	3:E:702:CB3:N3	2.30	0.46
1:B:368:LEU:HD22	1:B:368:LEU:H	1.80	0.46
1:F:25:TRP:HB3	1:F:178:PHE:CE2	2.51	0.46
1:D:19:ILE:HA	1:D:181:ASP:OD1	2.15	0.46
1:C:492:LEU:HD11	1:D:491:LEU:HD11	1.98	0.46
1:B:166:ALA:O	1:B:250:LYS:HE2	2.15	0.46
1:A:577:LEU:HA	6:A:952:HOH:O	2.15	0.46
1:G:492:LEU:CD1	1:H:491:LEU:HD11	2.46	0.46
1:H:489:CYS:SG	2:H:701:UMP:C6	3.09	0.46
1:A:158:GLU:HG3	6:A:926:HOH:O	2.14	0.46
1:E:173:ARG:HD3	1:E:244:ASP:OD1	2.15	0.46
1:A:151:VAL:HG13	4:A:703:FOL:H7	1.98	0.46
1:H:328:LEU:HD22	1:H:564:LEU:HD22	1.96	0.46
1:H:608:MET:HE2	3:H:702:CB3:H16	1.98	0.46
1:G:531:MET:HE3	1:G:588:PHE:CD2	2.49	0.46
1:A:502:GLU:HB3	1:A:541:LYS:HB2	1.98	0.46
1:H:478:PRO:HA	1:H:481:LEU:HG	1.98	0.46
5:B:704:NDP:C8A	5:B:704:NDP:C3B	2.93	0.46
1:G:27[A]:HIS:O	6:G:845:HOH:O	2.15	0.46
1:D:358:ARG:HD3	1:D:542:GLU:OE1	2.16	0.46
1:E:151:VAL:O	4:E:703:FOL:H7	2.16	0.46
1:A:42:THR:CG2	1:A:43:PRO:HD2	2.45	0.46
1:H:23:LEU:HD13	1:H:25:TRP:CZ3	2.51	0.46
1:E:368:LEU:HD23	1:E:519:PRO:HB3	1.97	0.46
1:E:31:ASP:OD2	4:E:703:FOL:N3	2.49	0.45
1:E:9:VAL:CG1	1:E:157:TYR:CZ	3.00	0.45
1:F:239:ASN:HB2	6:F:980:HOH:O	2.15	0.45
1:A:499:ASP:HB3	1:A:500:GLN:HG2	1.97	0.45
4:H:703:FOL:C7	5:H:704:NDP:H42N	2.46	0.45
1:F:176:ARG:HD2	1:F:596:VAL:CG1	2.46	0.45
1:E:173:ARG:HD2	1:E:246:VAL:HG13	1.98	0.45
1:F:537:ASN:HB3	6:F:905:HOH:O	2.16	0.45
1:G:85:GLU:OE2	6:G:871:HOH:O	2.21	0.45
1:C:324:GLU:OE1	1:C:370:THR:HB	2.16	0.45
1:B:608:MET:HE2	3:B:702:CB3:H16	1.97	0.45
1:E:296:TRP:CB	1:F:37:ARG:HG3	2.46	0.45
1:D:532:VAL:HA	6:D:914:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:701:UMP:H1'	3:G:702:CB3:N3	2.31	0.45
1:A:87:MET:HB3	1:A:87:MET:HE2	1.75	0.45
1:A:290:ILE:HG21	1:B:319:PHE:CE2	2.52	0.45
1:A:30:THR:HB	1:A:243:TYR:OH	2.16	0.45
1:B:4:PRO:HA	6:B:834:HOH:O	2.15	0.45
1:C:77:VAL:HG21	1:C:94:LEU:HD12	1.98	0.45
1:C:43:PRO:O	1:C:46:ALA:N	2.50	0.45
1:F:143:ASP:O	6:F:832:HOH:O	2.21	0.45
1:G:5:VAL:HG23	1:G:148:ILE:HG22	1.98	0.45
1:G:469:ARG:HD3	2:H:701:UMP:OP1	2.17	0.45
1:F:40:LYS:HA	1:F:75:ASN:HD22	1.81	0.45
1:F:4:PRO:HA	6:F:829:HOH:O	2.16	0.45
1:B:138:GLU:O	1:B:142:LYS:HB2	2.17	0.45
1:A:43:PRO:HD3	6:A:869:HOH:O	2.17	0.45
1:G:489:CYS:SG	2:G:701:UMP:C6	3.10	0.45
1:C:331:ILE:HD13	1:C:560:LEU:HD22	1.98	0.45
1:A:416:ASN:HB2	6:A:832:HOH:O	2.16	0.45
1:G:17:ILE:HG21	6:G:981:HOH:O	2.16	0.45
1:C:290:ILE:HD11	1:D:230:ILE:HG21	1.99	0.45
1:D:80:GLY:N	1:D:156:LEU:HD22	2.32	0.45
1:C:11:MET:SD	1:C:193:LEU:HD11	2.57	0.45
1:H:425:ILE:HG23	6:H:988:HOH:O	2.16	0.45
1:B:18:GLY:HA3	5:B:704:NDP:O3D	2.17	0.44
1:D:308:LYS:HE3	1:D:308:LYS:HA	1.99	0.44
1:F:368:LEU:HD22	6:F:1022:HOH:O	2.15	0.44
1:B:242:PRO:HG3	1:B:573:ILE:HG23	1.98	0.44
1:F:489:CYS:SG	2:F:701:UMP:C6	3.11	0.44
1:A:9:VAL:CG1	1:A:157:TYR:CZ	3.00	0.44
1:D:482:ASP:OD2	6:D:967:HOH:O	2.21	0.44
1:G:459:ILE:O	1:G:463:ARG:HG3	2.17	0.44
4:B:703:FOL:C7	5:B:704:NDP:H42N	2.47	0.44
1:B:489:CYS:SG	2:B:701:UMP:C6	3.11	0.44
1:H:358:ARG:HD3	1:H:542:GLU:OE1	2.17	0.44
2:D:701:UMP:H1'	3:D:702:CB3:C4	2.47	0.44
1:G:296:TRP:HB3	1:H:37:ARG:HG2	2.00	0.44
1:F:74:PHE:O	1:F:145:VAL:HA	2.17	0.44
1:H:334:ILE:CD1	1:H:514:VAL:HG21	2.47	0.44
1:D:99:ASN:HD22	1:D:99:ASN:N	2.16	0.44
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.98	0.44
1:G:9:VAL:HB	6:G:932:HOH:O	2.17	0.44
1:D:368:LEU:HD22	6:D:834:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HB3	6:A:830:HOH:O	2.17	0.44
1:A:375:TRP:CH2	1:A:379:LEU:HD22	2.52	0.44
1:C:459:ILE:O	1:C:463:ARG:HG3	2.17	0.44
1:A:469:ARG:HH12	2:B:701:UMP:P	2.41	0.44
1:A:416:ASN:C	1:A:418:PRO:HD3	2.38	0.44
1:F:502:GLU:HB3	1:F:541:LYS:HB2	2.00	0.44
1:B:472:LEU:HG	1:B:494:GLN:HG3	1.99	0.44
1:G:142:LYS:HD3	1:G:142:LYS:HA	1.83	0.44
1:B:481:LEU:HD23	1:B:484:MET:HE1	2.00	0.44
1:A:343:ASP:OD1	1:B:469:ARG:CZ	2.66	0.44
1:G:151:VAL:O	4:G:703:FOL:H7	2.18	0.44
1:H:334:ILE:HD11	1:H:550:THR:HG22	1.99	0.44
1:H:173:ARG:HD2	1:H:246:VAL:HG13	1.98	0.44
1:D:352:LYS:HD3	6:D:989:HOH:O	2.17	0.44
1:C:358:ARG:HD3	1:C:542:GLU:OE1	2.18	0.44
1:D:81:ARG:NE	5:D:704:NDP:O1X	2.38	0.44
3:H:702:CB3:C6	3:H:702:CB3:H15	2.47	0.44
1:A:11:MET:SD	1:A:193:LEU:HD11	2.57	0.44
1:B:92:ARG:NH1	6:B:877:HOH:O	2.40	0.44
1:E:192:ILE:HG23	1:E:567:GLU:HG3	1.99	0.44
1:A:97:ARG:O	1:A:99:ASN:ND2	2.51	0.44
1:F:242:PRO:HG2	6:F:952:HOH:O	2.17	0.44
1:F:551:HIS:NE2	2:F:701:UMP:O3'	2.40	0.44
1:C:9:VAL:CG1	1:C:157:TYR:CZ	3.01	0.44
1:F:142:LYS:HB3	6:F:841:HOH:O	2.18	0.44
1:H:227:TYR:CE2	1:H:250:LYS:HG3	2.52	0.44
1:F:534:HIS:HD2	6:F:909:HOH:O	2.00	0.44
1:B:80:GLY:N	1:B:156:LEU:HD22	2.33	0.43
2:B:701:UMP:H1'	3:B:702:CB3:C4	2.48	0.43
1:A:489:CYS:SG	2:A:701:UMP:C6	3.11	0.43
2:H:701:UMP:H1'	3:H:702:CB3:C4	2.48	0.43
3:F:702:CB3:H15	3:F:702:CB3:C6	2.48	0.43
1:C:37:ARG:O	1:C:41:THR:HG23	2.18	0.43
1:F:192:ILE:HD11	1:F:229:PRO:HD3	2.00	0.43
1:G:502:GLU:HB3	1:G:541:LYS:HB2	2.00	0.43
1:A:91:PHE:HB2	6:A:992:HOH:O	2.18	0.43
1:A:242:PRO:HB2	6:A:999:HOH:O	2.17	0.43
1:F:81:ARG:HA	6:F:894:HOH:O	2.18	0.43
1:C:316:HIS:HB2	6:C:879:HOH:O	2.17	0.43
1:B:502:GLU:HB3	1:B:541:LYS:HB2	1.99	0.43
6:G:916:HOH:O	1:H:344:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:THR:HG23	6:A:927:HOH:O	2.17	0.43
1:H:516:LEU:HD22	6:H:886:HOH:O	2.19	0.43
1:E:333:ASP:OD1	1:E:337:ASN:ND2	2.48	0.43
1:B:328:LEU:HD22	1:B:564:LEU:HD22	2.00	0.43
1:E:551:HIS:NE2	2:E:701:UMP:O3'	2.36	0.43
1:D:328:LEU:HD13	6:D:891:HOH:O	2.17	0.43
1:D:311:ILE:HD11	1:D:332:ALA:HA	2.00	0.43
1:H:512:CYS:SG	1:H:547:MET:HB3	2.58	0.43
1:G:559:ALA:HB1	1:G:604:ILE:HG21	1.99	0.43
1:D:502:GLU:HB3	1:D:541:LYS:HB2	2.00	0.43
1:F:234:LYS:HG2	1:F:235:THR:N	2.33	0.43
1:C:252:ARG:NH2	6:C:976:HOH:O	2.43	0.43
1:E:291:ALA:O	1:E:295:ALA:N	2.43	0.43
1:B:191:ASP:HB2	6:B:856:HOH:O	2.19	0.43
1:F:9:VAL:CG1	1:F:157:TYR:CZ	3.02	0.43
1:B:81:ARG:HD3	1:B:103:SER:OG	2.18	0.43
1:D:79:MET:HE2	6:D:901:HOH:O	2.19	0.43
1:C:551:HIS:NE2	2:C:701:UMP:O3'	2.31	0.43
1:H:139:GLU:HB2	6:H:838:HOH:O	2.19	0.43
1:B:397[A]:GLU:OE2	1:B:398:LYS:HG3	2.19	0.43
1:H:21:ASN:HA	5:H:704:NDP:H3D	2.00	0.43
1:H:9:VAL:CG1	1:H:157:TYR:CZ	3.02	0.43
1:F:299:GLU:OE2	6:F:870:HOH:O	2.21	0.43
1:D:459:ILE:O	1:D:463:ARG:HG3	2.19	0.43
1:D:3:LYS:N	1:D:4:PRO:HD3	2.33	0.43
1:E:489:CYS:SG	2:E:701:UMP:C6	3.12	0.43
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.71	0.43
1:H:459:ILE:O	1:H:463:ARG:HG3	2.18	0.43
1:F:155:GLY:HA2	1:F:158:GLU:CD	2.40	0.43
1:B:311:ILE:HD11	1:B:332:ALA:HA	2.01	0.43
1:C:32:PHE:HE2	4:C:703:FOL:C11	2.32	0.42
1:D:31:ASP:OD2	4:D:703:FOL:N3	2.52	0.42
3:C:702:CB3:C6	3:C:702:CB3:H15	2.49	0.42
1:B:527:LEU:HD11	1:B:593:PHE:CE2	2.54	0.42
1:A:486:LEU:HD23	1:A:487:PRO:HD2	2.01	0.42
1:E:30:THR:HB	1:E:243:TYR:OH	2.19	0.42
1:A:290:ILE:HD11	1:B:230:ILE:HG21	2.01	0.42
1:F:102:VAL:O	5:F:704:NDP:H1B	2.18	0.42
3:D:702:CB3:C6	3:D:702:CB3:H15	2.49	0.42
1:F:463:ARG:NH1	1:F:535:VAL:O	2.52	0.42
2:C:701:UMP:H1'	3:C:702:CB3:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ASN:C	1:C:418:PRO:HD3	2.39	0.42
1:C:230:ILE:HG23	1:D:290:ILE:HD11	2.01	0.42
1:G:515:GLY:O	1:G:606:MET:HE1	2.19	0.42
1:C:436:PHE:CE1	1:D:478:PRO:HD2	2.55	0.42
1:D:192:ILE:HD11	1:D:246:VAL:HG21	2.00	0.42
1:A:436:PHE:CZ	1:B:478:PRO:HD2	2.54	0.42
1:C:513:ASP:OD2	3:C:702:CB3:N3	2.52	0.42
1:E:331:ILE:HD13	1:E:560:LEU:HD22	2.01	0.42
1:C:158:GLU:HG3	6:C:902:HOH:O	2.19	0.42
1:E:87:MET:HE2	1:E:92:ARG:HB3	2.01	0.42
1:A:234:LYS:HE3	6:A:874:HOH:O	2.19	0.42
1:A:287:ALA:HA	1:A:290:ILE:CD1	2.47	0.42
1:C:74:PHE:O	1:C:145:VAL:HA	2.20	0.42
1:C:293:VAL:HA	1:C:296:TRP:CD1	2.54	0.42
2:F:701:UMP:H1'	3:F:702:CB3:C4	2.48	0.42
1:A:129:SER:HB2	1:A:131:PRO:HD2	2.02	0.42
1:D:7:LEU:HD22	1:D:150:VAL:HB	2.01	0.42
6:A:911:HOH:O	1:G:113:ALA:HB2	2.20	0.42
1:G:87:MET:HE2	1:G:92:ARG:HB3	2.01	0.42
1:A:230:ILE:HD13	1:B:286:SER:HB2	2.00	0.42
1:C:290:ILE:HG21	1:D:319:PHE:CD2	2.54	0.42
1:D:227:TYR:CZ	1:D:250:LYS:HG3	2.55	0.42
5:C:704:NDP:H52N	5:C:704:NDP:H2D	1.31	0.42
1:B:9:VAL:CG1	1:B:157:TYR:CZ	3.02	0.42
1:A:370:THR:HG23	1:A:563:GLN:CG	2.50	0.42
1:E:287:ALA:CA	1:E:290:ILE:HD12	2.47	0.42
1:C:313:ALA:HB2	1:C:564:LEU:HD22	2.01	0.42
1:H:3:LYS:NZ	6:H:863:HOH:O	2.52	0.42
1:D:23:LEU:HD13	1:D:25:TRP:CZ3	2.55	0.42
1:D:489:CYS:SG	2:D:701:UMP:C6	3.13	0.42
1:C:603:ARG:NE	6:C:988:HOH:O	2.40	0.42
1:C:30:THR:HB	1:C:243:TYR:OH	2.20	0.42
1:A:290:ILE:C	1:A:292:PRO:HD2	2.40	0.42
1:C:142:LYS:HA	1:C:142:LYS:HD3	1.77	0.42
1:B:80:GLY:HA2	1:B:102:VAL:HG23	2.01	0.41
1:F:176:ARG:N	6:F:952:HOH:O	2.53	0.41
1:H:384:TRP:CD1	1:H:389:ASP:HB3	2.55	0.41
1:A:99:ASN:HD22	1:A:99:ASN:N	2.17	0.41
1:E:87:MET:HE1	1:E:94:LEU:HG	2.01	0.41
1:F:469:ARG:HD3	6:F:850:HOH:O	2.20	0.41
1:C:502:GLU:HB3	1:C:541:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:THR:HB	1:D:243:TYR:OH	2.20	0.41
1:B:481:LEU:HA	1:B:484:MET:CE	2.45	0.41
1:A:151:VAL:O	4:A:703:FOL:H7	2.19	0.41
1:G:293:VAL:HA	1:G:296:TRP:CD1	2.55	0.41
1:F:192:ILE:HD13	1:F:248:LEU:HD11	2.02	0.41
1:G:169:LEU:HD12	1:G:248:LEU:HD12	2.01	0.41
1:C:344:ARG:NH1	6:C:963:HOH:O	2.52	0.41
1:A:5:VAL:HG21	1:A:150:VAL:HG23	2.02	0.41
1:F:308:LYS:HA	1:F:308:LYS:HE3	2.02	0.41
1:E:532:VAL:HA	6:E:894:HOH:O	2.20	0.41
1:C:36:SER:HB2	4:C:703:FOL:HB2	2.03	0.41
1:B:84:TRP:CE2	1:B:92:ARG:HD2	2.55	0.41
1:D:9:VAL:HG11	1:D:184:PHE:CD1	2.55	0.41
1:G:334:ILE:HG21	1:G:552:VAL:HG13	2.02	0.41
1:H:292:PRO:HB2	6:H:935:HOH:O	2.20	0.41
1:F:516:LEU:HD22	6:F:966:HOH:O	2.20	0.41
1:F:334:ILE:CD1	1:F:514:VAL:HG21	2.50	0.41
4:F:703:FOL:C6	5:F:704:NDP:H42N	2.51	0.41
1:C:469:ARG:NH1	2:D:701:UMP:OP3	2.52	0.41
1:G:37:ARG:O	1:G:41:THR:HG23	2.21	0.41
1:D:107:LYS:NZ	1:D:107:LYS:O	2.50	0.41
1:C:291:ALA:N	1:C:292:PRO:HD2	2.35	0.41
1:F:84:TRP:CZ2	1:F:92:ARG:HD2	2.56	0.41
1:C:296:TRP:CB	1:D:37:ARG:HG2	2.51	0.41
1:E:228:ARG:O	6:E:953:HOH:O	2.22	0.41
1:H:23:LEU:HA	1:H:24:PRO:HD3	1.89	0.41
1:C:489:CYS:SG	2:C:701:UMP:C6	3.13	0.41
1:F:225:ALA:HB3	6:F:892:HOH:O	2.18	0.41
5:E:704:NDP:H52N	5:E:704:NDP:H2D	1.31	0.41
1:D:87:MET:HA	1:D:88:PRO:HD2	1.88	0.41
1:F:40:LYS:O	1:F:41:THR:HG23	2.21	0.41
1:H:150:VAL:HG13	1:H:156:LEU:HD23	2.01	0.41
1:B:158:GLU:HG3	6:B:977:HOH:O	2.20	0.41
1:G:30:THR:HB	1:G:243:TYR:OH	2.20	0.41
1:E:329:ASP:OD2	6:E:838:HOH:O	2.22	0.41
1:H:384:TRP:HZ2	6:H:988:HOH:O	2.03	0.41
1:B:300:GLU:HA	1:B:301:ASP:HA	1.59	0.41
1:C:370:THR:HG23	1:C:563:GLN:CG	2.51	0.41
1:A:251:ARG:O	1:A:252:ARG:HB3	2.21	0.41
1:A:37:ARG:HG2	1:B:296:TRP:HB3	2.02	0.41
1:C:445:THR:HB	1:C:447:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:478:PRO:HA	1:F:481:LEU:HG	2.02	0.41
1:C:567:GLU:HA	1:C:568:PRO:HD3	1.93	0.41
1:C:11:MET:CG	1:C:15:ARG:HA	2.50	0.41
1:H:527:LEU:HD11	1:H:593:PHE:CE1	2.56	0.41
1:E:491:LEU:HD11	1:F:492:LEU:HD11	2.03	0.41
1:G:13:PRO:HD3	1:G:174:VAL:O	2.21	0.41
1:C:491:LEU:HD21	1:C:510:ARG:HB3	2.03	0.41
3:B:702:CB3:H15	3:B:702:CB3:C6	2.50	0.41
1:E:114:GLU:HG3	6:E:876:HOH:O	2.21	0.41
1:C:37:ARG:HG2	1:D:296:TRP:HB3	2.03	0.40
1:H:573:ILE:HD11	1:H:575:ASN:OD1	2.22	0.40
5:H:704:NDP:H3B	5:H:704:NDP:C8A	2.52	0.40
1:B:368:LEU:HD22	1:B:368:LEU:N	2.35	0.40
1:B:493:CYS:HA	1:B:506:ILE:O	2.21	0.40
2:C:701:UMP:H1'	3:C:702:CB3:C4	2.51	0.40
1:B:334:ILE:CD1	1:B:514:VAL:HG21	2.51	0.40
1:F:227:TYR:CZ	1:F:250:LYS:HG3	2.57	0.40
1:D:462:LEU:HD21	6:D:920:HOH:O	2.20	0.40
1:H:141:TYR:HE2	6:H:905:HOH:O	2.04	0.40
1:H:242:PRO:HG2	6:H:975:HOH:O	2.20	0.40
1:A:74:PHE:O	1:A:145:VAL:HA	2.21	0.40
1:F:23:LEU:HD13	1:F:25:TRP:CZ3	2.56	0.40
1:E:320:ARG:HD3	6:E:838:HOH:O	2.21	0.40
5:F:704:NDP:C8A	5:F:704:NDP:C3B	2.99	0.40
1:F:608:MET:HE2	3:F:702:CB3:H16	2.03	0.40
1:E:492:LEU:CD1	1:F:491:LEU:HD11	2.51	0.40
1:E:469:ARG:HD3	1:F:511:SER:OG	2.21	0.40
1:E:99:ASN:HD22	1:E:99:ASN:N	2.19	0.40
1:G:506:ILE:HG13	1:H:353:PHE:CE2	2.56	0.40
1:D:229:PRO:HA	1:D:248:LEU:HD12	2.03	0.40
1:H:89:ARG:HA	1:H:92:ARG:HG3	2.04	0.40
1:D:25:TRP:HB3	1:D:178:PHE:CE2	2.57	0.40
1:G:331:ILE:HD13	1:G:560:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/566 (89%)	487 (97%)	14 (3%)	1 (0%)	52	59
1	B	478/566 (84%)	456 (95%)	19 (4%)	3 (1%)	30	29
1	C	502/566 (89%)	488 (97%)	12 (2%)	2 (0%)	39	42
1	D	478/566 (84%)	449 (94%)	24 (5%)	5 (1%)	19	16
1	E	502/566 (89%)	489 (97%)	10 (2%)	3 (1%)	30	29
1	F	478/566 (84%)	454 (95%)	21 (4%)	3 (1%)	30	29
1	G	502/566 (89%)	488 (97%)	10 (2%)	4 (1%)	24	22
1	H	478/566 (84%)	456 (95%)	18 (4%)	4 (1%)	24	22
All	All	3920/4528 (87%)	3767 (96%)	128 (3%)	25 (1%)	30	29

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	TYR
1	B	429	TYR
1	C	286	SER
1	D	429	TYR
1	E	429	TYR
1	F	429	TYR
1	G	313	ALA
1	H	429	TYR
1	B	299	GLU
1	D	139	GLU
1	D	146	ASP
1	E	286	SER
1	G	286	SER
1	C	429	TYR
1	D	299	GLU
1	G	429	TYR
1	E	499	ASP

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Mol	Chain	Res	Type
1	F	139	GLU
1	G	499	ASP
1	H	144	SER
1	F	190	ASP
1	H	146	ASP
1	H	190	ASP
1	B	139	GLU
1	D	145	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/491 (90%)	410 (92%)	34 (8%)	16	16
1	B	431/491 (88%)	399 (93%)	32 (7%)	17	17
1	C	444/491 (90%)	406 (91%)	38 (9%)	13	12
1	D	431/491 (88%)	400 (93%)	31 (7%)	18	18
1	E	444/491 (90%)	414 (93%)	30 (7%)	20	21
1	F	431/491 (88%)	393 (91%)	38 (9%)	12	12
1	G	444/491 (90%)	407 (92%)	37 (8%)	14	13
1	H	431/491 (88%)	401 (93%)	30 (7%)	19	19
All	All	3500/3928 (89%)	3230 (92%)	270 (8%)	16	16

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	9	VAL
1	A	29	THR
1	A	37	ARG
1	A	89	ARG
1	A	90	LYS
1	A	106	LEU

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	123	ARG
1	A	137	LEU
1	A	142	LYS
1	A	145	VAL
1	A	156	LEU
1	A	161	LEU
1	A	192	ILE
1	A	234	LYS
1	A	252	ARG
1	A	310	LEU
1	A	320	ARG
1	A	330	LEU
1	A	368	LEU
1	A	370	THR
1	A	383	LEU
1	A	396	SER
1	A	397	GLU
1	A	410	GLU
1	A	441	LYS
1	A	486	LEU
1	A	492	LEU
1	A	499	ASP
1	A	539	LYS
1	A	554	THR
1	A	580	GLU
1	A	610	VAL
1	B	25	TRP
1	B	41	THR
1	B	79	MET
1	B	82	LYS
1	B	86	SER
1	B	89	ARG
1	B	107	LYS
1	B	136	LEU
1	B	144	SER
1	B	147	GLN
1	B	148	ILE
1	B	230	ILE
1	B	244	ASP
1	B	248	LEU
1	B	251	ARG

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Mol	Chain	Res	Type
1	B	285	SER
1	B	300	GLU
1	B	308	LYS
1	B	339	ARG
1	B	343	ASP
1	B	356	THR
1	B	360	SER
1	B	371	LYS
1	B	395	LEU
1	B	441	LYS
1	B	448	THR
1	B	486	LEU
1	B	558	GLU
1	B	564	LEU
1	B	567	GLU
1	B	573	ILE
1	B	579	LYS
1	C	5	VAL
1	C	8	VAL
1	C	29	THR
1	C	37	ARG
1	C	42	THR
1	C	89	ARG
1	C	90	LYS
1	C	109	GLU
1	C	137	LEU
1	C	139	GLU
1	C	142	LYS
1	C	143	ASP
1	C	144	SER
1	C	151	VAL
1	C	161	LEU
1	C	192	ILE
1	C	230	ILE
1	C	234	LYS
1	C	285	SER
1	C	299	GLU
1	C	310	LEU
1	C	320	ARG
1	C	330	LEU
1	C	343	ASP
1	C	349	VAL

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Mol	Chain	Res	Type
1	C	356	THR
1	C	370	THR
1	C	383	LEU
1	C	397	GLU
1	C	419	HIS
1	C	441	LYS
1	C	469	ARG
1	C	492	LEU
1	C	499	ASP
1	C	535	VAL
1	C	539	LYS
1	C	580	GLU
1	C	610	VAL
1	D	9	VAL
1	D	25	TRP
1	D	37	ARG
1	D	41	THR
1	D	79	MET
1	D	82	LYS
1	D	86	SER
1	D	89	ARG
1	D	102	VAL
1	D	107	LYS
1	D	136	LEU
1	D	145	VAL
1	D	148	ILE
1	D	230	ILE
1	D	234	LYS
1	D	244	ASP
1	D	248	LEU
1	D	250	LYS
1	D	251	ARG
1	D	300	GLU
1	D	308	LYS
1	D	310	LEU
1	D	339	ARG
1	D	356	THR
1	D	368	LEU
1	D	395	LEU
1	D	486	LEU
1	D	564	LEU
1	D	573	ILE

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Mol	Chain	Res	Type
1	D	579	LYS
1	D	580	GLU
1	E	5	VAL
1	E	37	ARG
1	E	42	THR
1	E	90	LYS
1	E	122	GLN
1	E	137	LEU
1	E	142	LYS
1	E	151	VAL
1	E	161	LEU
1	E	192	ILE
1	E	234	LYS
1	E	310	LEU
1	E	320	ARG
1	E	330	LEU
1	E	343	ASP
1	E	356	THR
1	E	368	LEU
1	E	370	THR
1	E	383	LEU
1	E	396	SER
1	E	397	GLU
1	E	414	SER
1	E	415	ARG
1	E	441	LYS
1	E	486	LEU
1	E	539	LYS
1	E	552	VAL
1	E	554	THR
1	E	580	GLU
1	E	610	VAL
1	F	25	TRP
1	F	36	SER
1	F	37	ARG
1	F	41	THR
1	F	82	LYS
1	F	89	ARG
1	F	102	VAL
1	F	127	CYS
1	F	140	GLU
1	F	143	ASP

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Mol	Chain	Res	Type
1	F	148	ILE
1	F	158	GLU
1	F	230	ILE
1	F	234	LYS
1	F	244	ASP
1	F	248	LEU
1	F	250	LYS
1	F	285	SER
1	F	300	GLU
1	F	301	ASP
1	F	308	LYS
1	F	310	LEU
1	F	318	HIS
1	F	320	ARG
1	F	331	ILE
1	F	344	ARG
1	F	356	THR
1	F	360	SER
1	F	368	LEU
1	F	376	LYS
1	F	395	LEU
1	F	441	LYS
1	F	486	LEU
1	F	500	GLN
1	F	564	LEU
1	F	573	ILE
1	F	579	LYS
1	F	605	GLN
1	G	8	VAL
1	G	29	THR
1	G	37	ARG
1	G	42	THR
1	G	90	LYS
1	G	122	GLN
1	G	123	ARG
1	G	137	LEU
1	G	142	LYS
1	G	143	ASP
1	G	161	LEU
1	G	192	ILE
1	G	234	LYS
1	G	252	ARG

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Mol	Chain	Res	Type
1	G	310	LEU
1	G	312	ARG
1	G	314	VAL
1	G	330	LEU
1	G	343	ASP
1	G	349	VAL
1	G	368	LEU
1	G	383	LEU
1	G	397	GLU
1	G	410	GLU
1	G	414	SER
1	G	415	ARG
1	G	441	LYS
1	G	486	LEU
1	G	492	LEU
1	G	499	ASP
1	G	530	LEU
1	G	537	ASN
1	G	539	LYS
1	G	552	VAL
1	G	554	THR
1	G	580	GLU
1	G	610	VAL
1	H	25	TRP
1	H	37	ARG
1	H	41	THR
1	H	79	MET
1	H	82	LYS
1	H	89	ARG
1	H	107	LYS
1	H	136	LEU
1	H	148	ILE
1	H	158	GLU
1	H	177	GLU
1	H	230	ILE
1	H	244	ASP
1	H	250	LYS
1	H	285	SER
1	H	300	GLU
1	H	308	LYS
1	H	310	LEU
1	H	339	ARG

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Mol	Chain	Res	Type
1	H	344	ARG
1	H	356	THR
1	H	360	SER
1	H	368	LEU
1	H	395	LEU
1	H	441	LYS
1	H	472	LEU
1	H	486	LEU
1	H	564	LEU
1	H	573	ILE
1	H	579	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	563	GLN

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](#)

32 ligands are modelled in this entry.

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
2	UMP	A	701	-	16,21,21	1.62	4 (25%)	23,31,31	5.46	11 (47%)
3	CB3	A	702	-	31,37,37	1.98	8 (25%)	35,51,51	1.61	5 (14%)
4	FOL	A	703	-	27,34,34	2.03	7 (25%)	31,47,47	1.73	9 (29%)
5	NDP	A	704	-	42,52,52	2.30	16 (38%)	55,80,80	4.01	23 (41%)
2	UMP	B	701	-	16,21,21	1.58	4 (25%)	23,31,31	5.52	9 (39%)
3	CB3	B	702	-	31,37,37	1.86	7 (22%)	35,51,51	1.40	4 (11%)
4	FOL	B	703	-	27,34,34	2.10	6 (22%)	31,47,47	1.50	5 (16%)
5	NDP	B	704	-	42,52,52	2.12	16 (38%)	55,80,80	3.99	18 (32%)
2	UMP	C	701	-	16,21,21	1.63	4 (25%)	23,31,31	5.54	10 (43%)
3	CB3	C	702	-	31,37,37	1.83	6 (19%)	35,51,51	1.42	4 (11%)
4	FOL	C	703	-	27,34,34	2.18	9 (33%)	31,47,47	2.07	9 (29%)
5	NDP	C	704	-	42,52,52	2.31	16 (38%)	55,80,80	4.01	23 (41%)
2	UMP	D	701	-	16,21,21	1.54	4 (25%)	23,31,31	5.47	10 (43%)
3	CB3	D	702	-	31,37,37	1.73	6 (19%)	35,51,51	1.43	5 (14%)
4	FOL	D	703	-	27,34,34	2.14	9 (33%)	31,47,47	1.60	4 (12%)
5	NDP	D	704	-	42,52,52	2.32	17 (40%)	55,80,80	3.79	23 (41%)
2	UMP	E	701	-	16,21,21	1.57	4 (25%)	23,31,31	5.53	11 (47%)
3	CB3	E	702	-	31,37,37	1.91	8 (25%)	35,51,51	1.43	4 (11%)
4	FOL	E	703	-	27,34,34	2.11	9 (33%)	31,47,47	2.14	12 (38%)
5	NDP	E	704	-	42,52,52	2.30	14 (33%)	55,80,80	3.96	25 (45%)
2	UMP	F	701	-	16,21,21	1.57	4 (25%)	23,31,31	5.50	10 (43%)
3	CB3	F	702	-	31,37,37	1.75	6 (19%)	35,51,51	1.37	5 (14%)
4	FOL	F	703	-	27,34,34	2.07	7 (25%)	31,47,47	1.52	6 (19%)
5	NDP	F	704	-	42,52,52	2.14	15 (35%)	55,80,80	4.16	19 (34%)
2	UMP	G	701	-	16,21,21	1.63	4 (25%)	23,31,31	5.47	10 (43%)
3	CB3	G	702	-	31,37,37	2.13	9 (29%)	35,51,51	1.80	6 (17%)
4	FOL	G	703	-	27,34,34	2.09	9 (33%)	31,47,47	2.11	11 (35%)
5	NDP	G	704	-	42,52,52	2.34	16 (38%)	55,80,80	4.00	24 (43%)
2	UMP	H	701	-	16,21,21	1.56	4 (25%)	23,31,31	5.51	10 (43%)
3	CB3	H	702	-	31,37,37	1.84	7 (22%)	35,51,51	1.26	3 (8%)
4	FOL	H	703	-	27,34,34	2.07	7 (25%)	31,47,47	1.72	6 (19%)
5	NDP	H	704	-	42,52,52	2.12	15 (35%)	55,80,80	4.00	19 (34%)

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
2	UMP	A	701	-	-	0/6/22/22	0/2/2/2
3	CB3	A	702	-	-	0/21/28/28	0/3/3/3
4	FOL	A	703	-	-	0/16/22/22	0/3/3/3
5	NDP	A	704	-	-	0/30/77/77	0/5/5/5
2	UMP	B	701	-	-	0/6/22/22	0/2/2/2
3	CB3	B	702	-	-	0/21/28/28	0/3/3/3
4	FOL	B	703	-	-	0/16/22/22	0/3/3/3
5	NDP	B	704	-	-	0/30/77/77	0/5/5/5
2	UMP	C	701	-	-	0/6/22/22	0/2/2/2
3	CB3	C	702	-	-	0/21/28/28	0/3/3/3
4	FOL	C	703	-	-	0/16/22/22	0/3/3/3
5	NDP	C	704	-	-	0/30/77/77	0/5/5/5
2	UMP	D	701	-	-	0/6/22/22	0/2/2/2
3	CB3	D	702	-	-	0/21/28/28	0/3/3/3
4	FOL	D	703	-	-	0/16/22/22	0/3/3/3
5	NDP	D	704	-	-	0/30/77/77	0/5/5/5
2	UMP	E	701	-	-	0/6/22/22	0/2/2/2
3	CB3	E	702	-	-	0/21/28/28	0/3/3/3
4	FOL	E	703	-	-	0/16/22/22	0/3/3/3
5	NDP	E	704	-	-	0/30/77/77	0/5/5/5
2	UMP	F	701	-	-	0/6/22/22	0/2/2/2
3	CB3	F	702	-	-	0/21/28/28	0/3/3/3
4	FOL	F	703	-	-	0/16/22/22	0/3/3/3
5	NDP	F	704	-	-	0/30/77/77	0/5/5/5
2	UMP	G	701	-	-	0/6/22/22	0/2/2/2
3	CB3	G	702	-	-	0/21/28/28	0/3/3/3
4	FOL	G	703	-	-	0/16/22/22	0/3/3/3
5	NDP	G	704	-	-	0/30/77/77	0/5/5/5
2	UMP	H	701	-	-	0/6/22/22	0/2/2/2
3	CB3	H	702	-	-	0/21/28/28	0/3/3/3
4	FOL	H	703	-	-	0/16/22/22	0/3/3/3
5	NDP	H	704	-	-	0/30/77/77	0/5/5/5

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	CB3	C9-C6	-5.74	1.40	1.51
4	D	703	FOL	C9-C6	-5.48	1.40	1.51
4	B	703	FOL	C9-C6	-5.48	1.40	1.51
3	G	702	CB3	C9-C6	-5.36	1.41	1.51
3	E	702	CB3	C9-C6	-5.32	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	CB3	C9-C6	-5.21	1.41	1.51
3	H	702	CB3	C9-C6	-5.14	1.41	1.51
3	A	702	CB3	C11-C	-5.14	1.39	1.50
4	F	703	FOL	C9-C6	-5.07	1.41	1.51
4	H	703	FOL	C9-C6	-5.04	1.41	1.51
3	C	702	CB3	C11-C	-4.96	1.39	1.50
5	C	704	NDP	C4N-C5N	-4.93	1.38	1.49
5	D	704	NDP	C4N-C5N	-4.93	1.38	1.49
3	C	702	CB3	C9-C6	-4.91	1.42	1.51
5	G	704	NDP	C4N-C5N	-4.90	1.38	1.49
5	E	704	NDP	C4N-C5N	-4.85	1.38	1.49
5	A	704	NDP	C4N-C5N	-4.83	1.38	1.49
4	E	703	FOL	C9-C6	-4.81	1.41	1.51
3	G	702	CB3	C11-C	-4.80	1.40	1.50
4	A	703	FOL	C11-C	-4.79	1.40	1.50
3	D	702	CB3	C9-C6	-4.73	1.42	1.51
4	C	703	FOL	C9-C6	-4.71	1.41	1.51
4	A	703	FOL	C9-C6	-4.69	1.41	1.51
3	E	702	CB3	C11-C	-4.64	1.40	1.50
3	F	702	CB3	C11-C	-4.62	1.40	1.50
4	B	703	FOL	C11-C	-4.62	1.40	1.50
3	G	702	CB3	CP2-CP3	-4.58	1.07	1.17
4	H	703	FOL	C11-C	-4.56	1.40	1.50
3	F	702	CB3	C9-C6	-4.56	1.43	1.51
3	H	702	CB3	C11-C	-4.55	1.40	1.50
5	F	704	NDP	C4N-C5N	-4.53	1.39	1.49
4	G	703	FOL	C9-C6	-4.51	1.42	1.51
3	D	702	CB3	C11-C	-4.48	1.40	1.50
5	B	704	NDP	C4N-C5N	-4.46	1.39	1.49
5	H	704	NDP	C4N-C5N	-4.45	1.39	1.49
4	F	703	FOL	C11-C	-4.43	1.40	1.50
5	A	704	NDP	C2D-C1D	-4.41	1.39	1.53
3	B	702	CB3	C11-C	-4.39	1.40	1.50
4	G	703	FOL	C11-C	-4.29	1.41	1.50
4	E	703	FOL	C11-C	-4.20	1.41	1.50
5	A	704	NDP	C3B-C4B	-4.20	1.41	1.53
5	E	704	NDP	C3B-C4B	-4.17	1.41	1.53
5	C	704	NDP	C3B-C4B	-4.15	1.41	1.53
5	C	704	NDP	C2D-C1D	-4.14	1.40	1.53
5	G	704	NDP	C3B-C4B	-4.12	1.41	1.53
4	D	703	FOL	C11-C	-4.02	1.41	1.50
4	C	703	FOL	C11-C	-3.87	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	704	NDP	C2D-C1D	-3.80	1.41	1.53
5	G	704	NDP	C2D-C1D	-3.76	1.41	1.53
5	F	704	NDP	C3B-C4B	-3.76	1.42	1.53
5	H	704	NDP	C3B-C4B	-3.69	1.43	1.53
5	D	704	NDP	C2D-C1D	-3.55	1.41	1.53
5	B	704	NDP	C3B-C4B	-3.42	1.43	1.53
5	D	704	NDP	C3B-C4B	-3.31	1.44	1.53
3	E	702	CB3	CP2-CP3	-3.08	1.10	1.17
3	A	702	CB3	CP2-CP3	-2.96	1.11	1.17
3	C	702	CB3	CP2-CP3	-2.82	1.11	1.17
3	B	702	CB3	CP2-CP3	-2.72	1.11	1.17
5	E	704	NDP	C5A-C4A	-2.60	1.34	1.40
5	G	704	NDP	C5A-C4A	-2.59	1.34	1.40
5	C	704	NDP	C5A-C4A	-2.57	1.34	1.40
5	A	704	NDP	C5A-C4A	-2.53	1.34	1.40
5	B	704	NDP	C5A-C4A	-2.49	1.34	1.40
5	D	704	NDP	C5A-C4A	-2.48	1.34	1.40
5	H	704	NDP	C5A-C4A	-2.42	1.35	1.40
5	F	704	NDP	C5A-C4A	-2.39	1.35	1.40
4	G	703	FOL	C4-C4A	-2.33	1.36	1.41
3	G	702	CB3	CP1-CP2	-2.31	1.44	1.47
2	A	701	UMP	P-OP2	-2.28	1.46	1.54
2	G	701	UMP	P-OP2	-2.26	1.46	1.54
4	A	703	FOL	C8A-N8	-2.24	1.33	1.37
4	B	703	FOL	C8A-N8	-2.22	1.33	1.37
4	H	703	FOL	C8A-N8	-2.22	1.33	1.37
4	F	703	FOL	C8A-N8	-2.20	1.33	1.37
4	G	703	FOL	C8A-N8	-2.20	1.33	1.37
4	C	703	FOL	C8A-N8	-2.19	1.33	1.37
4	E	703	FOL	C4-C4A	-2.18	1.36	1.41
2	D	701	UMP	P-OP2	-2.16	1.47	1.54
4	D	703	FOL	C4-C4A	-2.15	1.36	1.41
4	A	703	FOL	C4-C4A	-2.15	1.36	1.41
2	E	701	UMP	P-OP2	-2.15	1.47	1.54
2	C	701	UMP	P-OP2	-2.14	1.47	1.54
5	G	704	NDP	C5A-N7A	-2.13	1.32	1.39
4	C	703	FOL	C4-C4A	-2.13	1.37	1.41
2	H	701	UMP	P-OP2	-2.12	1.47	1.54
5	A	704	NDP	C5A-N7A	-2.11	1.32	1.39
5	H	704	NDP	C2D-C3D	-2.10	1.47	1.53
4	E	703	FOL	C8A-N8	-2.09	1.33	1.37
5	E	704	NDP	C5A-N7A	-2.08	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	704	NDP	C5A-N7A	-2.08	1.32	1.39
5	B	704	NDP	C5A-N7A	-2.07	1.32	1.39
5	C	704	NDP	C5A-N7A	-2.05	1.32	1.39
5	F	704	NDP	C5A-N7A	-2.05	1.32	1.39
2	B	701	UMP	P-OP2	-2.05	1.47	1.54
5	G	704	NDP	P2B-O2X	-2.05	1.47	1.54
5	C	704	NDP	P2B-O2X	-2.04	1.47	1.54
5	E	704	NDP	P2B-O2X	-2.04	1.47	1.54
4	H	703	FOL	C4-C4A	-2.04	1.37	1.41
5	F	704	NDP	P2B-O2X	-2.04	1.47	1.54
3	F	702	CB3	CP2-CP3	-2.03	1.13	1.17
5	A	704	NDP	P2B-O2X	-2.03	1.47	1.54
2	F	701	UMP	P-OP2	-2.03	1.47	1.54
5	B	704	NDP	C2D-C3D	-2.03	1.47	1.53
5	D	704	NDP	C5A-N7A	-2.02	1.32	1.39
5	B	704	NDP	P2B-O2X	-2.01	1.47	1.54
4	D	703	FOL	C8A-N8	-2.01	1.33	1.37
5	A	704	NDP	P2B-O2B	2.03	1.66	1.60
4	G	703	FOL	C9-N10	2.03	1.50	1.45
5	A	704	NDP	O2B-C2B	2.04	1.50	1.44
4	D	703	FOL	CB-CA	2.04	1.56	1.53
3	B	702	CB3	C9-N10	2.06	1.49	1.46
5	F	704	NDP	P2B-O2B	2.08	1.66	1.60
5	C	704	NDP	O2B-C2B	2.08	1.50	1.44
5	G	704	NDP	O2B-C2B	2.08	1.50	1.44
3	E	702	CB3	CB-CA	2.10	1.56	1.53
5	G	704	NDP	P2B-O2B	2.11	1.66	1.60
5	B	704	NDP	P2B-O2B	2.12	1.66	1.60
5	C	704	NDP	P2B-O2B	2.14	1.66	1.60
5	F	704	NDP	C2N-C3N	2.14	1.39	1.34
5	H	704	NDP	P2B-O2B	2.15	1.66	1.60
4	E	703	FOL	C9-N10	2.16	1.51	1.45
5	D	704	NDP	P2B-O2B	2.16	1.66	1.60
4	A	703	FOL	C2-N3	2.16	1.39	1.35
2	D	701	UMP	O4'-C4'	2.17	1.50	1.45
4	G	703	FOL	C2-N3	2.17	1.39	1.35
4	E	703	FOL	C2-N3	2.19	1.39	1.35
5	D	704	NDP	PN-O5D	2.21	1.69	1.59
5	H	704	NDP	C2N-C3N	2.23	1.40	1.34
5	B	704	NDP	C2N-C3N	2.24	1.40	1.34
4	H	703	FOL	C2-N3	2.25	1.39	1.35
3	H	702	CB3	C9-N10	2.27	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	O2B-C2B	2.28	1.51	1.44
3	D	702	CB3	C2-N3	2.29	1.39	1.35
5	B	704	NDP	O4B-C4B	2.29	1.50	1.45
5	D	704	NDP	O4B-C4B	2.31	1.50	1.45
5	D	704	NDP	O2B-C2B	2.31	1.51	1.44
5	A	704	NDP	C2N-C3N	2.31	1.40	1.34
3	A	702	CB3	CA-N	2.32	1.50	1.46
4	C	703	FOL	C2-N3	2.32	1.39	1.35
3	D	702	CB3	C9-N10	2.32	1.49	1.46
3	H	702	CB3	C2-N3	2.32	1.39	1.35
4	F	703	FOL	CA-N	2.32	1.50	1.46
4	F	703	FOL	C2-N3	2.33	1.39	1.35
2	F	701	UMP	O4'-C4'	2.33	1.50	1.45
3	E	702	CB3	C2-N3	2.34	1.39	1.35
3	G	702	CB3	C2-N3	2.35	1.39	1.35
3	A	702	CB3	C9-N10	2.36	1.49	1.46
5	H	704	NDP	PA-O5B	2.37	1.69	1.59
5	F	704	NDP	O2B-C2B	2.38	1.51	1.44
5	H	704	NDP	O2B-C2B	2.38	1.51	1.44
3	C	702	CB3	C9-N10	2.38	1.49	1.46
4	G	703	FOL	CA-N	2.39	1.50	1.46
5	C	704	NDP	C2N-C3N	2.40	1.40	1.34
2	B	701	UMP	O4'-C4'	2.40	1.50	1.45
4	C	703	FOL	CB-CA	2.41	1.56	1.53
3	F	702	CB3	C2-N3	2.42	1.39	1.35
3	A	702	CB3	C2-N3	2.44	1.39	1.35
3	H	702	CB3	CA-N	2.47	1.50	1.46
4	E	703	FOL	CA-N	2.47	1.50	1.46
5	A	704	NDP	C6N-C5N	2.48	1.38	1.33
2	H	701	UMP	O4'-C4'	2.48	1.50	1.45
2	E	701	UMP	O4'-C4'	2.49	1.50	1.45
3	G	702	CB3	C9-N10	2.49	1.49	1.46
4	D	703	FOL	C2-N3	2.51	1.39	1.35
5	F	704	NDP	O4D-C4D	2.53	1.50	1.45
5	C	704	NDP	C6N-C5N	2.53	1.38	1.33
5	G	704	NDP	C2N-C3N	2.53	1.40	1.34
5	D	704	NDP	C6N-C5N	2.55	1.38	1.33
4	B	703	FOL	C2-N3	2.56	1.39	1.35
2	G	701	UMP	O4'-C4'	2.56	1.50	1.45
2	A	701	UMP	O4'-C4'	2.56	1.50	1.45
4	E	703	FOL	C4-N3	2.56	1.37	1.33
3	B	702	CB3	C2-N3	2.57	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	702	CB3	C9-N10	2.57	1.49	1.46
3	D	702	CB3	CA-N	2.58	1.50	1.46
5	E	704	NDP	C2N-C3N	2.58	1.41	1.34
5	G	704	NDP	C6N-C5N	2.59	1.38	1.33
5	D	704	NDP	C2N-C3N	2.59	1.41	1.34
2	E	701	UMP	C6-N1	2.60	1.39	1.35
2	D	701	UMP	C6-N1	2.62	1.39	1.35
3	C	702	CB3	C2-N3	2.63	1.40	1.35
5	E	704	NDP	C6N-C5N	2.65	1.38	1.33
5	F	704	NDP	O4B-C4B	2.66	1.51	1.45
3	F	702	CB3	C9-N10	2.66	1.49	1.46
3	E	702	CB3	CA-N	2.67	1.50	1.46
5	C	704	NDP	C2A-N1A	2.70	1.39	1.33
3	A	702	CB3	CB-CA	2.70	1.57	1.53
2	C	701	UMP	O4'-C4'	2.72	1.51	1.45
2	A	701	UMP	C6-N1	2.73	1.39	1.35
2	F	701	UMP	C6-N1	2.74	1.39	1.35
5	G	704	NDP	C2A-N1A	2.77	1.39	1.33
4	G	703	FOL	C4-N3	2.78	1.38	1.33
4	A	703	FOL	C4-N3	2.81	1.38	1.33
3	B	702	CB3	CA-N	2.81	1.50	1.46
4	D	703	FOL	CA-N	2.81	1.50	1.46
2	B	701	UMP	C6-N1	2.82	1.39	1.35
4	C	703	FOL	C4-N3	2.83	1.38	1.33
5	E	704	NDP	C2A-N1A	2.85	1.39	1.33
5	A	704	NDP	C2A-N1A	2.86	1.39	1.33
2	G	701	UMP	C6-N1	2.91	1.39	1.35
4	F	703	FOL	C4-N3	2.96	1.38	1.33
2	C	701	UMP	C6-N1	2.98	1.40	1.35
4	H	703	FOL	C4-N3	3.00	1.38	1.33
4	D	703	FOL	C4-N3	3.00	1.38	1.33
2	H	701	UMP	C6-N1	3.01	1.40	1.35
5	F	704	NDP	C2A-N1A	3.01	1.39	1.33
3	H	702	CB3	CB-CA	3.02	1.57	1.53
3	G	702	CB3	CB-CA	3.03	1.57	1.53
5	B	704	NDP	O4D-C4D	3.06	1.52	1.45
5	D	704	NDP	C2A-N1A	3.11	1.39	1.33
4	B	703	FOL	C4-N3	3.15	1.39	1.33
5	H	704	NDP	C2A-N1A	3.17	1.39	1.33
5	B	704	NDP	C2A-N1A	3.17	1.39	1.33
3	G	702	CB3	CA-N	3.17	1.51	1.46
5	H	704	NDP	C6N-C5N	3.19	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	CB3	C4-N3	3.20	1.39	1.33
5	H	704	NDP	O4D-C4D	3.20	1.52	1.45
5	F	704	NDP	C6N-C5N	3.23	1.39	1.33
5	B	704	NDP	C6N-C5N	3.26	1.39	1.33
3	E	702	CB3	C4-N3	3.28	1.39	1.33
3	H	702	CB3	C4-N3	3.35	1.39	1.33
2	H	701	UMP	C4-N3	3.38	1.39	1.33
3	G	702	CB3	C4-N3	3.40	1.39	1.33
3	C	702	CB3	C4-N3	3.42	1.39	1.33
3	B	702	CB3	C4-N3	3.50	1.39	1.33
3	F	702	CB3	C4-N3	3.53	1.39	1.33
5	A	704	NDP	C2D-C3D	3.53	1.63	1.53
3	D	702	CB3	C4-N3	3.54	1.39	1.33
2	C	701	UMP	C4-N3	3.56	1.39	1.33
5	C	704	NDP	O4B-C1B	3.61	1.45	1.41
2	A	701	UMP	C4-N3	3.62	1.39	1.33
2	B	701	UMP	C4-N3	3.64	1.39	1.33
2	D	701	UMP	C4-N3	3.64	1.39	1.33
2	E	701	UMP	C4-N3	3.66	1.39	1.33
5	E	704	NDP	C2D-C3D	3.68	1.63	1.53
4	C	703	FOL	CA-N	3.69	1.52	1.46
5	G	704	NDP	C2D-C3D	3.70	1.63	1.53
5	C	704	NDP	C2D-C3D	3.71	1.63	1.53
5	B	704	NDP	O4B-C1B	3.74	1.45	1.41
2	G	701	UMP	C4-N3	3.77	1.40	1.33
2	F	701	UMP	C4-N3	3.83	1.40	1.33
5	E	704	NDP	O4B-C1B	3.90	1.46	1.41
5	D	704	NDP	O4B-C1B	3.92	1.46	1.41
5	A	704	NDP	O4D-C1D	3.93	1.51	1.42
5	E	704	NDP	C2A-N3A	3.96	1.39	1.32
5	A	704	NDP	O4B-C1B	3.96	1.46	1.41
5	G	704	NDP	C2A-N3A	3.97	1.39	1.32
5	D	704	NDP	C2D-C3D	3.99	1.64	1.53
5	D	704	NDP	C2A-N3A	4.05	1.39	1.32
5	H	704	NDP	C2A-N3A	4.10	1.39	1.32
5	A	704	NDP	C2A-N3A	4.12	1.39	1.32
5	H	704	NDP	O4B-C1B	4.13	1.46	1.41
5	C	704	NDP	C2A-N3A	4.16	1.39	1.32
5	G	704	NDP	O4B-C1B	4.24	1.46	1.41
5	B	704	NDP	C2A-N3A	4.40	1.40	1.32
5	F	704	NDP	O4B-C1B	4.41	1.46	1.41
5	E	704	NDP	O4D-C1D	4.43	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	704	NDP	O4D-C1D	4.47	1.53	1.42
5	D	704	NDP	O4D-C1D	4.48	1.53	1.42
5	F	704	NDP	C2A-N3A	4.59	1.40	1.32
5	G	704	NDP	O4D-C1D	4.67	1.53	1.42
5	H	704	NDP	C3B-C2B	5.06	1.64	1.53
5	D	704	NDP	C3B-C2B	5.07	1.64	1.53
5	E	704	NDP	C3B-C2B	5.18	1.64	1.53
4	B	703	FOL	C7-N8	5.30	1.40	1.31
5	F	704	NDP	C3B-C2B	5.35	1.65	1.53
4	F	703	FOL	C7-N8	5.41	1.41	1.31
5	G	704	NDP	C3B-C2B	5.42	1.65	1.53
5	C	704	NDP	C3B-C2B	5.42	1.65	1.53
4	H	703	FOL	C7-N8	5.45	1.41	1.31
5	A	704	NDP	C3B-C2B	5.49	1.65	1.53
5	B	704	NDP	C3B-C2B	5.50	1.65	1.53
4	D	703	FOL	C7-N8	5.62	1.41	1.31
4	A	703	FOL	C7-N8	5.75	1.41	1.31
4	C	703	FOL	C7-N8	5.92	1.41	1.31
4	G	703	FOL	C7-N8	6.06	1.42	1.31
4	E	703	FOL	C7-N8	6.09	1.42	1.31

All (353) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	UMP	O4'-C1'-C2'	-19.85	66.69	106.27
2	F	701	UMP	O4'-C1'-C2'	-19.84	66.71	106.27
2	C	701	UMP	O4'-C1'-C2'	-19.83	66.74	106.27
2	H	701	UMP	O4'-C1'-C2'	-19.82	66.76	106.27
2	B	701	UMP	O4'-C1'-C2'	-19.80	66.80	106.27
2	D	701	UMP	O4'-C1'-C2'	-19.73	66.94	106.27
2	A	701	UMP	O4'-C1'-C2'	-19.56	67.28	106.27
2	G	701	UMP	O4'-C1'-C2'	-19.49	67.42	106.27
5	F	704	NDP	O4D-C1D-C2D	-14.46	73.04	106.58
5	B	704	NDP	O4D-C1D-C2D	-13.99	74.12	106.58
5	H	704	NDP	O4D-C1D-C2D	-13.84	74.48	106.58
5	F	704	NDP	N3A-C2A-N1A	-13.11	118.86	128.89
5	E	704	NDP	N3A-C2A-N1A	-13.07	118.89	128.89
5	C	704	NDP	N3A-C2A-N1A	-12.93	118.99	128.89
5	B	704	NDP	N3A-C2A-N1A	-12.83	119.07	128.89
5	H	704	NDP	N3A-C2A-N1A	-12.73	119.15	128.89
5	A	704	NDP	N3A-C2A-N1A	-12.60	119.24	128.89
5	D	704	NDP	N3A-C2A-N1A	-12.58	119.26	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	704	NDP	N3A-C2A-N1A	-12.45	119.36	128.89
5	G	704	NDP	O4B-C1B-C2B	-10.79	87.08	106.60
5	A	704	NDP	O4B-C1B-C2B	-10.74	87.18	106.60
5	H	704	NDP	O4B-C1B-C2B	-10.47	87.65	106.60
5	C	704	NDP	O4B-C1B-C2B	-10.30	87.97	106.60
2	E	701	UMP	O4'-C4'-C5'	-10.22	72.76	109.32
5	E	704	NDP	O4B-C1B-C2B	-10.20	88.16	106.60
5	D	704	NDP	O4B-C1B-C2B	-10.19	88.16	106.60
2	A	701	UMP	O4'-C4'-C5'	-10.15	73.03	109.32
2	C	701	UMP	O4'-C4'-C5'	-10.14	73.04	109.32
5	B	704	NDP	O4B-C1B-C2B	-10.12	88.30	106.60
2	H	701	UMP	O4'-C4'-C5'	-10.11	73.16	109.32
2	B	701	UMP	O4'-C4'-C5'	-10.10	73.18	109.32
2	D	701	UMP	O4'-C4'-C5'	-10.08	73.25	109.32
2	F	701	UMP	O4'-C4'-C5'	-10.08	73.27	109.32
2	G	701	UMP	O4'-C4'-C5'	-10.07	73.29	109.32
5	F	704	NDP	O4B-C1B-C2B	-9.86	88.76	106.60
5	H	704	NDP	O4D-C4D-C3D	-9.29	86.42	105.15
5	B	704	NDP	O4D-C4D-C3D	-9.10	86.81	105.15
5	F	704	NDP	O4D-C4D-C5D	-8.77	77.97	109.32
5	F	704	NDP	O4D-C4D-C3D	-8.74	87.53	105.15
2	B	701	UMP	O4'-C4'-C3'	-8.40	84.54	105.67
2	C	701	UMP	O4'-C4'-C3'	-8.40	84.55	105.67
5	H	704	NDP	O4D-C4D-C5D	-8.37	79.37	109.32
5	B	704	NDP	O4D-C4D-C5D	-8.36	79.42	109.32
5	G	704	NDP	C5D-C4D-C3D	-8.34	82.12	115.21
2	E	701	UMP	O4'-C4'-C3'	-8.29	84.81	105.67
5	E	704	NDP	C5D-C4D-C3D	-8.29	82.32	115.21
2	F	701	UMP	O4'-C4'-C3'	-8.28	84.84	105.67
2	H	701	UMP	O4'-C4'-C3'	-8.27	84.87	105.67
5	C	704	NDP	C5D-C4D-C3D	-8.27	82.39	115.21
2	G	701	UMP	O4'-C4'-C3'	-8.24	84.96	105.67
5	A	704	NDP	C5D-C4D-C3D	-8.23	82.53	115.21
2	A	701	UMP	O4'-C4'-C3'	-8.20	85.05	105.67
2	D	701	UMP	O4'-C4'-C3'	-8.12	85.24	105.67
5	D	704	NDP	C5D-C4D-C3D	-8.12	83.00	115.21
5	A	704	NDP	C3D-C2D-C1D	-7.09	87.16	101.40
5	C	704	NDP	C3D-C2D-C1D	-6.99	87.35	101.40
5	D	704	NDP	C3D-C2D-C1D	-6.98	87.38	101.40
5	E	704	NDP	C3D-C2D-C1D	-6.97	87.40	101.40
5	G	704	NDP	C3D-C2D-C1D	-6.87	87.59	101.40
5	C	704	NDP	O4D-C4D-C3D	-6.84	91.36	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NDP	O4D-C4D-C3D	-6.77	91.50	105.15
5	E	704	NDP	O4D-C4D-C3D	-6.68	91.70	105.15
5	G	704	NDP	O4D-C4D-C3D	-6.66	91.73	105.15
5	D	704	NDP	O4D-C4D-C3D	-6.64	91.77	105.15
5	B	704	NDP	C2B-C3B-C4B	-6.52	86.42	101.85
5	D	704	NDP	C2B-C3B-C4B	-6.48	86.52	101.85
5	G	704	NDP	C2B-C3B-C4B	-6.23	87.09	101.85
5	C	704	NDP	C2B-C3B-C4B	-6.23	87.11	101.85
5	F	704	NDP	C2B-C3B-C4B	-6.19	87.19	101.85
5	A	704	NDP	C2B-C3B-C4B	-6.07	87.49	101.85
5	E	704	NDP	C2B-C3B-C4B	-5.96	87.75	101.85
5	H	704	NDP	C2B-C3B-C4B	-5.92	87.84	101.85
5	G	704	NDP	C1D-N1N-C6N	-5.50	108.50	120.81
5	E	704	NDP	C1D-N1N-C6N	-5.50	108.51	120.81
5	A	704	NDP	C1D-N1N-C6N	-5.27	109.03	120.81
5	C	704	NDP	C1D-N1N-C6N	-5.25	109.06	120.81
5	H	704	NDP	O3-PN-O5D	-5.07	89.48	102.94
5	D	704	NDP	O3-PN-O5D	-5.07	89.49	102.94
5	D	704	NDP	C1D-N1N-C6N	-5.04	109.53	120.81
5	F	704	NDP	O3-PN-O5D	-4.94	89.83	102.94
5	C	704	NDP	O3-PN-O5D	-4.91	89.92	102.94
2	E	701	UMP	C2'-C1'-N1	-4.82	102.44	114.16
5	B	704	NDP	O3-PN-O5D	-4.78	90.25	102.94
2	C	701	UMP	C2'-C1'-N1	-4.74	102.63	114.16
5	G	704	NDP	O3-PN-O5D	-4.71	90.45	102.94
3	G	702	CB3	N1-C2-N3	-4.68	120.32	127.44
2	B	701	UMP	C2'-C1'-N1	-4.67	102.81	114.16
2	H	701	UMP	C2'-C1'-N1	-4.66	102.83	114.16
3	B	702	CB3	N1-C2-N3	-4.64	120.38	127.44
2	F	701	UMP	C2'-C1'-N1	-4.63	102.90	114.16
2	D	701	UMP	C2'-C1'-N1	-4.54	103.12	114.16
3	F	702	CB3	N1-C2-N3	-4.54	120.53	127.44
2	A	701	UMP	C2'-C1'-N1	-4.53	103.13	114.16
5	E	704	NDP	O3-PN-O5D	-4.52	90.95	102.94
3	D	702	CB3	N1-C2-N3	-4.52	120.57	127.44
3	E	702	CB3	N1-C2-N3	-4.50	120.60	127.44
2	G	701	UMP	C2'-C1'-N1	-4.50	103.22	114.16
5	H	704	NDP	C3D-C2D-C1D	-4.50	92.37	101.40
3	H	702	CB3	N1-C2-N3	-4.49	120.61	127.44
3	C	702	CB3	N1-C2-N3	-4.42	120.70	127.44
5	A	704	NDP	O3-PN-O5D	-4.42	91.22	102.94
5	F	704	NDP	C3D-C2D-C1D	-4.29	92.77	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	CB3	N1-C2-N3	-4.27	120.93	127.44
4	F	703	FOL	N1-C2-N3	-4.27	120.94	127.44
4	B	703	FOL	N1-C2-N3	-4.26	120.95	127.44
4	H	703	FOL	N1-C2-N3	-4.18	121.08	127.44
4	A	703	FOL	N1-C2-N3	-4.16	121.10	127.44
5	A	704	NDP	C3N-C2N-N1N	-4.12	117.24	123.14
5	B	704	NDP	C3D-C2D-C1D	-4.12	93.13	101.40
4	C	703	FOL	N1-C2-N3	-4.09	121.21	127.44
4	D	703	FOL	N1-C2-N3	-4.04	121.28	127.44
4	G	703	FOL	N1-C2-N3	-4.01	121.33	127.44
5	G	704	NDP	O3B-C3B-C4B	-3.97	99.15	111.05
5	A	704	NDP	O3B-C3B-C4B	-3.91	99.34	111.05
4	E	703	FOL	N1-C2-N3	-3.86	121.56	127.44
3	C	702	CB3	CG-CB-CA	-3.80	105.26	112.99
5	E	704	NDP	O3B-C3B-C4B	-3.73	99.85	111.05
5	C	704	NDP	C3N-C2N-N1N	-3.68	117.88	123.14
5	G	704	NDP	O2D-C2D-C1D	-3.52	97.65	109.94
5	E	704	NDP	O2D-C2D-C1D	-3.52	97.65	109.94
5	C	704	NDP	O3B-C3B-C4B	-3.51	100.52	111.05
5	C	704	NDP	O2D-C2D-C1D	-3.44	97.92	109.94
5	E	704	NDP	C3N-C2N-N1N	-3.41	118.26	123.14
4	B	703	FOL	C4A-C4-N3	-3.32	119.05	123.59
5	G	704	NDP	C3N-C2N-N1N	-3.32	118.39	123.14
4	D	703	FOL	C4A-C4-N3	-3.29	119.09	123.59
5	D	704	NDP	C3N-C2N-N1N	-3.24	118.50	123.14
4	E	703	FOL	C4A-C4-N3	-3.23	119.18	123.59
5	A	704	NDP	O2D-C2D-C1D	-3.22	98.68	109.94
5	A	704	NDP	O2D-C2D-C3D	-3.16	101.53	111.83
4	C	703	FOL	C4A-C4-N3	-3.11	119.33	123.59
4	A	703	FOL	C4A-C4-N3	-3.09	119.36	123.59
4	E	703	FOL	C4-C4A-N5	-3.08	114.98	118.72
4	G	703	FOL	C4A-C4-N3	-3.07	119.39	123.59
4	F	703	FOL	C4A-C4-N3	-3.06	119.40	123.59
5	D	704	NDP	O2D-C2D-C1D	-3.05	99.28	109.94
4	G	703	FOL	C4-C4A-N5	-3.02	115.05	118.72
5	E	704	NDP	O2D-C2D-C3D	-3.00	102.09	111.83
4	H	703	FOL	C4A-C4-N3	-2.99	119.50	123.59
5	G	704	NDP	O2D-C2D-C3D	-2.96	102.21	111.83
5	C	704	NDP	O2D-C2D-C3D	-2.95	102.25	111.83
3	G	702	CB3	O-C-C11	-2.85	116.10	120.97
2	A	701	UMP	OP2-P-O5'	-2.85	98.36	106.56
5	A	704	NDP	C4N-C5N-C6N	-2.79	117.98	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	704	NDP	O3B-C3B-C4B	-2.78	102.72	111.05
2	E	701	UMP	OP2-P-O5'	-2.76	98.60	106.56
3	D	702	CB3	C11-C-N	-2.75	112.03	116.93
4	G	703	FOL	CB-CG-CD	-2.72	101.91	113.02
2	C	701	UMP	OP2-P-O5'	-2.70	98.78	106.56
4	E	703	FOL	CB-CG-CD	-2.70	102.01	113.02
2	G	701	UMP	OP2-P-O5'	-2.69	98.82	106.56
5	H	704	NDP	O3B-C3B-C4B	-2.58	103.31	111.05
2	B	701	UMP	C3'-C2'-C1'	-2.57	96.21	102.40
4	A	703	FOL	C4-C4A-N5	-2.55	115.62	118.72
5	C	704	NDP	C4N-C5N-C6N	-2.55	118.38	122.58
2	F	701	UMP	C3'-C2'-C1'	-2.54	96.28	102.40
4	C	703	FOL	C4-C4A-N5	-2.54	115.64	118.72
2	H	701	UMP	C3'-C2'-C1'	-2.48	96.42	102.40
5	D	704	NDP	O2D-C2D-C3D	-2.40	104.02	111.83
4	D	703	FOL	C4-C4A-N5	-2.40	115.81	118.72
5	E	704	NDP	C4N-C5N-C6N	-2.37	118.67	122.58
5	B	704	NDP	O3B-C3B-C4B	-2.35	103.99	111.05
2	E	701	UMP	C3'-C2'-C1'	-2.34	96.77	102.40
5	D	704	NDP	C4N-C5N-C6N	-2.33	118.74	122.58
2	D	701	UMP	C3'-C2'-C1'	-2.30	96.86	102.40
5	F	704	NDP	C2D-C1D-N1N	-2.29	107.15	113.34
5	G	704	NDP	C4N-C5N-C6N	-2.28	118.81	122.58
3	E	702	CB3	O-C-C11	-2.26	117.11	120.97
5	D	704	NDP	O3B-C3B-C4B	-2.22	104.39	111.05
3	F	702	CB3	C11-C-N	-2.22	112.98	116.93
2	G	701	UMP	C3'-C2'-C1'	-2.21	97.07	102.40
5	E	704	NDP	O2B-P2B-O1X	-2.20	101.62	107.11
2	C	701	UMP	C3'-C2'-C1'	-2.20	97.11	102.40
4	A	703	FOL	CG-CB-CA	-2.19	108.53	112.99
2	A	701	UMP	C2'-C3'-C4'	-2.14	98.33	102.77
5	G	704	NDP	O2B-P2B-O1X	-2.14	101.76	107.11
5	E	704	NDP	O3B-C3B-C2B	-2.13	105.00	111.16
4	C	703	FOL	C4A-C8A-N8	-2.12	117.96	121.81
5	C	704	NDP	O3-PA-O5B	-2.11	97.33	102.94
2	H	701	UMP	OP2-P-O5'	-2.10	100.51	106.56
2	D	701	UMP	C2'-C3'-C4'	-2.08	98.46	102.77
4	G	703	FOL	C4A-C8A-N8	-2.07	118.04	121.81
5	H	704	NDP	O3B-C3B-C2B	-2.06	105.20	111.16
3	B	702	CB3	C6-C9-N10	-2.06	111.08	114.51
2	F	701	UMP	OP2-P-O5'	-2.05	100.65	106.56
4	A	703	FOL	C4A-C8A-N8	-2.04	118.09	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	703	FOL	C4A-C8A-N8	-2.04	118.10	121.81
5	G	704	NDP	O3-PA-O5B	-2.04	97.53	102.94
2	A	701	UMP	C3'-C2'-C1'	-2.02	97.54	102.40
2	E	701	UMP	C2'-C3'-C4'	-2.01	98.62	102.77
4	G	703	FOL	C9-N10-C14	2.01	127.62	122.15
2	H	701	UMP	OP3-P-OP2	2.07	115.25	107.38
4	E	703	FOL	C4-N3-C2	2.07	118.81	115.94
2	D	701	UMP	OP3-P-OP2	2.07	115.26	107.38
4	G	703	FOL	C4-N3-C2	2.07	118.81	115.94
5	E	704	NDP	O5B-C5B-C4B	2.08	116.79	109.12
3	C	702	CB3	C9-N10-C14	2.12	124.75	120.93
2	F	701	UMP	OP3-P-OP2	2.13	115.51	107.38
4	E	703	FOL	C16-C15-C14	2.14	122.70	120.28
4	B	703	FOL	C9-C6-N5	2.17	120.93	116.81
4	C	703	FOL	C4-N3-C2	2.20	119.00	115.94
3	F	702	CB3	CG-CB-CA	2.20	117.47	112.99
5	A	704	NDP	C2D-C3D-C4D	2.20	107.14	102.61
5	A	704	NDP	O5B-C5B-C4B	2.20	117.25	109.12
5	B	704	NDP	O2B-C2B-C1B	2.21	118.63	110.02
5	C	704	NDP	P2B-O2B-C2B	2.22	126.88	121.56
2	B	701	UMP	OP3-P-OP2	2.23	115.86	107.38
4	F	703	FOL	C6-C9-N10	2.23	118.25	113.32
4	E	703	FOL	C9-C6-N5	2.24	121.05	116.81
4	H	703	FOL	C4-N3-C2	2.24	119.05	115.94
4	A	703	FOL	C4-N3-C2	2.25	119.06	115.94
4	B	703	FOL	C4-N3-C2	2.25	119.07	115.94
3	D	702	CB3	C9-N10-C14	2.26	124.98	120.93
3	F	702	CB3	C9-N10-C14	2.27	125.01	120.93
4	F	703	FOL	C4-N3-C2	2.27	119.09	115.94
5	F	704	NDP	O2B-C2B-C1B	2.28	118.91	110.02
3	C	702	CB3	C4-N3-C2	2.30	119.14	115.94
3	F	702	CB3	C4-N3-C2	2.30	119.14	115.94
3	D	702	CB3	C4-N3-C2	2.31	119.15	115.94
4	E	703	FOL	C9-N10-C14	2.32	128.45	122.15
2	C	701	UMP	OP3-P-OP2	2.33	116.25	107.38
3	A	702	CB3	CB-CG-CD	2.35	122.59	113.02
2	G	701	UMP	OP3-P-OP2	2.35	116.33	107.38
5	F	704	NDP	O5B-C5B-C4B	2.35	117.80	109.12
2	E	701	UMP	OP3-P-OP2	2.35	116.35	107.38
2	A	701	UMP	OP3-P-OP2	2.36	116.36	107.38
5	D	704	NDP	O5B-C5B-C4B	2.37	117.85	109.12
3	E	702	CB3	C4-N3-C2	2.37	119.23	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	702	CB3	C9-N10-C14	2.37	125.20	120.93
5	C	704	NDP	C2D-C3D-C4D	2.38	107.51	102.61
2	A	701	UMP	O3'-C3'-C4'	2.39	119.72	110.05
5	E	704	NDP	C2D-C3D-C4D	2.39	107.53	102.61
3	H	702	CB3	C4-N3-C2	2.40	119.28	115.94
3	D	702	CB3	O-C-N	2.41	126.80	122.44
5	A	704	NDP	P2B-O2B-C2B	2.43	127.40	121.56
3	B	702	CB3	C9-N10-C14	2.43	125.31	120.93
3	E	702	CB3	C9-N10-C14	2.44	125.32	120.93
5	G	704	NDP	C2D-C3D-C4D	2.45	107.64	102.61
5	B	704	NDP	O5B-C5B-C4B	2.45	118.15	109.12
3	A	702	CB3	C4-N3-C2	2.46	119.35	115.94
2	G	701	UMP	O3'-C3'-C4'	2.51	120.20	110.05
5	E	704	NDP	P2B-O2B-C2B	2.52	127.61	121.56
5	H	704	NDP	O5B-C5B-C4B	2.52	118.41	109.12
2	D	701	UMP	O3'-C3'-C4'	2.55	120.34	110.05
4	C	703	FOL	C9-C6-N5	2.57	121.69	116.81
3	G	702	CB3	C9-N10-C14	2.60	125.61	120.93
5	D	704	NDP	C2D-C3D-C4D	2.61	107.97	102.61
3	G	702	CB3	C4-N3-C2	2.62	119.57	115.94
3	B	702	CB3	C4-N3-C2	2.63	119.59	115.94
2	C	701	UMP	O3'-C3'-C4'	2.63	120.67	110.05
4	F	703	FOL	C9-C6-N5	2.63	121.80	116.81
5	B	704	NDP	C5N-C4N-C3N	2.67	119.88	112.52
2	E	701	UMP	O3'-C3'-C4'	2.67	120.85	110.05
5	H	704	NDP	C1B-N9A-C4A	2.68	130.97	126.94
5	G	704	NDP	P2B-O2B-C2B	2.68	127.99	121.56
5	H	704	NDP	C5N-C4N-C3N	2.69	119.93	112.52
2	B	701	UMP	O3'-C3'-C4'	2.70	120.93	110.05
5	H	704	NDP	O2B-C2B-C1B	2.73	120.66	110.02
2	F	701	UMP	O3'-C3'-C4'	2.74	121.10	110.05
5	D	704	NDP	O2B-C2B-C1B	2.74	120.70	110.02
5	G	704	NDP	C5N-C4N-C3N	2.77	120.14	112.52
4	B	703	FOL	N8-C8A-N1	2.77	120.11	116.14
3	A	702	CB3	C9-N10-C14	2.79	125.94	120.93
2	H	701	UMP	O3'-C3'-C4'	2.80	121.38	110.05
5	B	704	NDP	O5D-C5D-C4D	2.87	119.71	109.12
5	H	704	NDP	O5D-C5D-C4D	2.89	119.78	109.12
4	G	703	FOL	C9-C6-N5	2.91	122.32	116.81
5	F	704	NDP	C5N-C4N-C3N	2.93	120.59	112.52
5	E	704	NDP	C5N-C4N-C3N	2.94	120.61	112.52
4	A	703	FOL	C9-C6-N5	2.95	122.39	116.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NDP	C5N-C4N-C3N	3.02	120.83	112.52
3	G	702	CB3	CB-CG-CD	3.02	125.34	113.02
5	C	704	NDP	C5N-C4N-C3N	3.04	120.91	112.52
5	D	704	NDP	C5N-C4N-C3N	3.09	121.04	112.52
4	F	703	FOL	N8-C8A-N1	3.12	120.61	116.14
4	H	703	FOL	N8-C8A-N1	3.18	120.70	116.14
4	C	703	FOL	C6-C9-N10	3.19	120.36	113.32
5	C	704	NDP	C3B-C2B-C1B	3.22	108.95	102.73
5	E	704	NDP	C3B-C2B-C1B	3.23	108.97	102.73
5	B	704	NDP	C3B-C2B-C1B	3.26	109.03	102.73
4	H	703	FOL	C9-C6-N5	3.27	123.02	116.81
5	A	704	NDP	C3B-C2B-C1B	3.30	109.11	102.73
5	H	704	NDP	C3B-C2B-C1B	3.32	109.14	102.73
4	A	703	FOL	C6-C9-N10	3.35	120.72	113.32
5	F	704	NDP	O5D-C5D-C4D	3.35	121.47	109.12
5	F	704	NDP	C3B-C2B-C1B	3.45	109.40	102.73
5	D	704	NDP	C3B-C2B-C1B	3.47	109.43	102.73
4	D	703	FOL	N8-C8A-N1	3.56	121.24	116.14
4	A	703	FOL	N8-C8A-N1	3.59	121.28	116.14
5	G	704	NDP	C3B-C2B-C1B	3.61	109.71	102.73
4	C	703	FOL	N8-C8A-N1	3.75	121.51	116.14
4	E	703	FOL	C6-C9-N10	3.79	121.69	113.32
5	F	704	NDP	C5D-C4D-C3D	3.80	130.29	115.21
4	G	703	FOL	N8-C8A-N1	3.84	121.64	116.14
5	D	704	NDP	C1B-N9A-C4A	3.87	132.77	126.94
4	E	703	FOL	N8-C8A-N1	3.96	121.81	116.14
5	F	704	NDP	C4B-O4B-C1B	4.23	114.36	109.72
5	B	704	NDP	C5D-C4D-C3D	4.23	132.01	115.21
4	G	703	FOL	C6-C9-N10	4.32	122.87	113.32
4	H	703	FOL	C6-C9-N10	4.35	122.92	113.32
5	H	704	NDP	C5D-C4D-C3D	4.41	132.70	115.21
3	A	702	CB3	CG-CB-CA	4.44	122.00	112.99
5	D	704	NDP	C4B-O4B-C1B	4.73	114.92	109.72
5	B	704	NDP	C4B-O4B-C1B	4.73	114.92	109.72
4	G	703	FOL	CG-CB-CA	4.89	122.92	112.99
2	A	701	UMP	O3'-C3'-C2'	4.90	126.97	110.74
5	E	704	NDP	C4B-O4B-C1B	5.00	115.21	109.72
5	B	704	NDP	C1B-N9A-C4A	5.02	134.51	126.94
5	C	704	NDP	C4B-O4B-C1B	5.09	115.31	109.72
2	D	701	UMP	O3'-C3'-C2'	5.16	127.83	110.74
2	E	701	UMP	O3'-C3'-C2'	5.17	127.84	110.74
2	B	701	UMP	O3'-C3'-C2'	5.17	127.84	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	701	UMP	O3'-C3'-C2'	5.19	127.91	110.74
2	C	701	UMP	O3'-C3'-C2'	5.24	128.09	110.74
5	A	704	NDP	C1D-N1N-C2N	5.24	130.04	120.91
2	H	701	UMP	O3'-C3'-C2'	5.28	128.21	110.74
4	E	703	FOL	CG-CB-CA	5.33	123.81	112.99
2	F	701	UMP	O3'-C3'-C2'	5.34	128.41	110.74
3	G	702	CB3	CG-CB-CA	5.34	123.84	112.99
5	G	704	NDP	C4B-O4B-C1B	5.54	115.80	109.72
4	C	703	FOL	CG-CB-CA	5.61	124.39	112.99
5	C	704	NDP	C1D-N1N-C2N	5.63	130.71	120.91
5	H	704	NDP	C4B-O4B-C1B	5.65	115.93	109.72
5	F	704	NDP	C5B-C4B-C3B	5.68	137.73	115.21
5	B	704	NDP	C5B-C4B-C3B	5.80	138.22	115.21
5	D	704	NDP	C1D-N1N-C2N	5.80	131.00	120.91
5	D	704	NDP	C5B-C4B-C3B	5.82	138.32	115.21
5	A	704	NDP	C4B-O4B-C1B	5.87	116.17	109.72
5	G	704	NDP	C5B-C4B-C3B	5.95	138.83	115.21
5	C	704	NDP	C5B-C4B-C3B	6.01	139.05	115.21
5	E	704	NDP	C5B-C4B-C3B	6.03	139.14	115.21
5	H	704	NDP	C5B-C4B-C3B	6.04	139.19	115.21
5	A	704	NDP	C5B-C4B-C3B	6.13	139.53	115.21
5	E	704	NDP	C1D-N1N-C2N	6.22	131.75	120.91
5	G	704	NDP	C1D-N1N-C2N	6.45	132.15	120.91
2	E	701	UMP	C4-N3-C2	6.83	120.91	114.14
2	D	701	UMP	C4-N3-C2	6.86	120.94	114.14
2	F	701	UMP	C4-N3-C2	6.87	120.94	114.14
2	B	701	UMP	C4-N3-C2	7.00	121.07	114.14
2	H	701	UMP	C4-N3-C2	7.01	121.08	114.14
2	A	701	UMP	C4-N3-C2	7.01	121.09	114.14
2	C	701	UMP	C4-N3-C2	7.06	121.13	114.14
5	E	704	NDP	C1B-N9A-C4A	7.14	137.71	126.94
2	G	701	UMP	C4-N3-C2	7.16	121.23	114.14
5	G	704	NDP	C2D-C1D-N1N	7.66	134.02	113.34
5	C	704	NDP	C2D-C1D-N1N	7.73	134.21	113.34
5	G	704	NDP	C1B-N9A-C4A	7.75	138.62	126.94
5	E	704	NDP	C2D-C1D-N1N	7.78	134.36	113.34
5	A	704	NDP	C2D-C1D-N1N	7.79	134.39	113.34
5	D	704	NDP	C2D-C1D-N1N	7.90	134.69	113.34
5	A	704	NDP	C1B-N9A-C4A	8.23	139.36	126.94
5	C	704	NDP	C1B-N9A-C4A	8.64	139.98	126.94
5	F	704	NDP	C1B-N9A-C4A	9.29	140.95	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	UMP	3	0
3	A	702	CB3	2	0
4	A	703	FOL	4	0
5	A	704	NDP	3	0
2	B	701	UMP	7	0
3	B	702	CB3	4	0
4	B	703	FOL	2	0
5	B	704	NDP	7	0
2	C	701	UMP	4	0
3	C	702	CB3	4	0
4	C	703	FOL	5	0
5	C	704	NDP	5	0
2	D	701	UMP	4	0
3	D	702	CB3	3	0
4	D	703	FOL	2	0
5	D	704	NDP	7	0
2	E	701	UMP	3	0
3	E	702	CB3	1	0
4	E	703	FOL	4	0
5	E	704	NDP	4	0
2	F	701	UMP	4	0
3	F	702	CB3	4	0
4	F	703	FOL	3	0
5	F	704	NDP	8	0
2	G	701	UMP	2	0
3	G	702	CB3	1	0
4	G	703	FOL	4	0
5	G	704	NDP	3	0
2	H	701	UMP	5	0
3	H	702	CB3	4	0
4	H	703	FOL	2	0
5	H	704	NDP	7	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, 95th 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	510/566 (90%)	0.10	19 (3%)	45	44	25, 39, 75, 107	0
1	B	491/566 (86%)	0.25	31 (6%)	23	23	27, 40, 90, 113	0
1	C	510/566 (90%)	0.06	21 (4%)	41	39	25, 39, 73, 105	0
1	D	491/566 (86%)	0.24	31 (6%)	23	23	25, 40, 89, 112	0
1	E	510/566 (90%)	0.09	22 (4%)	39	38	27, 39, 74, 109	0
1	F	491/566 (86%)	0.21	31 (6%)	23	23	26, 41, 87, 114	0
1	G	510/566 (90%)	0.09	16 (3%)	52	51	26, 39, 74, 107	0
1	H	491/566 (86%)	0.21	29 (5%)	26	25	26, 40, 86, 118	0
All	All	4004/4528 (88%)	0.15	200 (4%)	32	32	25, 40, 83, 118	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	106	LEU	6.5
1	F	106	LEU	6.4
1	H	136	LEU	6.4
1	E	610	VAL	6.0
1	F	105	SER	5.9
1	C	294	LEU	5.9
1	C	143	ASP	5.7
1	A	298	ASP	5.7
1	G	143	ASP	5.6
1	B	106	LEU	5.5
1	C	295	ALA	4.9
1	D	145	VAL	4.9
1	F	136	LEU	4.8
1	D	137	LEU	4.7
1	B	105	SER	4.6
1	H	105	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	137	LEU	4.6
1	D	106	LEU	4.6
1	D	105	SER	4.5
1	F	134	LEU	4.4
1	D	146	ASP	4.4
1	E	43	PRO	4.3
1	B	144	SER	4.3
1	B	136	LEU	4.3
1	D	136	LEU	4.3
1	D	91	PHE	4.3
1	G	298	ASP	4.3
1	B	134	LEU	4.3
1	F	137	LEU	4.2
1	C	610	VAL	4.2
1	D	134	LEU	4.2
1	H	144	SER	4.2
1	A	294	LEU	4.1
1	B	91	PHE	4.0
1	A	296	TRP	3.9
1	A	225	ALA	3.8
1	B	196	LYS	3.8
1	C	297	MET	3.8
1	E	294	LEU	3.8
1	D	308	LYS	3.8
1	G	294	LEU	3.7
1	A	285	SER	3.7
1	A	46	ALA	3.7
1	H	126	VAL	3.7
1	H	134	LEU	3.7
1	C	298	ASP	3.6
1	A	610	VAL	3.6
1	C	285	SER	3.6
1	G	46	ALA	3.6
1	H	146	ASP	3.6
1	A	47	SER	3.5
1	H	319	PHE	3.5
1	B	133	ALA	3.5
1	D	74	PHE	3.5
1	B	141	TYR	3.5
1	D	319	PHE	3.5
1	D	144	SER	3.4
1	F	91	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	46	ALA	3.4
1	C	46	ALA	3.3
1	H	139	GLU	3.3
1	G	43	PRO	3.3
1	A	295	ALA	3.3
1	A	297	MET	3.3
1	F	319	PHE	3.3
1	G	252	ARG	3.3
1	B	163	LEU	3.3
1	G	295	ALA	3.3
1	G	297	MET	3.2
1	F	145	VAL	3.2
1	E	252	ARG	3.2
1	E	143	ASP	3.2
1	E	225	ALA	3.2
1	A	143	ASP	3.1
1	D	104	SER	3.1
1	B	74	PHE	3.1
1	B	143	ASP	3.1
1	F	143	ASP	3.1
1	F	300	GLU	3.1
1	D	139	GLU	3.1
1	C	296	TRP	3.1
1	A	311	ILE	3.1
1	E	297	MET	3.0
1	D	196	LYS	3.0
1	F	101	VAL	3.0
1	F	308	LYS	3.0
1	F	146	ASP	3.0
1	D	6	CYS	3.0
1	G	225	ALA	3.0
1	E	310	LEU	3.0
1	B	76	ALA	3.0
1	B	104	SER	3.0
1	H	127	CYS	3.0
1	F	126	VAL	2.9
1	F	6	CYS	2.9
1	C	47	SER	2.9
1	B	146	ASP	2.9
1	D	133	ALA	2.9
1	D	300	GLU	2.9
1	B	126	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	300	GLU	2.9
1	C	43	PRO	2.9
1	B	103	SER	2.8
1	H	137	LEU	2.8
1	E	296	TRP	2.8
1	F	127	CYS	2.8
1	F	133	ALA	2.8
1	H	74	PHE	2.8
1	F	104	SER	2.8
1	G	285	SER	2.8
1	B	4	PRO	2.7
1	B	308	LYS	2.7
1	B	298	ASP	2.7
1	H	91	PHE	2.7
1	H	145	VAL	2.7
1	H	143	ASP	2.7
1	D	5	VAL	2.7
1	A	299	GLU	2.7
1	C	299	GLU	2.7
1	D	140	GLU	2.7
1	A	42	THR	2.7
1	E	546	PHE	2.7
1	B	41	THR	2.7
1	E	295	ALA	2.7
1	H	196	LYS	2.6
1	E	298	ASP	2.6
1	F	102	VAL	2.6
1	G	546	PHE	2.6
1	F	139	GLU	2.6
1	G	47	SER	2.6
1	H	308	LYS	2.6
1	C	292	PRO	2.5
1	C	225	ALA	2.5
1	F	144	SER	2.5
1	B	94	LEU	2.5
1	D	98	LEU	2.5
1	B	300	GLU	2.5
1	B	145	VAL	2.5
1	A	43	PRO	2.5
1	C	42	THR	2.5
1	D	163	LEU	2.5
1	H	101	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	141	TYR	2.5
1	C	48	ARG	2.5
1	D	165	VAL	2.5
1	E	291	ALA	2.4
1	B	138	GLU	2.4
1	H	76	ALA	2.4
1	D	132	ALA	2.4
1	E	419	HIS	2.4
1	H	94	LEU	2.4
1	G	419	HIS	2.4
1	A	48	ARG	2.4
1	H	89	ARG	2.4
1	C	291	ALA	2.3
1	H	104	SER	2.3
1	C	546	PHE	2.3
1	F	298	ASP	2.3
1	C	252	ARG	2.3
1	H	102	VAL	2.3
1	E	47	SER	2.3
1	D	94	LEU	2.3
1	E	292	PRO	2.3
1	D	141	TYR	2.3
1	G	610	VAL	2.3
1	H	4	PRO	2.3
1	C	289	ALA	2.3
1	D	89	ARG	2.3
1	G	296	TRP	2.3
1	F	544	ILE	2.3
1	A	410	GLU	2.3
1	B	140	GLU	2.3
1	F	170	TYR	2.2
1	H	298	ASP	2.2
1	F	41	THR	2.2
1	E	48	ARG	2.2
1	E	89	ARG	2.2
1	G	91	PHE	2.2
1	D	101	VAL	2.2
1	B	355	CYS	2.2
1	F	155	GLY	2.2
1	B	101	VAL	2.2
1	D	170	TYR	2.1
1	H	225	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	129	SER	2.1
1	E	489	CYS	2.1
1	B	139	GLU	2.1
1	B	128	ALA	2.1
1	E	375	TRP	2.1
1	E	547	MET	2.1
1	F	196	LYS	2.1
1	D	130	LEU	2.1
1	A	291	ALA	2.1
1	F	128	ALA	2.1
1	C	375	TRP	2.1
1	F	355	CYS	2.1
1	H	163	LEU	2.0
1	A	292	PRO	2.0
1	H	155	GLY	2.0
1	D	143	ASP	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, 95th 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	FOL	E	703	32/32	0.92	0.19	3.02	30,57,81,94	0
4	FOL	G	703	32/32	0.90	0.20	2.76	32,57,85,109	0
4	FOL	H	703	32/32	0.90	0.23	2.34	37,71,89,102	0
4	FOL	C	703	32/32	0.89	0.18	2.27	33,53,75,84	0
4	FOL	A	703	32/32	0.90	0.20	2.19	28,52,83,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	FOL	F	703	32/32	0.90	0.22	1.85	33,70,96,101	0
4	FOL	B	703	32/32	0.90	0.24	1.74	38,71,99,107	0
4	FOL	D	703	32/32	0.89	0.22	1.38	34,71,93,102	0
5	NDP	E	704	48/48	0.95	0.13	1.28	24,41,58,61	0
3	CB3	D	702	35/35	0.90	0.15	0.87	26,35,101,111	0
2	UMP	F	701	20/20	0.95	0.14	0.79	27,35,42,52	0
5	NDP	A	704	48/48	0.96	0.12	0.74	25,42,56,64	0
5	NDP	C	704	48/48	0.96	0.12	0.70	24,41,53,62	0
5	NDP	G	704	48/48	0.96	0.12	0.50	23,41,53,67	0
3	CB3	F	702	35/35	0.92	0.14	0.43	21,34,103,108	0
2	UMP	C	701	20/20	0.95	0.15	0.40	31,38,50,54	0
2	UMP	D	701	20/20	0.96	0.13	0.38	27,36,43,52	0
3	CB3	B	702	35/35	0.93	0.14	0.35	26,36,82,106	0
2	UMP	B	701	20/20	0.95	0.13	0.33	28,33,41,54	0
2	UMP	H	701	20/20	0.96	0.13	0.28	25,34,44,54	0
2	UMP	G	701	20/20	0.95	0.15	0.24	29,37,51,65	0
3	CB3	H	702	35/35	0.94	0.12	0.12	22,33,84,109	0
2	UMP	E	701	20/20	0.97	0.14	-0.07	27,39,50,58	0
3	CB3	C	702	35/35	0.93	0.13	-0.10	30,41,86,93	0
2	UMP	A	701	20/20	0.96	0.13	-0.18	28,36,50,57	0
5	NDP	H	704	48/48	0.94	0.14	-0.26	31,62,108,114	0
5	NDP	D	704	48/48	0.92	0.15	-0.29	38,66,111,114	0
3	CB3	E	702	35/35	0.93	0.13	-0.31	30,44,86,91	0
5	NDP	B	704	48/48	0.93	0.13	-0.39	35,65,114,126	0
3	CB3	G	702	35/35	0.94	0.12	-0.49	32,40,86,90	0
5	NDP	F	704	48/48	0.94	0.13	-0.54	38,61,107,116	0
3	CB3	A	702	35/35	0.94	0.12	-0.61	27,41,88,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.