



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 04:39 PM EST

PDB ID : 5HHU  
Title : Plasmodium vivax hypoxanthine-guanine phosphoribosyltransferase in complex with [3R,4R]-4-guanin-9-yl-3-((S)-2-hydroxy-2-phosphonoethyl)oxy-1-N-(phosphonopropionyl)pyrrolidine  
Authors : Guddat, L.W.; Keough, D.T.; Rejman, D.  
Deposited on : 2016-01-11  
Resolution : 3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

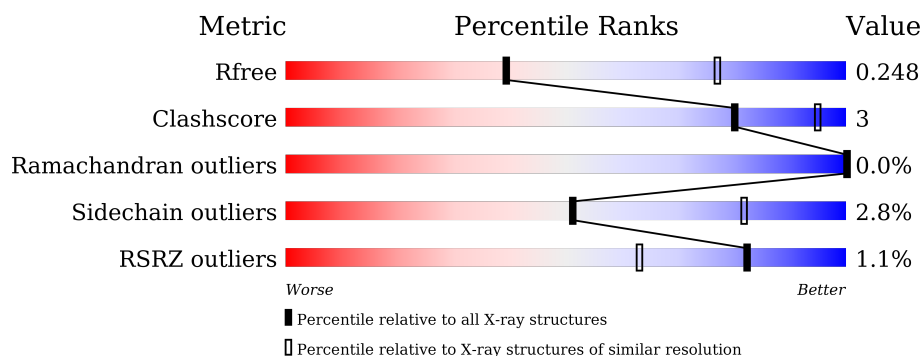
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	238	
1	B	238	
1	C	238	
1	D	238	
1	E	238	
1	F	238	

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Mol	Chain	Length	Quality of chain
1	G	238	
1	H	238	
1	I	238	
1	J	238	
1	K	238	
1	L	238	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	L	303	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21914 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 Hypoxanthine-guanine-xanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1813	1182	301	325	5			
1	B	220	Total	C	N	O	S	0	0	0
			1813	1182	301	325	5			
1	C	219	Total	C	N	O	S	0	0	0
			1799	1173	296	325	5			
1	D	218	Total	C	N	O	S	0	0	0
			1789	1167	293	324	5			
1	E	211	Total	C	N	O	S	0	0	0
			1736	1133	285	313	5			
1	F	220	Total	C	N	O	S	0	0	0
			1809	1179	299	326	5			
1	G	218	Total	C	N	O	S	0	0	0
			1789	1167	293	324	5			
1	H	218	Total	C	N	O	S	0	0	0
			1789	1167	293	324	5			
1	I	217	Total	C	N	O	S	0	0	0
			1783	1164	292	322	5			
1	J	218	Total	C	N	O	S	0	0	0
			1789	1167	293	324	5			
1	K	217	Total	C	N	O	S	0	0	0
			1783	1164	292	322	5			
1	L	216	Total	C	N	O	S	0	0	0
			1774	1158	290	321	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP A0A0J9SD35
A	-3	HIS	-	expression tag	UNP A0A0J9SD35
A	-2	HIS	-	expression tag	UNP A0A0J9SD35
A	-1	HIS	-	expression tag	UNP A0A0J9SD35
A	0	HIS	-	expression tag	UNP A0A0J9SD35

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP A0A0J9SD35
B	-4	HIS	-	expression tag	UNP A0A0J9SD35
B	-3	HIS	-	expression tag	UNP A0A0J9SD35
B	-2	HIS	-	expression tag	UNP A0A0J9SD35
B	-1	HIS	-	expression tag	UNP A0A0J9SD35
B	0	HIS	-	expression tag	UNP A0A0J9SD35
B	1	HIS	-	expression tag	UNP A0A0J9SD35
C	-4	HIS	-	expression tag	UNP A0A0J9SD35
C	-3	HIS	-	expression tag	UNP A0A0J9SD35
C	-2	HIS	-	expression tag	UNP A0A0J9SD35
C	-1	HIS	-	expression tag	UNP A0A0J9SD35
C	0	HIS	-	expression tag	UNP A0A0J9SD35
C	1	HIS	-	expression tag	UNP A0A0J9SD35
D	-4	HIS	-	expression tag	UNP A0A0J9SD35
D	-3	HIS	-	expression tag	UNP A0A0J9SD35
D	-2	HIS	-	expression tag	UNP A0A0J9SD35
D	-1	HIS	-	expression tag	UNP A0A0J9SD35
D	0	HIS	-	expression tag	UNP A0A0J9SD35
D	1	HIS	-	expression tag	UNP A0A0J9SD35
E	-4	HIS	-	expression tag	UNP A0A0J9SD35
E	-3	HIS	-	expression tag	UNP A0A0J9SD35
E	-2	HIS	-	expression tag	UNP A0A0J9SD35
E	-1	HIS	-	expression tag	UNP A0A0J9SD35
E	0	HIS	-	expression tag	UNP A0A0J9SD35
E	1	HIS	-	expression tag	UNP A0A0J9SD35
F	-4	HIS	-	expression tag	UNP A0A0J9SD35
F	-3	HIS	-	expression tag	UNP A0A0J9SD35
F	-2	HIS	-	expression tag	UNP A0A0J9SD35
F	-1	HIS	-	expression tag	UNP A0A0J9SD35
F	0	HIS	-	expression tag	UNP A0A0J9SD35
F	1	HIS	-	expression tag	UNP A0A0J9SD35
G	-4	HIS	-	expression tag	UNP A0A0J9SD35
G	-3	HIS	-	expression tag	UNP A0A0J9SD35
G	-2	HIS	-	expression tag	UNP A0A0J9SD35
G	-1	HIS	-	expression tag	UNP A0A0J9SD35
G	0	HIS	-	expression tag	UNP A0A0J9SD35
G	1	HIS	-	expression tag	UNP A0A0J9SD35
H	-4	HIS	-	expression tag	UNP A0A0J9SD35
H	-3	HIS	-	expression tag	UNP A0A0J9SD35
H	-2	HIS	-	expression tag	UNP A0A0J9SD35
H	-1	HIS	-	expression tag	UNP A0A0J9SD35
H	0	HIS	-	expression tag	UNP A0A0J9SD35

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1	HIS	-	expression tag	UNP A0A0J9SD35
I	-4	HIS	-	expression tag	UNP A0A0J9SD35
I	-3	HIS	-	expression tag	UNP A0A0J9SD35
I	-2	HIS	-	expression tag	UNP A0A0J9SD35
I	-1	HIS	-	expression tag	UNP A0A0J9SD35
I	0	HIS	-	expression tag	UNP A0A0J9SD35
I	1	HIS	-	expression tag	UNP A0A0J9SD35
J	-4	HIS	-	expression tag	UNP A0A0J9SD35
J	-3	HIS	-	expression tag	UNP A0A0J9SD35
J	-2	HIS	-	expression tag	UNP A0A0J9SD35
J	-1	HIS	-	expression tag	UNP A0A0J9SD35
J	0	HIS	-	expression tag	UNP A0A0J9SD35
J	1	HIS	-	expression tag	UNP A0A0J9SD35
K	-4	HIS	-	expression tag	UNP A0A0J9SD35
K	-3	HIS	-	expression tag	UNP A0A0J9SD35
K	-2	HIS	-	expression tag	UNP A0A0J9SD35
K	-1	HIS	-	expression tag	UNP A0A0J9SD35
K	0	HIS	-	expression tag	UNP A0A0J9SD35
K	1	HIS	-	expression tag	UNP A0A0J9SD35
L	-4	HIS	-	expression tag	UNP A0A0J9SD35
L	-3	HIS	-	expression tag	UNP A0A0J9SD35
L	-2	HIS	-	expression tag	UNP A0A0J9SD35
L	-1	HIS	-	expression tag	UNP A0A0J9SD35
L	0	HIS	-	expression tag	UNP A0A0J9SD35
L	1	HIS	-	expression tag	UNP A0A0J9SD35

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

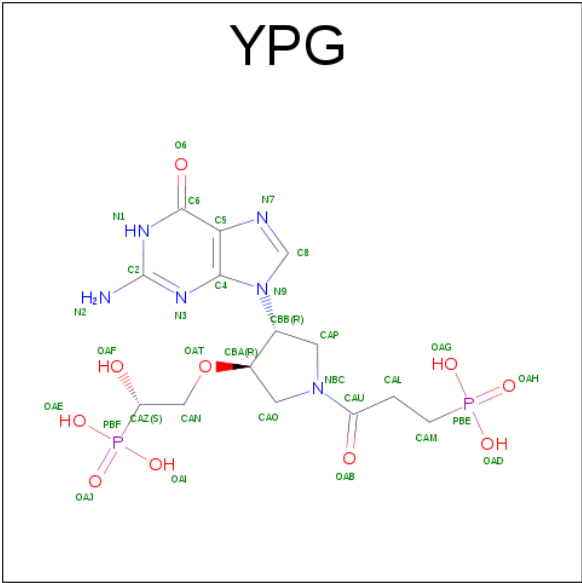
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	K	3	Total Mg 3 3	0	0
2	E	3	Total Mg 3 3	0	0
2	H	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	3	Total	Mg	0	0
			3	3		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is [3-[(3 {R},4 {R})-3-(2-azanyl-6-oxidanylidene-1 {H}-purin-9-yl)-4-[(2 {S})-2-oxidanyl-2-phosphono-ethoxy]pyrrolidin-1-yl]-3-oxidanylidene-propyl]phosphonic acid (three-letter code: YPG) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>6</sub>O<sub>10</sub>P<sub>2</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	G	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	H	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	I	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	J	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	K	1	Total	C	N	O	P	0	0
			32	14	6	10	2		
3	L	1	Total	C	N	O	P	0	0
			32	14	6	10	2		

- Molecule 4 is water.

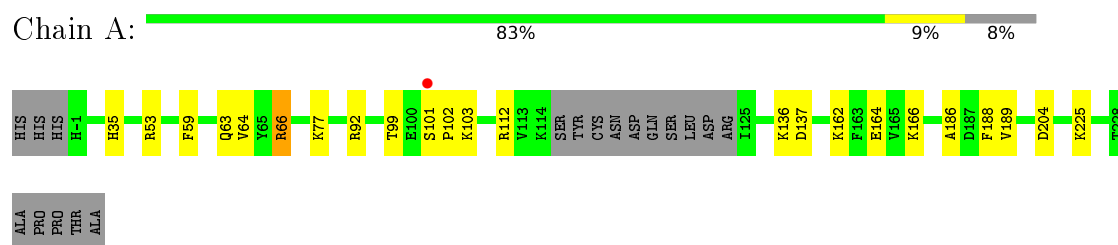
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		
4	C	5	Total	O	0	0
			5	5		
4	D	2	Total	O	0	0
			2	2		
4	E	2	Total	O	0	0
			2	2		
4	F	3	Total	O	0	0
			3	3		
4	G	4	Total	O	0	0
			4	4		
4	H	4	Total	O	0	0
			4	4		
4	I	2	Total	O	0	0
			2	2		
4	J	2	Total	O	0	0
			2	2		
4	K	2	Total	O	0	0
			2	2		
4	L	4	Total	O	0	0
			4	4		



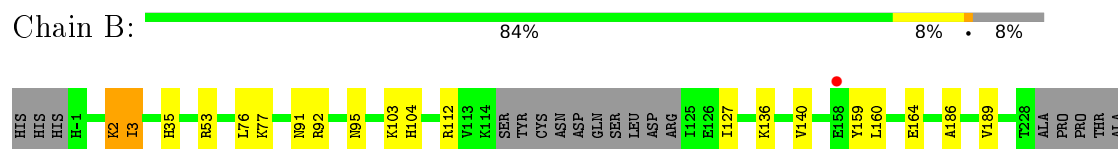
### 3 Residue-property plots [i](#)

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.

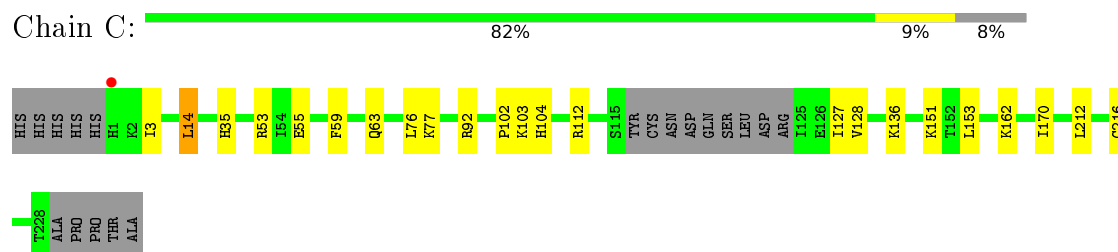
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



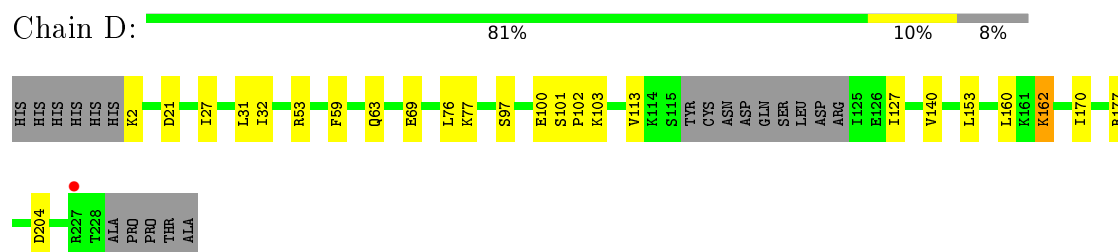
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



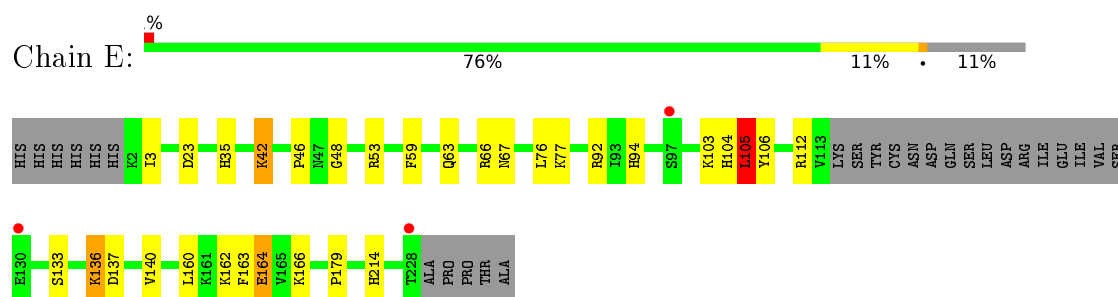
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



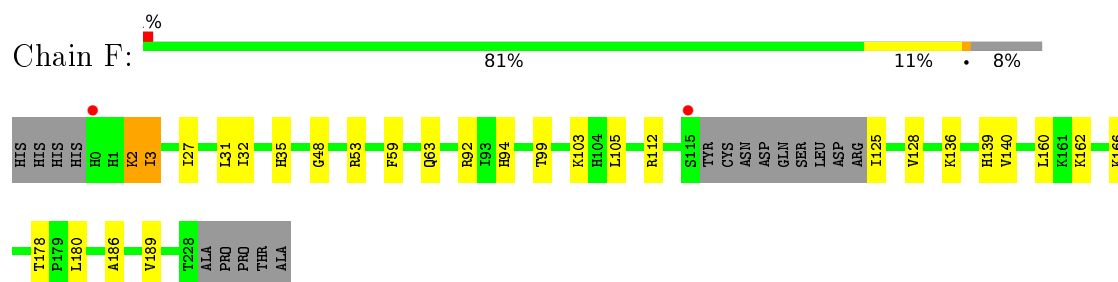
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



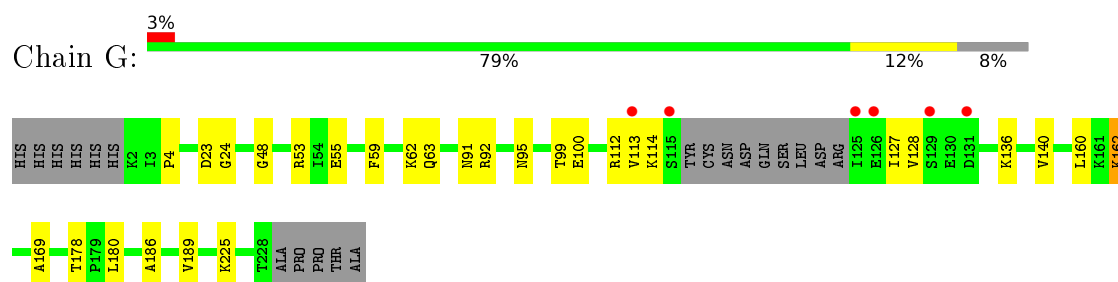
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



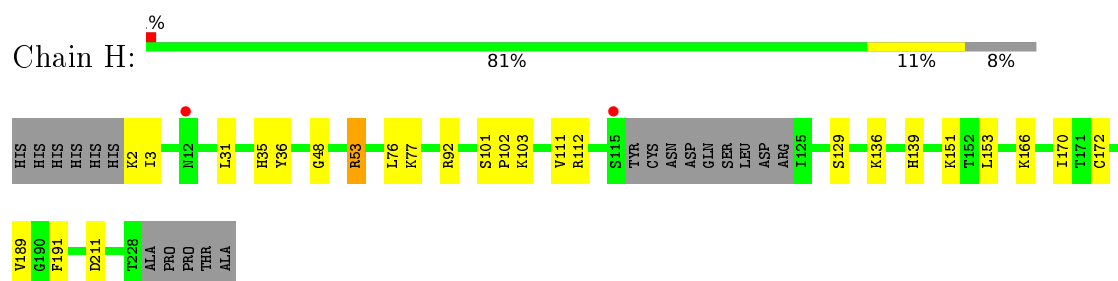
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase



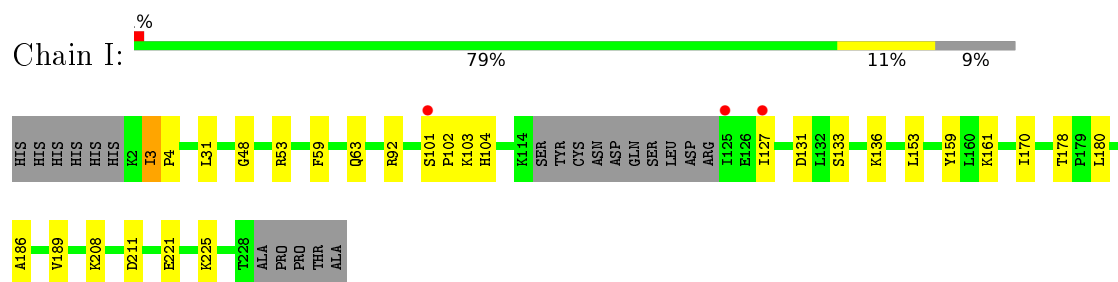
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase




- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

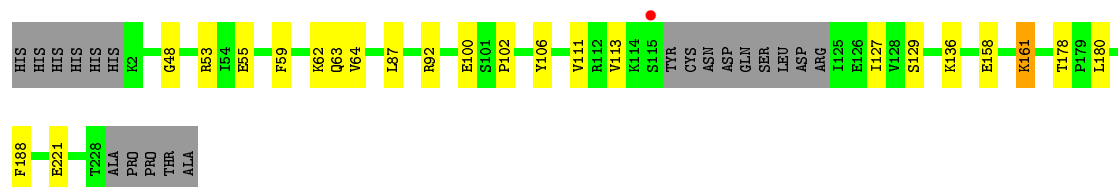


- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase




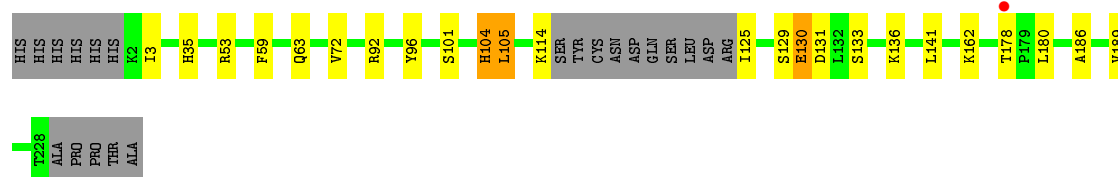
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain J: 




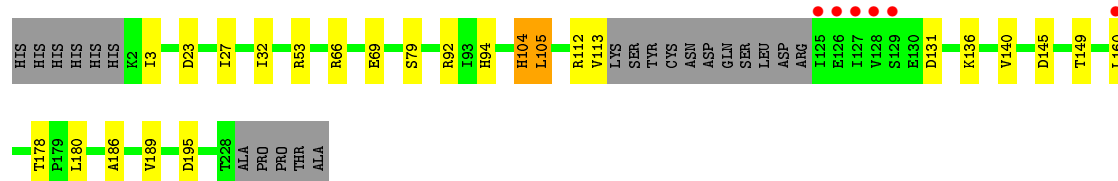
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain K: 



- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.83Å 254.23Å 55.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 3.05 48.01 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.01-3.05) 98.9 (48.01-3.05)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.188 , 0.247 0.187 , 0.248	Depositor DCC
$R_{free}$ test set	1998 reflections (3.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, YPG

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	0.47	0/1857	0.63	0/2507
1	B	0.45	0/1857	0.61	0/2507
1	C	0.45	0/1841	0.63	0/2485
1	D	0.45	0/1830	0.64	0/2470
1	E	0.44	0/1777	0.66	0/2399
1	F	0.43	0/1852	0.61	0/2500
1	G	0.44	0/1830	0.59	0/2470
1	H	0.41	0/1830	0.62	0/2470
1	I	0.44	0/1824	0.64	0/2462
1	J	0.41	0/1830	0.60	0/2470
1	K	0.39	0/1824	0.61	0/2462
1	L	0.41	0/1815	0.63	0/2451
All	All	0.43	0/21967	0.62	0/29653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	1826	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1813	0	1826	10	0
1	C	1799	0	1817	15	0
1	D	1789	0	1807	13	1
1	E	1736	0	1747	18	0
1	F	1809	0	1824	14	0
1	G	1789	0	1807	16	0
1	H	1789	0	1807	14	0
1	I	1783	0	1802	17	0
1	J	1789	0	1807	12	0
1	K	1783	0	1802	15	0
1	L	1774	0	1789	12	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
3	C	32	0	0	0	0
3	D	32	0	0	0	0
3	E	32	0	0	0	0
3	F	32	0	0	0	0
3	G	32	0	0	0	0
3	H	32	0	0	0	0
3	I	32	0	0	0	0
3	J	32	0	0	0	0
3	K	32	0	0	0	0
3	L	32	0	0	0	0
4	A	4	0	0	1	0
4	B	3	0	0	0	0
4	C	5	0	0	0	0
4	D	2	0	0	1	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	4	0	0	0	0
All	All	21914	0	21661	146	1

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 3.

All (146) 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:F:2:LYS:HE2	1:F:3:ILE:H	1.51	0.76
1:E:94:HIS:CD2	1:E:105:LEU:HD23	2.23	0.73
1:C:112:ARG:HB3	1:C:128:VAL:HB	1.72	0.72
1:G:92:ARG:HD2	1:K:92:ARG:HD2	1.71	0.72
1:F:140:VAL:HG11	1:F:160:LEU:HD21	1.72	0.70
1:B:92:ARG:HD2	1:C:92:ARG:HD2	1.75	0.67
1:B:91:ASN:O	1:B:95:ASN:ND2	2.27	0.65
1:D:204:ASP:OD1	4:D:401:HOH:O	2.13	0.65
1:E:23:ASP:O	1:E:42:LYS:NZ	2.29	0.65
1:C:103:LYS:O	1:C:104:HIS:ND1	2.30	0.65
1:G:62:LYS:NZ	1:G:100:GLU:OE2	2.29	0.64
1:L:105:LEU:HD23	1:L:105:LEU:H	1.60	0.64
1:A:66:ARG:NH1	1:A:99:THR:O	2.20	0.61
1:H:153:LEU:HD21	1:H:170:ILE:HG21	1.82	0.61
1:A:136:LYS:HG2	1:A:164:GLU:HB2	1.84	0.60
1:E:140:VAL:HG11	1:E:160:LEU:HD21	1.84	0.59
1:D:140:VAL:HG11	1:D:160:LEU:HD21	1.85	0.58
1:K:129:SER:OG	1:K:130:GLU:N	2.35	0.58
1:A:77:LYS:HE3	1:A:112:ARG:NH1	2.18	0.58
1:E:137:ASP:HA	1:E:166:LYS:HG3	1.86	0.57
1:A:204:ASP:OD1	4:A:401:HOH:O	2.18	0.57
1:F:92:ARG:HD2	1:I:92:ARG:HD2	1.88	0.56
1:L:69:GLU:OE2	1:L:104:HIS:HE1	1.88	0.55
1:G:23:ASP:OD1	1:G:24:GLY:N	2.39	0.55
1:E:105:LEU:HD11	1:I:211:ASP:OD2	2.07	0.55
1:L:140:VAL:HG11	1:L:160:LEU:HD21	1.89	0.55
1:E:104:HIS:NE2	1:I:208:LYS:HD2	2.24	0.53
1:C:14:LEU:HD12	1:C:14:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:VAL:HG12	1:J:129:SER:HB3	1.92	0.52
1:F:112:ARG:HB3	1:F:128:VAL:HB	1.91	0.52
1:E:48:GLY:HA3	1:F:48:GLY:HA3	1.91	0.52
1:B:127:ILE:HG13	1:B:159:TYR:CE2	2.46	0.51
1:L:94:HIS:CE1	1:L:105:LEU:HB3	2.45	0.51
1:F:27:ILE:HG23	1:F:32:ILE:HD12	1.92	0.51
1:E:92:ARG:HD3	1:J:92:ARG:HD2	1.93	0.50
1:D:153:LEU:HD21	1:D:170:ILE:HG21	1.92	0.50
1:G:140:VAL:HG11	1:G:160:LEU:HD21	1.93	0.50
1:F:94:HIS:CD2	1:F:105:LEU:HD22	2.47	0.50
1:J:64:VAL:HG21	1:J:188:PHE:HZ	1.77	0.50
1:E:105:LEU:HD11	1:I:211:ASP:CG	2.33	0.50
1:H:102:PRO:HD3	1:K:35:HIS:HB2	1.94	0.50
1:E:35:HIS:HB2	1:I:102:PRO:HD3	1.94	0.49
1:I:221:GLU:O	1:I:225:LYS:HD3	2.11	0.49
1:J:87:LEU:HD22	1:J:106:TYR:CE1	2.47	0.49
1:G:91:ASN:O	1:G:95:ASN:HB2	2.11	0.49
1:K:186:ALA:HB3	1:K:189:VAL:HG22	1.93	0.49
1:H:92:ARG:HD2	1:L:92:ARG:HD2	1.93	0.49
1:A:162:LYS:O	1:A:162:LYS:HG2	2.11	0.49
1:A:137:ASP:HA	1:A:166:LYS:HG3	1.93	0.49
1:G:113:VAL:HG22	1:G:127:ILE:HD12	1.95	0.49
1:I:31:LEU:HD12	1:J:55:GLU:HG2	1.95	0.48
1:A:59:PHE:O	1:A:63:GLN:HG2	2.14	0.48
1:C:153:LEU:HD21	1:C:170:ILE:HG21	1.95	0.48
1:D:97:SER:HB3	1:D:100:GLU:HG2	1.96	0.48
1:F:178:THR:HG22	1:F:180:LEU:H	1.79	0.48
1:L:149:THR:HG22	1:L:180:LEU:HB3	1.96	0.48
1:B:140:VAL:HG11	1:B:160:LEU:HD21	1.96	0.47
1:B:35:HIS:HB2	1:D:102:PRO:HD3	1.96	0.47
1:K:72:VAL:HG12	1:K:141:LEU:HD23	1.97	0.47
1:K:131:ASP:OD2	1:K:133:SER:OG	2.31	0.47
1:L:27:ILE:HG23	1:L:32:ILE:HD12	1.95	0.47
1:H:77:LYS:HE3	1:H:112:ARG:NH1	2.30	0.47
1:C:55:GLU:HG2	1:D:31:LEU:HD12	1.97	0.47
1:A:77:LYS:HE3	1:A:112:ARG:HH12	1.79	0.46
1:B:136:LYS:HD3	1:B:164:GLU:HB2	1.97	0.46
1:J:62:LYS:NZ	1:J:100:GLU:OE2	2.40	0.46
1:L:94:HIS:ND1	1:L:105:LEU:HD13	2.31	0.46
1:A:101:SER:C	1:A:103:LYS:H	2.19	0.46
1:B:103:LYS:O	1:B:104:HIS:ND1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:LEU:HD21	1:I:170:ILE:HG21	1.96	0.46
1:K:59:PHE:O	1:K:63:GLN:HG2	2.16	0.46
1:D:113:VAL:HG22	1:D:127:ILE:HD12	1.98	0.46
1:G:55:GLU:OE2	1:K:96:TYR:OH	2.34	0.46
1:A:35:HIS:HB2	1:C:102:PRO:HD3	1.98	0.45
1:F:59:PHE:O	1:F:63:GLN:HG2	2.15	0.45
1:G:112:ARG:HB3	1:G:128:VAL:HG23	1.98	0.45
1:J:158:GLU:O	1:J:161:LYS:HG2	2.16	0.45
1:H:101:SER:C	1:H:103:LYS:H	2.20	0.45
1:I:103:LYS:O	1:I:104:HIS:ND1	2.49	0.45
1:I:178:THR:HG22	1:I:180:LEU:H	1.81	0.45
1:G:4:PRO:HG2	1:G:169:ALA:HB2	1.99	0.45
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.79	0.45
1:A:102:PRO:HD3	1:C:35:HIS:HB2	1.98	0.45
1:E:106:TYR:CD1	1:E:106:TYR:C	2.90	0.45
1:D:101:SER:C	1:D:103:LYS:H	2.21	0.44
1:K:104:HIS:O	1:K:105:LEU:HB2	2.17	0.44
1:G:186:ALA:HB3	1:G:189:VAL:HG22	2.00	0.44
1:H:36:TYR:HE2	1:H:211:ASP:OD1	2.01	0.44
1:L:186:ALA:HB3	1:L:189:VAL:HG22	1.98	0.44
1:G:55:GLU:HG2	1:H:31:LEU:HD12	1.98	0.44
1:A:186:ALA:HB3	1:A:189:VAL:HG22	1.99	0.44
1:F:35:HIS:HB2	1:J:102:PRO:HD3	1.99	0.44
1:E:163:PHE:C	1:E:164:GLU:HG2	2.38	0.44
1:C:127:ILE:HG12	1:E:179:PRO:HB2	1.99	0.44
1:C:59:PHE:O	1:C:63:GLN:HG2	2.18	0.44
1:C:162:LYS:HG2	1:C:162:LYS:O	2.16	0.43
1:H:111:VAL:HG12	1:H:129:SER:HB3	2.00	0.43
1:B:186:ALA:HB3	1:B:189:VAL:HG22	2.01	0.43
1:D:59:PHE:O	1:D:63:GLN:HG2	2.19	0.43
1:H:35:HIS:HB3	1:K:101:SER:O	2.18	0.43
1:I:48:GLY:HA3	1:J:48:GLY:HA3	2.00	0.43
1:E:46:PRO:HA	1:E:214:HIS:ND1	2.34	0.43
1:E:59:PHE:O	1:E:63:GLN:HG2	2.19	0.43
1:G:59:PHE:O	1:G:63:GLN:HG2	2.19	0.43
1:K:105:LEU:HD12	1:K:105:LEU:HA	1.72	0.43
1:C:212:LEU:HD21	1:C:216:CYS:SG	2.59	0.43
1:B:2:LYS:HD3	1:B:3:ILE:O	2.18	0.43
1:E:76:LEU:HA	1:E:77:LYS:HA	1.82	0.43
1:D:76:LEU:HA	1:D:77:LYS:HA	1.74	0.43
1:J:113:VAL:HG22	1:J:127:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HA	1:B:77:LYS:HA	1.79	0.42
1:J:59:PHE:O	1:J:63:GLN:HG2	2.19	0.42
1:L:79:SER:HA	1:L:145:ASP:HB3	2.02	0.42
1:F:139:HIS:CE1	1:F:166:LYS:HD3	2.54	0.42
1:I:131:ASP:C	1:I:133:SER:H	2.21	0.42
1:K:178:THR:HG22	1:K:180:LEU:H	1.83	0.42
1:A:64:VAL:HG21	1:A:188:PHE:HZ	1.84	0.42
1:H:53:ARG:HG3	1:H:191:PHE:CZ	2.55	0.42
1:I:101:SER:C	1:I:103:LYS:H	2.22	0.42
1:I:127:ILE:HG13	1:I:159:TYR:CD2	2.53	0.42
1:K:104:HIS:CG	1:K:105:LEU:H	2.38	0.42
1:G:178:THR:HG22	1:G:180:LEU:H	1.85	0.42
1:L:178:THR:HG22	1:L:180:LEU:H	1.83	0.42
1:F:125:ILE:HG23	1:F:125:ILE:O	2.19	0.42
1:G:48:GLY:HA3	1:H:48:GLY:HA3	2.01	0.42
1:F:186:ALA:HB3	1:F:189:VAL:HG22	2.01	0.41
1:H:139:HIS:NE2	1:H:166:LYS:HD3	2.35	0.41
1:L:105:LEU:H	1:L:105:LEU:CD2	2.32	0.41
1:K:104:HIS:CG	1:K:105:LEU:N	2.89	0.41
1:C:153:LEU:HA	1:C:153:LEU:HD12	1.93	0.41
1:C:76:LEU:HA	1:C:77:LYS:HA	1.76	0.41
1:E:66:ARG:HB3	1:E:67:ASN:H	1.63	0.41
1:D:27:ILE:HG23	1:D:32:ILE:HD12	2.02	0.41
1:G:162:LYS:O	1:G:162:LYS:HG2	2.19	0.41
1:H:76:LEU:HA	1:H:77:LYS:HA	1.74	0.41
1:D:21:ASP:OD1	1:D:177:ARG:NH2	2.45	0.41
1:E:133:SER:O	1:E:136:LYS:HG2	2.20	0.41
1:K:125:ILE:HG23	1:K:125:ILE:O	2.21	0.41
1:I:186:ALA:HB3	1:I:189:VAL:HG22	2.02	0.40
1:I:3:ILE:HA	1:I:4:PRO:HD3	1.95	0.40
1:I:59:PHE:O	1:I:63:GLN:HG2	2.21	0.40
1:G:99:THR:O	1:G:99:THR:HG23	2.21	0.40
1:J:178:THR:HG22	1:J:180:LEU:HB2	2.04	0.40
1:A:225:LYS:HE3	1:C:103:LYS:HE2	2.03	0.40
1:F:99:THR:O	1:F:99:THR:HG23	2.22	0.40
1:H:172:CYS:O	1:H:189:VAL:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LYS:NZ	1:L:195:ASP:OD2[4_555]	1.83	0.37

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/238 (91%)	203 (94%)	13 (6%)	0	100	100
1	B	216/238 (91%)	201 (93%)	15 (7%)	0	100	100
1	C	215/238 (90%)	200 (93%)	15 (7%)	0	100	100
1	D	214/238 (90%)	202 (94%)	12 (6%)	0	100	100
1	E	207/238 (87%)	198 (96%)	8 (4%)	1 (0%)	34	70
1	F	216/238 (91%)	205 (95%)	11 (5%)	0	100	100
1	G	214/238 (90%)	204 (95%)	10 (5%)	0	100	100
1	H	214/238 (90%)	204 (95%)	10 (5%)	0	100	100
1	I	213/238 (90%)	198 (93%)	15 (7%)	0	100	100
1	J	214/238 (90%)	204 (95%)	10 (5%)	0	100	100
1	K	213/238 (90%)	202 (95%)	11 (5%)	0	100	100
1	L	212/238 (89%)	201 (95%)	11 (5%)	0	100	100
All	All	2564/2856 (90%)	2422 (94%)	141 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	105	LEU

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/218 (93%)	199 (98%)	3 (2%)	72	90
1	B	202/218 (93%)	198 (98%)	4 (2%)	63	87
1	C	201/218 (92%)	196 (98%)	5 (2%)	55	84
1	D	200/218 (92%)	196 (98%)	4 (2%)	63	87
1	E	193/218 (88%)	184 (95%)	9 (5%)	32	68
1	F	202/218 (93%)	195 (96%)	7 (4%)	43	78
1	G	200/218 (92%)	195 (98%)	5 (2%)	55	84
1	H	200/218 (92%)	195 (98%)	5 (2%)	55	84
1	I	199/218 (91%)	195 (98%)	4 (2%)	63	87
1	J	200/218 (92%)	196 (98%)	4 (2%)	63	87
1	K	199/218 (91%)	191 (96%)	8 (4%)	38	74
1	L	198/218 (91%)	188 (95%)	10 (5%)	29	65
All	All	2396/2616 (92%)	2328 (97%)	68 (3%)	51	82

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	66	ARG
1	A	92	ARG
1	B	2	LYS
1	B	3	ILE
1	B	53	ARG
1	B	112	ARG
1	C	3	ILE
1	C	14	LEU
1	C	53	ARG
1	C	136	LYS
1	C	151	LYS
1	D	2	LYS
1	D	53	ARG
1	D	69	GLU
1	D	162	LYS
1	E	3	ILE
1	E	42	LYS

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Mol	Chain	Res	Type
1	E	53	ARG
1	E	103	LYS
1	E	105	LEU
1	E	112	ARG
1	E	136	LYS
1	E	162	LYS
1	E	164	GLU
1	F	2	LYS
1	F	3	ILE
1	F	31	LEU
1	F	53	ARG
1	F	103	LYS
1	F	136	LYS
1	F	162	LYS
1	G	53	ARG
1	G	114	LYS
1	G	136	LYS
1	G	162	LYS
1	G	225	LYS
1	H	2	LYS
1	H	3	ILE
1	H	53	ARG
1	H	136	LYS
1	H	151	LYS
1	I	3	ILE
1	I	53	ARG
1	I	136	LYS
1	I	161	LYS
1	J	53	ARG
1	J	136	LYS
1	J	161	LYS
1	J	221	GLU
1	K	3	ILE
1	K	53	ARG
1	K	104	HIS
1	K	105	LEU
1	K	114	LYS
1	K	130	GLU
1	K	136	LYS
1	K	162	LYS
1	L	3	ILE
1	L	23	ASP

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Mol	Chain	Res	Type
1	L	53	ARG
1	L	66	ARG
1	L	104	HIS
1	L	105	LEU
1	L	112	ARG
1	L	113	VAL
1	L	131	ASP
1	L	136	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	E	94	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 27 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	YPG	A	303	2	30,34,34	3.27	11 (36%)	27,52,52	2.55	9 (33%)
3	YPG	B	303	2	30,34,34	3.21	9 (30%)	27,52,52	2.42	9 (33%)
3	YPG	C	303	2	30,34,34	3.34	12 (40%)	27,52,52	2.32	11 (40%)
3	YPG	D	303	2	30,34,34	3.23	10 (33%)	27,52,52	2.23	9 (33%)
3	YPG	E	304	2	30,34,34	3.28	10 (33%)	27,52,52	2.46	10 (37%)
3	YPG	F	303	2	30,34,34	3.32	9 (30%)	27,52,52	2.64	10 (37%)
3	YPG	G	303	2	30,34,34	3.28	10 (33%)	27,52,52	2.43	9 (33%)
3	YPG	H	303	2	30,34,34	3.34	10 (33%)	27,52,52	2.41	8 (29%)
3	YPG	I	303	2	30,34,34	3.26	10 (33%)	27,52,52	2.12	10 (37%)
3	YPG	J	303	2	30,34,34	3.30	10 (33%)	27,52,52	2.32	8 (29%)
3	YPG	K	304	2	30,34,34	3.27	11 (36%)	27,52,52	2.27	8 (29%)
3	YPG	L	304	2	30,34,34	3.26	9 (30%)	27,52,52	2.37	10 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YPG	A	303	2	-	0/15/37/37	0/3/3/3
3	YPG	B	303	2	-	0/15/37/37	0/3/3/3
3	YPG	C	303	2	-	0/15/37/37	0/3/3/3
3	YPG	D	303	2	-	0/15/37/37	0/3/3/3
3	YPG	E	304	2	-	0/15/37/37	0/3/3/3
3	YPG	F	303	2	-	0/15/37/37	0/3/3/3
3	YPG	G	303	2	-	0/15/37/37	0/3/3/3
3	YPG	H	303	2	-	0/15/37/37	0/3/3/3
3	YPG	I	303	2	-	0/15/37/37	0/3/3/3
3	YPG	J	303	2	-	0/15/37/37	0/3/3/3
3	YPG	K	304	2	-	0/15/37/37	0/3/3/3
3	YPG	L	304	2	-	0/15/37/37	0/3/3/3

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	YPG	CAO-CBA	-8.15	1.32	1.52
3	G	303	YPG	CAO-CBA	-7.99	1.32	1.52
3	L	304	YPG	CAO-CBA	-7.96	1.32	1.52
3	D	303	YPG	CAO-CBA	-7.90	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	YPG	CAO-CBA	-7.89	1.33	1.52
3	E	304	YPG	CAO-CBA	-7.89	1.33	1.52
3	K	304	YPG	CAO-CBA	-7.87	1.33	1.52
3	B	303	YPG	CAO-CBA	-7.87	1.33	1.52
3	I	303	YPG	CAO-CBA	-7.86	1.33	1.52
3	J	303	YPG	CAO-CBA	-7.86	1.33	1.52
3	H	303	YPG	CAO-CBA	-7.78	1.33	1.52
3	F	303	YPG	CAO-CBA	-7.72	1.33	1.52
3	L	304	YPG	CAP-NBC	-6.27	1.32	1.46
3	C	303	YPG	CAP-NBC	-6.25	1.32	1.46
3	I	303	YPG	CAP-NBC	-6.21	1.32	1.46
3	D	303	YPG	CAP-NBC	-6.03	1.32	1.46
3	K	304	YPG	CAP-NBC	-6.00	1.32	1.46
3	B	303	YPG	CAP-NBC	-6.00	1.32	1.46
3	E	304	YPG	CAP-NBC	-5.97	1.32	1.46
3	A	303	YPG	CAP-NBC	-5.92	1.33	1.46
3	G	303	YPG	CAP-NBC	-5.87	1.33	1.46
3	H	303	YPG	CAP-NBC	-5.78	1.33	1.46
3	F	303	YPG	CAP-NBC	-5.74	1.33	1.46
3	J	303	YPG	CAP-NBC	-5.73	1.33	1.46
3	G	303	YPG	PBF-OAI	-2.86	1.50	1.54
3	A	303	YPG	PBF-OAI	-2.58	1.50	1.54
3	I	303	YPG	PBF-OAE	-2.52	1.50	1.54
3	D	303	YPG	PBF-OAI	-2.49	1.50	1.54
3	K	304	YPG	PBF-OAI	-2.49	1.50	1.54
3	A	303	YPG	OAT-CAN	-2.44	1.39	1.43
3	H	303	YPG	PBF-OAI	-2.42	1.51	1.54
3	J	303	YPG	PBF-OAI	-2.40	1.51	1.54
3	B	303	YPG	PBF-OAI	-2.37	1.51	1.54
3	E	304	YPG	PBF-OAI	-2.31	1.51	1.54
3	I	303	YPG	PBF-OAI	-2.28	1.51	1.54
3	L	304	YPG	PBF-OAI	-2.26	1.51	1.54
3	C	303	YPG	PBF-OAE	-2.26	1.51	1.54
3	G	303	YPG	PBF-OAE	-2.21	1.51	1.54
3	A	303	YPG	PBF-OAE	-2.14	1.51	1.54
3	C	303	YPG	OAT-CAN	-2.12	1.39	1.43
3	H	303	YPG	PBF-OAE	-2.10	1.51	1.54
3	D	303	YPG	OAT-CAN	-2.10	1.39	1.43
3	E	304	YPG	OAT-CAN	-2.09	1.39	1.43
3	K	304	YPG	PBF-OAE	-2.07	1.51	1.54
3	C	303	YPG	OAB-CAU	-2.06	1.18	1.23
3	F	303	YPG	PBF-OAI	-2.04	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	YPG	PBF-OAI	-2.03	1.51	1.54
3	K	304	YPG	OAT-CAN	-2.01	1.40	1.43
3	J	303	YPG	OAT-CAN	-2.01	1.40	1.43
3	I	303	YPG	PBF-CAZ	2.13	1.85	1.82
3	A	303	YPG	PBF-CAZ	2.69	1.85	1.82
3	F	303	YPG	PBF-CAZ	2.85	1.86	1.82
3	J	303	YPG	PBF-CAZ	2.97	1.86	1.82
3	E	304	YPG	PBF-CAZ	3.00	1.86	1.82
3	K	304	YPG	PBF-CAZ	3.04	1.86	1.82
3	H	303	YPG	PBF-CAZ	3.10	1.86	1.82
3	L	304	YPG	PBF-CAZ	3.10	1.86	1.82
3	G	303	YPG	PBF-CAZ	3.13	1.86	1.82
3	B	303	YPG	PBF-CAZ	3.16	1.86	1.82
3	D	303	YPG	PBF-CAZ	3.28	1.86	1.82
3	L	304	YPG	CAU-NBC	3.87	1.44	1.35
3	C	303	YPG	PBF-CAZ	3.90	1.87	1.82
3	G	303	YPG	CAU-NBC	4.24	1.45	1.35
3	K	304	YPG	CAU-NBC	4.36	1.45	1.35
3	D	303	YPG	CAU-NBC	4.43	1.45	1.35
3	I	303	YPG	CAU-NBC	4.45	1.45	1.35
3	C	303	YPG	CAU-NBC	4.47	1.45	1.35
3	H	303	YPG	CAU-NBC	4.56	1.45	1.35
3	A	303	YPG	CAU-NBC	4.58	1.45	1.35
3	B	303	YPG	CAU-NBC	4.66	1.46	1.35
3	G	303	YPG	C2-N2	4.89	1.44	1.34
3	E	304	YPG	CAU-NBC	4.90	1.46	1.35
3	J	303	YPG	CAU-NBC	5.01	1.46	1.35
3	B	303	YPG	C2-N2	5.04	1.44	1.34
3	D	303	YPG	C2-N2	5.09	1.44	1.34
3	F	303	YPG	CAU-NBC	5.10	1.47	1.35
3	E	304	YPG	C2-N2	5.18	1.45	1.34
3	I	303	YPG	C2-N2	5.19	1.45	1.34
3	K	304	YPG	C2-N2	5.29	1.45	1.34
3	H	303	YPG	C2-N2	5.30	1.45	1.34
3	A	303	YPG	C2-N2	5.30	1.45	1.34
3	C	303	YPG	C2-N2	5.44	1.45	1.34
3	J	303	YPG	C2-N2	5.50	1.45	1.34
3	L	304	YPG	C2-N2	5.53	1.45	1.34
3	B	303	YPG	O6-C6	5.62	1.38	1.24
3	F	303	YPG	C2-N2	5.87	1.46	1.34
3	D	303	YPG	O6-C6	5.89	1.39	1.24
3	C	303	YPG	O6-C6	5.94	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	304	YPG	O6-C6	5.99	1.39	1.24
3	I	303	YPG	O6-C6	6.05	1.39	1.24
3	A	303	YPG	O6-C6	6.05	1.39	1.24
3	H	303	YPG	O6-C6	6.08	1.40	1.24
3	K	304	YPG	O6-C6	6.09	1.40	1.24
3	E	304	YPG	O6-C6	6.12	1.40	1.24
3	G	303	YPG	O6-C6	6.16	1.40	1.24
3	J	303	YPG	O6-C6	6.17	1.40	1.24
3	F	303	YPG	O6-C6	6.30	1.40	1.24
3	B	303	YPG	CAO-NBC	6.43	1.61	1.46
3	A	303	YPG	CAO-NBC	6.45	1.61	1.46
3	L	304	YPG	CAO-NBC	6.50	1.61	1.46
3	I	303	YPG	CAO-NBC	6.51	1.61	1.46
3	D	303	YPG	CAO-NBC	6.52	1.61	1.46
3	E	304	YPG	CAO-NBC	6.68	1.61	1.46
3	K	304	YPG	CAO-NBC	6.68	1.61	1.46
3	G	303	YPG	CAO-NBC	6.68	1.61	1.46
3	D	303	YPG	PBE-CAM	6.70	1.85	1.78
3	H	303	YPG	CAO-NBC	6.71	1.61	1.46
3	C	303	YPG	CAO-NBC	6.78	1.62	1.46
3	J	303	YPG	PBE-CAM	6.82	1.85	1.78
3	J	303	YPG	CAO-NBC	6.86	1.62	1.46
3	C	303	YPG	PBE-CAM	6.87	1.85	1.78
3	F	303	YPG	CAO-NBC	6.88	1.62	1.46
3	B	303	YPG	PBE-CAM	6.90	1.85	1.78
3	L	304	YPG	PBE-CAM	6.98	1.85	1.78
3	K	304	YPG	PBE-CAM	6.99	1.85	1.78
3	I	303	YPG	PBE-CAM	7.02	1.85	1.78
3	F	303	YPG	PBE-CAM	7.04	1.85	1.78
3	E	304	YPG	PBE-CAM	7.05	1.85	1.78
3	A	303	YPG	PBE-CAM	7.20	1.86	1.78
3	G	303	YPG	PBE-CAM	7.20	1.86	1.78
3	H	303	YPG	PBE-CAM	8.13	1.86	1.78

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	303	YPG	N3-C2-N1	-6.42	118.82	127.56
3	L	304	YPG	N3-C2-N1	-5.56	119.99	127.56
3	H	303	YPG	N3-C2-N1	-5.52	120.04	127.56
3	C	303	YPG	N3-C2-N1	-5.40	120.21	127.56
3	E	304	YPG	N3-C2-N1	-5.37	120.25	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	YPG	N3-C2-N1	-5.36	120.27	127.56
3	B	303	YPG	N3-C2-N1	-5.23	120.44	127.56
3	J	303	YPG	N3-C2-N1	-5.15	120.55	127.56
3	K	304	YPG	N3-C2-N1	-5.15	120.56	127.56
3	D	303	YPG	N3-C2-N1	-4.91	120.88	127.56
3	G	303	YPG	N3-C2-N1	-4.78	121.05	127.56
3	G	303	YPG	C5-C6-N1	-4.52	117.62	123.52
3	A	303	YPG	C5-C6-N1	-4.42	117.75	123.52
3	I	303	YPG	N3-C2-N1	-4.40	121.57	127.56
3	E	304	YPG	C5-C6-N1	-4.07	118.20	123.52
3	H	303	YPG	CBB-CAP-NBC	-3.93	96.26	102.84
3	F	303	YPG	C5-C6-N1	-3.89	118.44	123.52
3	H	303	YPG	C5-C6-N1	-3.87	118.47	123.52
3	F	303	YPG	C6-C5-C4	-3.84	116.47	120.86
3	J	303	YPG	C5-C6-N1	-3.80	118.56	123.52
3	B	303	YPG	C6-C5-C4	-3.75	116.57	120.86
3	L	304	YPG	CBB-CAP-NBC	-3.75	96.57	102.84
3	C	303	YPG	CBB-CAP-NBC	-3.70	96.64	102.84
3	E	304	YPG	CAP-NBC-CAO	-3.69	107.02	112.35
3	K	304	YPG	C6-C5-C4	-3.65	116.68	120.86
3	B	303	YPG	CBB-CAP-NBC	-3.64	96.75	102.84
3	G	303	YPG	CBB-CAP-NBC	-3.63	96.76	102.84
3	A	303	YPG	CAP-NBC-CAO	-3.62	107.13	112.35
3	A	303	YPG	C6-C5-C4	-3.58	116.76	120.86
3	I	303	YPG	C5-C6-N1	-3.57	118.86	123.52
3	J	303	YPG	CAP-NBC-CAO	-3.55	107.23	112.35
3	K	304	YPG	C5-C6-N1	-3.53	118.91	123.52
3	E	304	YPG	C6-C5-C4	-3.50	116.86	120.86
3	L	304	YPG	C6-C5-C4	-3.47	116.89	120.86
3	F	303	YPG	CAP-NBC-CAO	-3.44	107.40	112.35
3	B	303	YPG	C5-C6-N1	-3.41	119.06	123.52
3	L	304	YPG	C5-C6-N1	-3.41	119.07	123.52
3	D	303	YPG	C6-C5-C4	-3.40	116.97	120.86
3	G	303	YPG	C6-C5-C4	-3.34	117.04	120.86
3	B	303	YPG	CAP-NBC-CAO	-3.34	107.54	112.35
3	D	303	YPG	C5-C6-N1	-3.33	119.17	123.52
3	F	303	YPG	CBB-CAP-NBC	-3.33	97.26	102.84
3	I	303	YPG	CBB-CAP-NBC	-3.27	97.37	102.84
3	D	303	YPG	CBB-CAP-NBC	-3.24	97.42	102.84
3	K	304	YPG	CBB-CAP-NBC	-3.24	97.42	102.84
3	H	303	YPG	CAP-NBC-CAO	-3.20	107.74	112.35
3	C	303	YPG	CAP-NBC-CAO	-3.19	107.74	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	303	YPG	CBB-CAP-NBC	-3.16	97.55	102.84
3	I	303	YPG	CAP-NBC-CAO	-3.11	107.86	112.35
3	C	303	YPG	C6-C5-C4	-3.09	117.33	120.86
3	J	303	YPG	C6-C5-C4	-3.08	117.33	120.86
3	H	303	YPG	C6-C5-C4	-3.07	117.35	120.86
3	C	303	YPG	C5-C6-N1	-2.95	119.67	123.52
3	G	303	YPG	CAP-NBC-CAO	-2.85	108.24	112.35
3	K	304	YPG	CAP-NBC-CAO	-2.76	108.36	112.35
3	A	303	YPG	CBB-CAP-NBC	-2.72	98.30	102.84
3	D	303	YPG	CAP-NBC-CAO	-2.69	108.46	112.35
3	I	303	YPG	C6-C5-C4	-2.69	117.78	120.86
3	L	304	YPG	CAP-NBC-CAO	-2.64	108.54	112.35
3	L	304	YPG	OAI-PBF-OAJ	-2.53	106.93	113.58
3	E	304	YPG	CBB-CAP-NBC	-2.50	98.65	102.84
3	E	304	YPG	OAI-PBF-OAJ	-2.48	107.04	113.58
3	I	303	YPG	OAE-PBF-OAJ	-2.48	107.06	113.58
3	A	303	YPG	OAI-PBF-OAJ	-2.31	107.51	113.58
3	F	303	YPG	OAJ-PBF-CAZ	-2.19	107.64	112.68
3	G	303	YPG	OAI-PBF-OAJ	-2.14	107.96	113.58
3	F	303	YPG	OAB-CAU-CAL	-2.13	117.30	121.36
3	B	303	YPG	OAI-PBF-OAJ	-2.09	108.08	113.58
3	L	304	YPG	OAH-PBE-CAM	-2.05	107.21	111.30
3	E	304	YPG	OAB-CAU-CAL	-2.04	117.47	121.36
3	C	303	YPG	OAE-PBF-OAJ	-2.02	108.26	113.58
3	H	303	YPG	N2-C2-N1	2.01	120.52	117.20
3	B	303	YPG	N2-C2-N1	2.05	120.59	117.20
3	L	304	YPG	N2-C2-N1	2.06	120.60	117.20
3	I	303	YPG	OAD-PBE-CAM	2.10	112.38	106.82
3	C	303	YPG	CAL-CAU-NBC	2.13	120.88	117.87
3	D	303	YPG	N2-C2-N1	2.14	120.73	117.20
3	I	303	YPG	N2-C2-N1	2.14	120.74	117.20
3	C	303	YPG	N2-C2-N1	2.30	121.00	117.20
3	C	303	YPG	PBF-CAZ-OAF	2.36	113.27	107.38
3	D	303	YPG	CAL-CAU-NBC	2.37	121.21	117.87
3	E	304	YPG	N2-C2-N1	2.38	121.13	117.20
3	K	304	YPG	N2-C2-N1	2.38	121.13	117.20
3	G	303	YPG	CAN-OAT-CBA	2.50	118.88	115.19
3	J	303	YPG	N2-C2-N1	2.82	121.85	117.20
3	A	303	YPG	N2-C2-N1	3.26	122.59	117.20
3	I	303	YPG	CBA-CAO-NBC	3.30	107.24	103.59
3	L	304	YPG	CBA-CAO-NBC	3.55	107.52	103.59
3	D	303	YPG	CBA-CAO-NBC	3.55	107.52	103.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	303	YPG	N2-C2-N1	3.55	123.06	117.20
3	K	304	YPG	CBA-CAO-NBC	3.67	107.66	103.59
3	H	303	YPG	CBA-CAO-NBC	3.97	107.98	103.59
3	F	303	YPG	CBA-CAO-NBC	3.99	108.00	103.59
3	A	303	YPG	CBA-CAO-NBC	4.14	108.17	103.59
3	B	303	YPG	CBA-CAO-NBC	4.22	108.26	103.59
3	E	304	YPG	CBA-CAO-NBC	4.26	108.31	103.59
3	G	303	YPG	CBA-CAO-NBC	4.32	108.37	103.59
3	C	303	YPG	CBA-CAO-NBC	4.32	108.37	103.59
3	C	303	YPG	C6-N1-C2	4.44	121.08	115.88
3	J	303	YPG	CBA-CAO-NBC	4.44	108.51	103.59
3	I	303	YPG	C6-N1-C2	4.46	121.11	115.88
3	D	303	YPG	C6-N1-C2	4.84	121.55	115.88
3	J	303	YPG	C6-N1-C2	5.05	121.79	115.88
3	K	304	YPG	C6-N1-C2	5.17	121.95	115.88
3	L	304	YPG	C6-N1-C2	5.33	122.13	115.88
3	B	303	YPG	C6-N1-C2	5.48	122.30	115.88
3	H	303	YPG	C6-N1-C2	5.56	122.40	115.88
3	E	304	YPG	C6-N1-C2	5.77	122.64	115.88
3	G	303	YPG	C6-N1-C2	5.93	122.83	115.88
3	F	303	YPG	C6-N1-C2	6.19	123.14	115.88
3	A	303	YPG	C6-N1-C2	6.21	123.16	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	220/238 (92%)	-0.35	1 (0%) 91 81	23, 43, 95, 115	0
1	B	220/238 (92%)	-0.23	1 (0%) 91 81	21, 46, 99, 135	0
1	C	219/238 (92%)	-0.24	1 (0%) 91 81	32, 55, 91, 118	0
1	D	218/238 (91%)	-0.29	1 (0%) 91 81	24, 49, 83, 113	0
1	E	211/238 (88%)	-0.21	3 (1%) 78 57	22, 50, 95, 131	0
1	F	220/238 (92%)	-0.25	2 (0%) 85 69	22, 48, 88, 120	0
1	G	218/238 (91%)	-0.21	6 (2%) 56 30	25, 49, 93, 137	0
1	H	218/238 (91%)	-0.16	2 (0%) 85 69	27, 58, 91, 111	0
1	I	217/238 (91%)	-0.22	3 (1%) 78 57	23, 47, 91, 136	0
1	J	218/238 (91%)	-0.21	1 (0%) 91 81	24, 54, 90, 120	0
1	K	217/238 (91%)	-0.15	1 (0%) 91 81	29, 61, 100, 127	0
1	L	216/238 (90%)	-0.11	6 (2%) 56 30	23, 51, 105, 135	0
All	All	2612/2856 (91%)	-0.22	28 (1%) 82 63	21, 50, 95, 137	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	125	ILE	6.7
1	L	125	ILE	5.1
1	I	125	ILE	4.5
1	G	115	SER	4.4
1	J	115	SER	3.9
1	L	126	GLU	3.9
1	H	115	SER	3.7
1	L	127	ILE	3.6
1	G	131	ASP	3.6
1	G	126	GLU	3.4
1	B	158	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	0	HIS	3.0
1	I	101	SER	3.0
1	K	178	THR	2.8
1	A	101	SER	2.7
1	L	128	VAL	2.7
1	L	160	LEU	2.6
1	L	129	SER	2.6
1	F	115	SER	2.5
1	I	127	ILE	2.4
1	D	227	ARG	2.3
1	E	97	SER	2.3
1	C	1	HIS	2.2
1	G	113	VAL	2.2
1	G	129	SER	2.1
1	H	12	ASN	2.1
1	E	130	GLU	2.1
1	E	228	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	L	303	1/1	0.81	0.41	3.42	68,68,68,68	0
2	MG	E	303	1/1	0.90	0.28	0.66	62,62,62,62	0
2	MG	J	301	1/1	0.98	0.18	0.44	33,33,33,33	0
3	YPG	E	304	32/32	0.96	0.14	-0.61	29,44,57,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	K	303	1/1	0.89	0.23	-0.70	54,54,54,54	0
3	YPG	D	303	32/32	0.95	0.14	-0.72	35,48,59,77	0
3	YPG	I	303	32/32	0.96	0.14	-0.75	26,31,51,61	0
3	YPG	A	303	32/32	0.97	0.15	-0.76	25,39,56,58	0
3	YPG	J	303	32/32	0.95	0.15	-0.97	35,52,69,70	0
3	YPG	G	303	32/32	0.95	0.14	-1.01	34,44,55,57	0
3	YPG	B	303	32/32	0.96	0.14	-1.03	25,39,53,59	0
3	YPG	L	304	32/32	0.97	0.12	-1.11	25,38,52,57	0
3	YPG	K	304	32/32	0.95	0.12	-1.34	46,59,76,83	0
3	YPG	H	303	32/32	0.95	0.12	-1.45	40,66,87,93	0
3	YPG	C	303	32/32	0.96	0.12	-1.55	41,49,59,63	0
3	YPG	F	303	32/32	0.97	0.11	-2.10	31,48,76,81	0
2	MG	G	302	1/1	0.99	0.10	-	37,37,37,37	0
2	MG	F	301	1/1	0.92	0.07	-	34,34,34,34	0
2	MG	C	301	1/1	0.98	0.14	-	74,74,74,74	0
2	MG	B	301	1/1	0.96	0.16	-	61,61,61,61	0
2	MG	E	302	1/1	0.97	0.22	-	39,39,39,39	0
2	MG	I	301	1/1	0.98	0.19	-	23,23,23,23	0
2	MG	E	301	1/1	0.92	0.15	-	36,36,36,36	0
2	MG	G	301	1/1	0.94	0.20	-	39,39,39,39	0
2	MG	K	302	1/1	0.95	0.08	-	49,49,49,49	0
2	MG	L	302	1/1	0.90	0.15	-	35,35,35,35	0
2	MG	L	301	1/1	0.98	0.12	-	38,38,38,38	0
2	MG	I	302	1/1	0.98	0.21	-	32,32,32,32	0
2	MG	C	302	1/1	0.95	0.09	-	43,43,43,43	0
2	MG	A	301	1/1	0.95	0.09	-	48,48,48,48	0
2	MG	H	302	1/1	0.94	0.10	-	46,46,46,46	0
2	MG	K	301	1/1	0.95	0.15	-	44,44,44,44	0
2	MG	F	302	1/1	0.94	0.09	-	75,75,75,75	0
2	MG	J	302	1/1	0.93	0.17	-	48,48,48,48	0
2	MG	D	302	1/1	0.96	0.07	-	41,41,41,41	0
2	MG	A	302	1/1	0.97	0.19	-	38,38,38,38	0
2	MG	B	302	1/1	0.90	0.19	-	43,43,43,43	0
2	MG	H	301	1/1	0.93	0.19	-	50,50,50,50	0
2	MG	D	301	1/1	0.96	0.23	-	55,55,55,55	0

## 6.5 Other polymers

There are no such residues in this entry.