



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:38 PM GMT

PDB ID : 1JJK  
Title : Selenomethionine Substitution of Orotidine-5'-monophosphateDecarboxylase  
from E. coli Causes a Change in Crystal Contacts and Space Group  
Authors : Poulsen, J.-C.N.; Harris, P.; Jensen, K.F.; Larsen, S.  
Deposited on : 2001-07-06  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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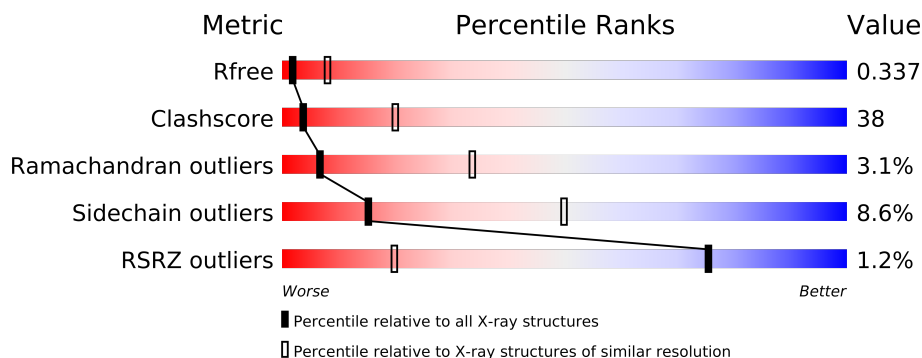
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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.



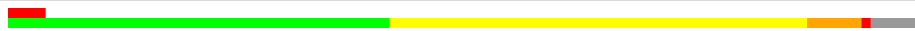
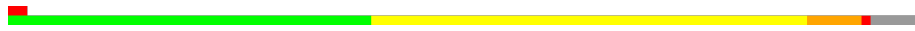
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
1	C	245	
1	D	245	
1	E	245	
1	F	245	
1	G	245	
1	H	245	
1	I	245	
1	J	245	
1	K	245	
1	L	245	
1	M	245	
1	N	245	

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Mol	Chain	Length	Quality of chain
1	O	245	
1	P	245	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28336 atoms, of which 0 are hydrogen and 0 are deuterium.

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 OROTIDINE 5'-PHOSPHATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	C	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	D	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	E	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	F	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	G	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	H	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	I	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	J	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	K	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	L	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	M	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	N	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	O	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	P	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	133	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
E	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	95	MSE	MET	MODIFIED RESIDUE	UNP P08244

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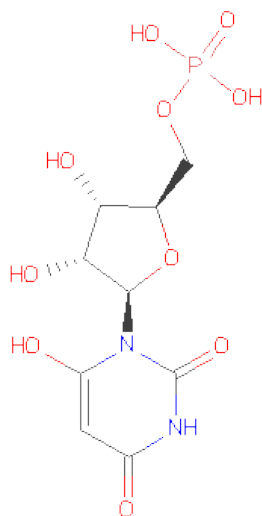
Chain	Residue	Modelled	Actual	Comment	Reference
J	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
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L	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
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M	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
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O	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

- Molecule 2 is 6-HYDROXYURIDINE-5'-PHOSPHATE (three-letter code: BMP) (formula:  $C_9H_{13}N_2O_{10}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	B	1	Total	C	N	O	P	0	0
			22	9	2	10	1		

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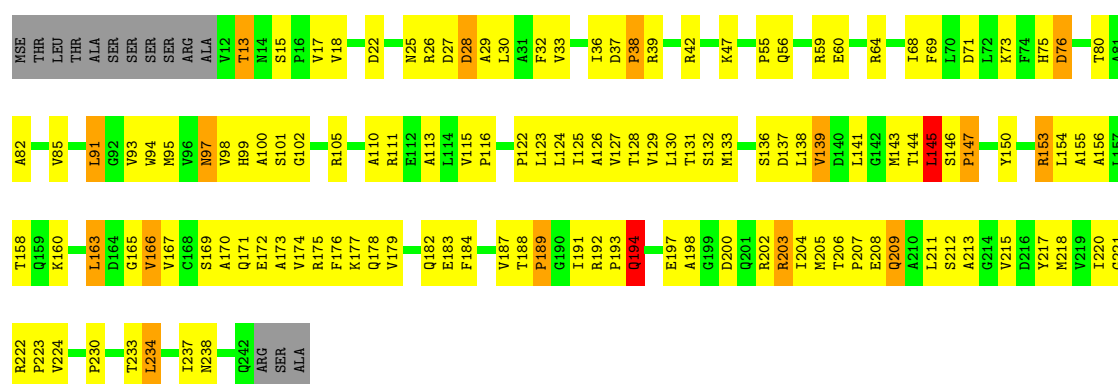
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	D	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	E	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	F	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	G	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	H	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	I	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	J	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	K	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	L	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	M	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	N	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	O	1	Total 22	C 9	N 2	O 10	P 1	0	0
2	P	1	Total 22	C 9	N 2	O 10	P 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

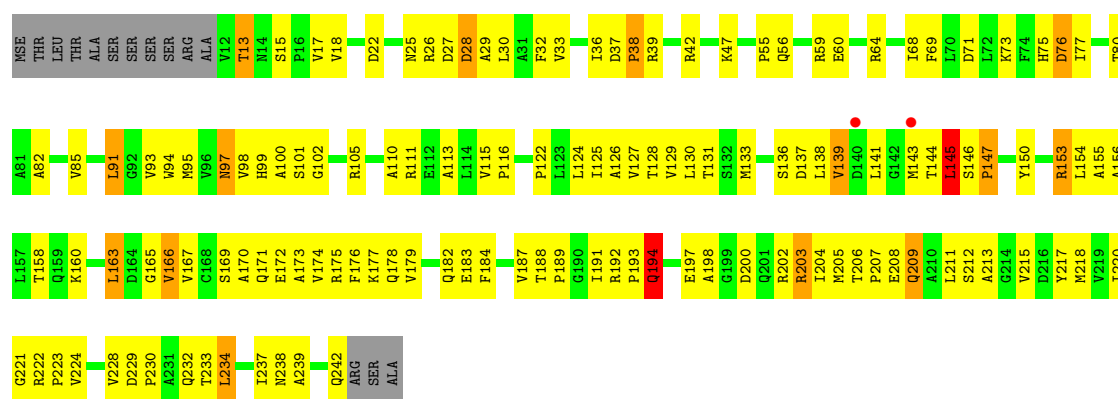
#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain A:



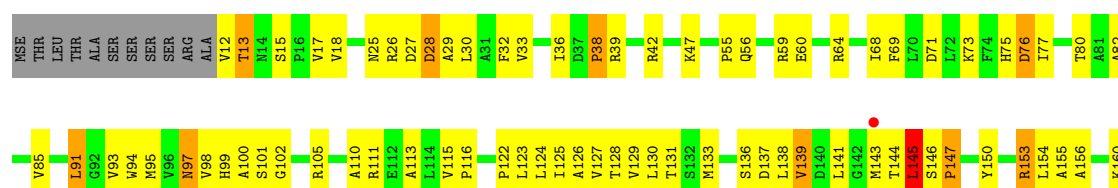
#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

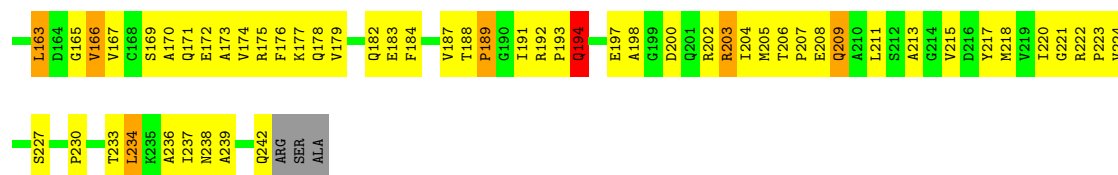
Chain B:



#### • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

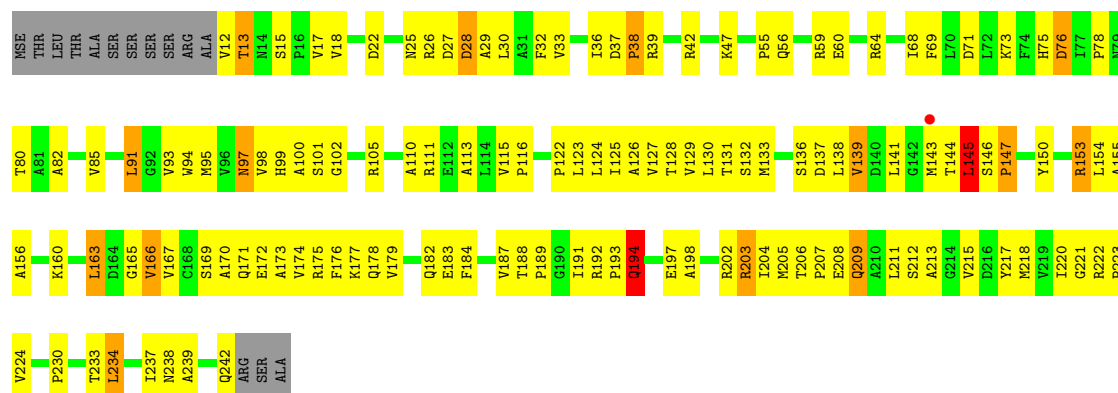
Chain C:





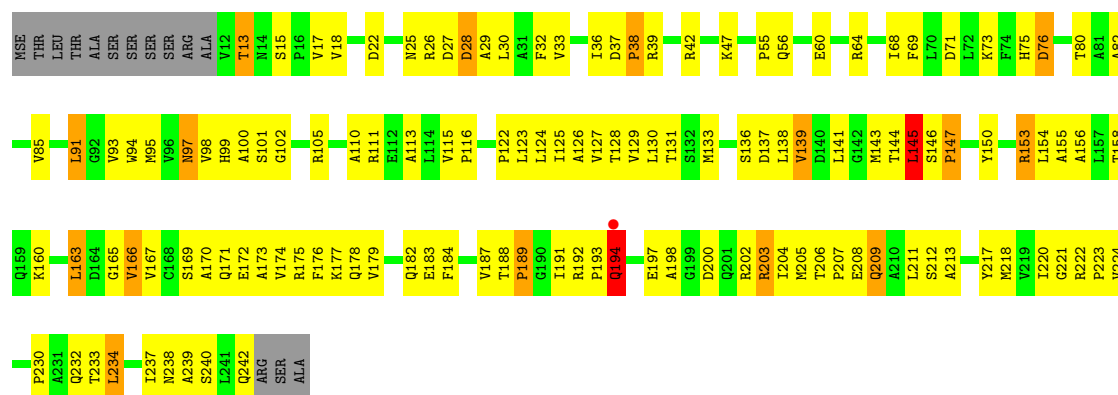
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain D:



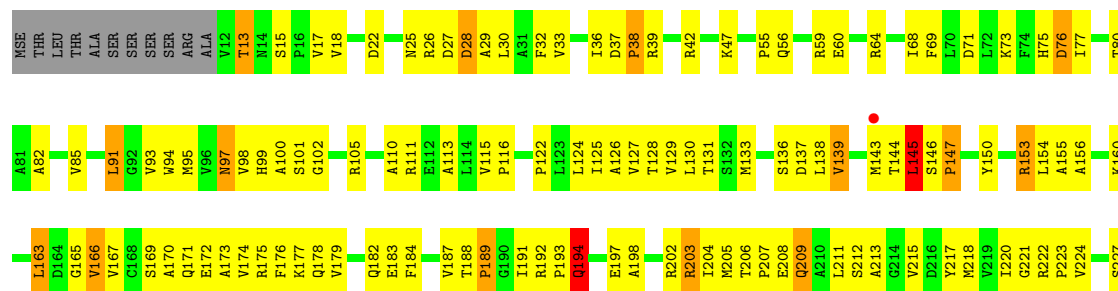
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

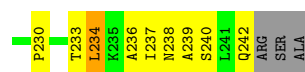
Chain E:



• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

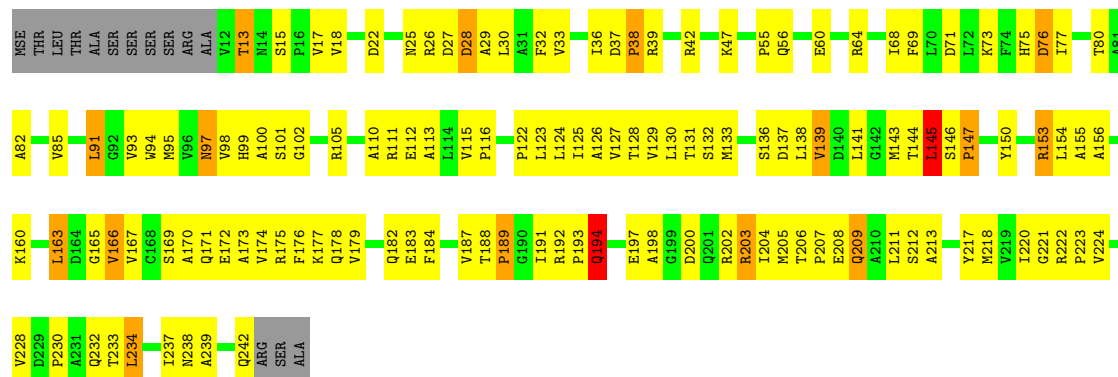
Chain F:





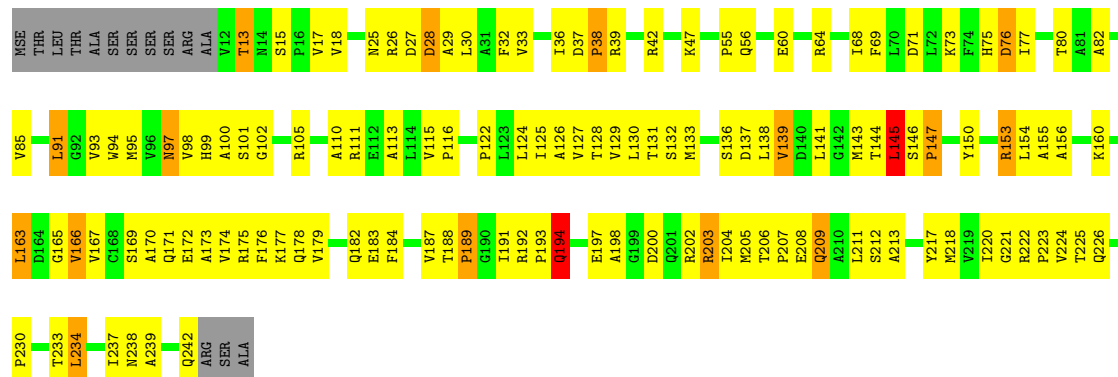
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain G:



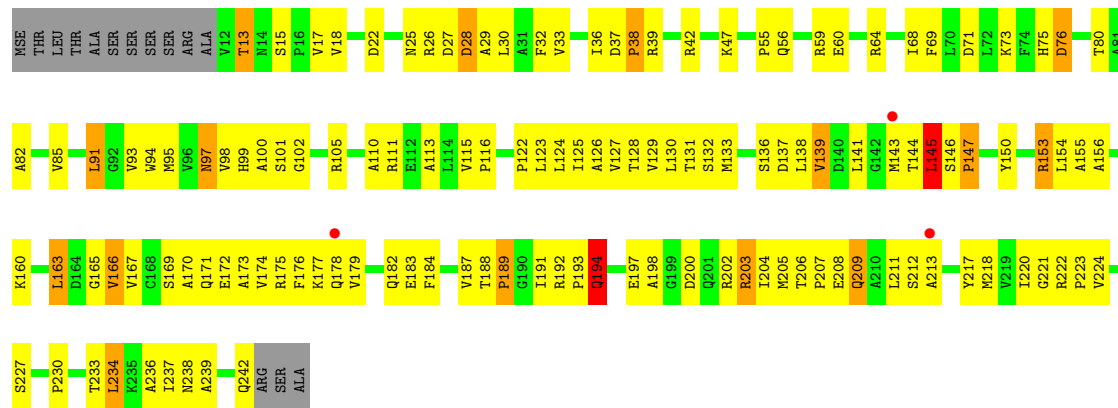
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain H:



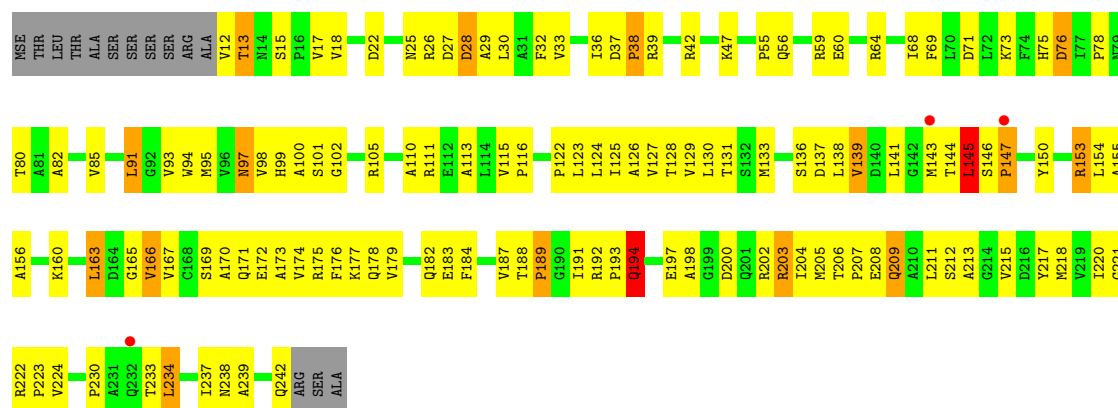
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain I:



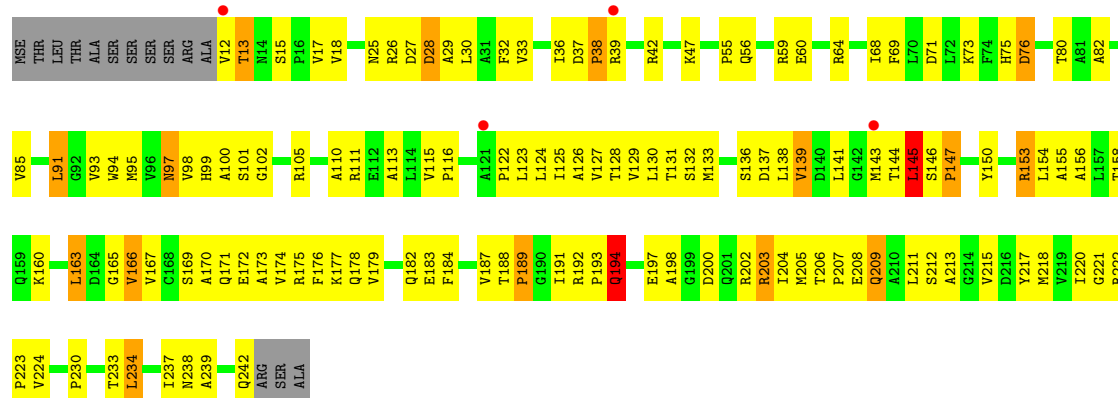
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

## Chain J:



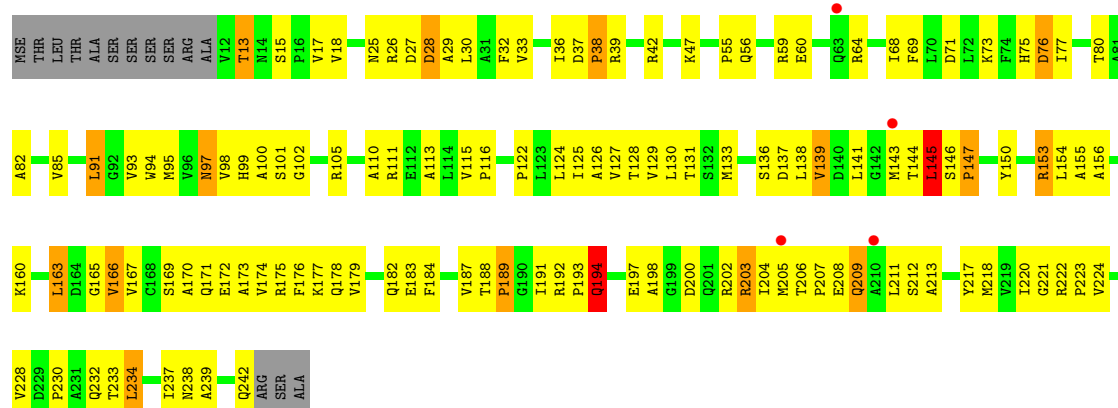
## • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

## Chain K:



## • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

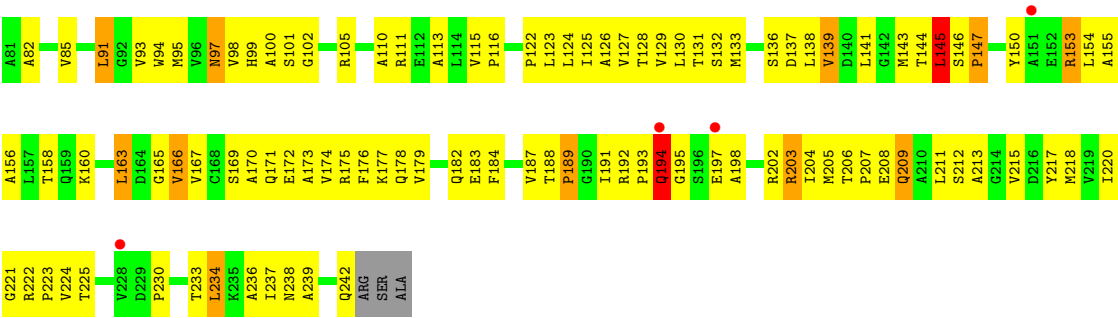
## Chain L:



## • Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

## Chain M:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.50Å 149.00Å 115.60Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-3.00) 91.1 (29.82-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.41 (at 3.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.344 , 0.344 0.342 , 0.337	Depositor DCC
$R_{free}$ test set	3274 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -1.1	EDS
Estimated twinning fraction	0.376 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	3 of 64895 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	28336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1146e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.40	0/1772	0.67	0/2392
1	B	0.40	0/1772	0.67	0/2392
1	C	0.40	0/1772	0.67	0/2392
1	D	0.40	0/1772	0.67	0/2392
1	E	0.40	0/1772	0.67	0/2392
1	F	0.40	0/1772	0.67	0/2392
1	G	0.40	0/1772	0.67	0/2392
1	H	0.40	0/1772	0.67	0/2392
1	I	0.40	0/1772	0.67	0/2392
1	J	0.40	0/1772	0.67	0/2392
1	K	0.40	0/1772	0.67	0/2392
1	L	0.40	0/1772	0.67	0/2392
1	M	0.40	0/1772	0.67	0/2392
1	N	0.40	0/1772	0.67	0/2392
1	O	0.40	0/1772	0.67	0/2392
1	P	0.40	0/1772	0.67	0/2392
All	All	0.40	0/28352	0.67	0/38272

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1749	0	1758	139	1
1	B	1749	0	1758	162	0
1	C	1749	0	1758	163	0
1	D	1749	0	1758	141	0
1	E	1749	0	1758	138	3
1	F	1749	0	1758	152	0
1	G	1749	0	1758	155	0
1	H	1749	0	1758	135	1
1	I	1749	0	1758	138	2
1	J	1749	0	1758	148	1
1	K	1749	0	1758	145	2
1	L	1749	0	1758	138	2
1	M	1749	0	1758	144	2
1	N	1749	0	1758	143	0
1	O	1749	0	1758	135	1
1	P	1749	0	1758	141	3
2	A	22	0	11	2	0
2	B	22	0	11	2	0
2	C	22	0	11	2	0
2	D	22	0	11	2	0
2	E	22	0	11	3	0
2	F	22	0	11	2	0
2	G	22	0	11	2	0
2	H	22	0	11	2	0
2	I	22	0	11	2	0
2	J	22	0	11	2	0
2	K	22	0	11	2	0
2	L	22	0	11	2	0
2	M	22	0	11	3	0
2	N	22	0	11	4	0
2	O	22	0	11	2	0
2	P	22	0	11	2	0
All	All	28336	0	28304	2177	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 2177 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:182:GLN:HG3	1:J:12:VAL:CG1	1.65	1.26

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:GLN:NE2	1:C:227:SER:HA	1.53	1.22
1:F:236:ALA:CB	1:G:228:VAL:HG21	1.77	1.13
1:F:236:ALA:CB	1:G:228:VAL:CG2	2.26	1.11
1:F:236:ALA:HB3	1:G:228:VAL:HG21	1.37	1.04

The worst 5 of 9 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	Distance(Å)	Clash(Å)
1:A:178:GLN:OE1	1:O:242:GLN:OE1[2_545]	1.39	0.81
1:E:242:GLN:OE1	1:K:178:GLN:OE1[1_454]	1.53	0.67
1:M:228:VAL:CG2	1:P:236:ALA:CB[1_455]	1.84	0.36
1:J:56:GLN:NE2	1:P:27:ASP:CB[2_646]	2.01	0.19
1:M:236:ALA:CB	1:P:195:GLY:O[1_455]	2.07	0.13

## 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	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	B	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	C	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	D	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	E	229/245 (94%)	185 (81%)	37 (16%)	7 (3%)	7	34
1	F	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	G	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	H	229/245 (94%)	183 (80%)	39 (17%)	7 (3%)	7	34
1	I	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	J	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	K	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	L	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	N	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	O	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
1	P	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	7	34
All	All	3664/3920 (94%)	2944 (80%)	608 (17%)	112 (3%)	7	34

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	194	GLN
1	B	145	LEU
1	B	194	GLN
1	C	145	LEU

### 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	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	B	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	C	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	D	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	E	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	F	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	G	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	H	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	I	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	J	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	K	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	L	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	M	185/187 (99%)	169 (91%)	16 (9%)	15	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	O	185/187 (99%)	169 (91%)	16 (9%)	15	50
1	P	185/187 (99%)	169 (91%)	16 (9%)	15	50
All	All	2960/2992 (99%)	2704 (91%)	256 (9%)	15	50

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	76	ASP
1	I	234	LEU
1	O	184	PHE
1	H	139	VAL
1	I	39	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	56	GLN
1	I	238	ASN
1	O	226	GLN
1	H	83	HIS
1	I	25	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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	BMP	A	301	-	23,23,23	1.95	7 (30%)	29,35,35	1.52	5 (17%)
2	BMP	B	302	-	23,23,23	1.95	7 (30%)	29,35,35	1.53	5 (17%)
2	BMP	C	303	-	23,23,23	1.94	7 (30%)	29,35,35	1.53	5 (17%)
2	BMP	D	304	-	23,23,23	1.95	5 (21%)	29,35,35	1.52	5 (17%)
2	BMP	E	305	-	23,23,23	1.95	6 (26%)	29,35,35	1.53	5 (17%)
2	BMP	F	306	-	23,23,23	1.95	6 (26%)	29,35,35	1.53	5 (17%)
2	BMP	G	307	-	23,23,23	1.94	6 (26%)	29,35,35	1.53	5 (17%)
2	BMP	H	308	-	23,23,23	1.95	7 (30%)	29,35,35	1.52	5 (17%)
2	BMP	I	309	-	23,23,23	1.94	5 (21%)	29,35,35	1.53	5 (17%)
2	BMP	J	310	-	23,23,23	1.95	7 (30%)	29,35,35	1.53	5 (17%)
2	BMP	K	311	-	23,23,23	1.95	7 (30%)	29,35,35	1.52	5 (17%)
2	BMP	L	312	-	23,23,23	1.94	6 (26%)	29,35,35	1.52	5 (17%)
2	BMP	M	313	-	23,23,23	1.94	6 (26%)	29,35,35	1.52	5 (17%)
2	BMP	N	314	-	23,23,23	1.95	6 (26%)	29,35,35	1.53	5 (17%)
2	BMP	O	315	-	23,23,23	1.95	7 (30%)	29,35,35	1.53	5 (17%)
2	BMP	P	316	-	23,23,23	1.95	6 (26%)	29,35,35	1.52	5 (17%)

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	BMP	A	301	-	-	0/6/26/26	0/2/2/2
2	BMP	B	302	-	-	0/6/26/26	0/2/2/2
2	BMP	C	303	-	-	0/6/26/26	0/2/2/2
2	BMP	D	304	-	-	0/6/26/26	0/2/2/2
2	BMP	E	305	-	-	0/6/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMP	F	306	-	-	0/6/26/26	0/2/2/2
2	BMP	G	307	-	-	0/6/26/26	0/2/2/2
2	BMP	H	308	-	-	0/6/26/26	0/2/2/2
2	BMP	I	309	-	-	0/6/26/26	0/2/2/2
2	BMP	J	310	-	-	0/6/26/26	0/2/2/2
2	BMP	K	311	-	-	0/6/26/26	0/2/2/2
2	BMP	L	312	-	-	0/6/26/26	0/2/2/2
2	BMP	M	313	-	-	0/6/26/26	0/2/2/2
2	BMP	N	314	-	-	0/6/26/26	0/2/2/2
2	BMP	O	315	-	-	0/6/26/26	0/2/2/2
2	BMP	P	316	-	-	0/6/26/26	0/2/2/2

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	314	BMP	O2-C2	4.87	1.33	1.23
2	J	310	BMP	O2-C2	4.86	1.33	1.23
2	P	316	BMP	O2-C2	4.86	1.33	1.23
2	O	315	BMP	O2-C2	4.86	1.33	1.23
2	E	305	BMP	O2-C2	4.85	1.33	1.23

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	310	BMP	C4'-O4'-C1'	-4.32	105.05	109.75
2	O	315	BMP	C4'-O4'-C1'	-4.32	105.06	109.75
2	I	309	BMP	C4'-O4'-C1'	-4.31	105.06	109.75
2	F	306	BMP	C4'-O4'-C1'	-4.31	105.07	109.75
2	A	301	BMP	C4'-O4'-C1'	-4.29	105.09	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	231/245 (94%)	0.14	0 100 100	1, 23, 45, 70	0
1	B	231/245 (94%)	0.15	2 (0%) 81 24	1, 23, 45, 70	0
1	C	231/245 (94%)	0.07	1 (0%) 90 41	1, 23, 45, 70	0
1	D	231/245 (94%)	0.12	1 (0%) 90 41	1, 23, 45, 70	0
1	E	231/245 (94%)	0.20	1 (0%) 90 41	1, 23, 45, 70	0
1	F	231/245 (94%)	0.27	1 (0%) 90 41	1, 23, 45, 70	0
1	G	231/245 (94%)	0.16	0 100 100	1, 23, 45, 70	0
1	H	231/245 (94%)	0.11	0 100 100	1, 23, 45, 70	0
1	I	231/245 (94%)	0.22	3 (1%) 74 19	1, 23, 45, 70	0
1	J	231/245 (94%)	0.34	3 (1%) 74 19	1, 23, 45, 70	0
1	K	231/245 (94%)	0.44	4 (1%) 67 15	1, 23, 45, 70	0
1	L	231/245 (94%)	0.44	4 (1%) 67 15	1, 23, 45, 70	0
1	M	231/245 (94%)	0.46	0 100 100	1, 23, 45, 70	0
1	N	231/245 (94%)	0.54	9 (3%) 37 7	1, 23, 45, 70	0
1	O	231/245 (94%)	0.68	9 (3%) 37 7	1, 23, 45, 70	0
1	P	231/245 (94%)	0.49	4 (1%) 67 15	1, 23, 45, 70	0
All	All	3696/3920 (94%)	0.30	42 (1%) 75 21	1, 23, 46, 70	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	143	MSE	3.8
1	B	143	MSE	3.8
1	N	143	MSE	3.6
1	O	197	GLU	3.5
1	L	143	MSE	3.4

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMP	B	302	22/22	0.23	0.12	6,8,12,13	0
2	BMP	E	305	22/22	0.25	-0.06	6,8,12,13	0
2	BMP	M	313	22/22	0.29	-0.22	6,8,12,13	0
2	BMP	O	315	22/22	0.32	-0.31	6,8,12,13	0
2	BMP	N	314	22/22	0.28	-0.34	6,8,12,13	0
2	BMP	A	301	22/22	0.21	-0.41	6,8,12,13	0
2	BMP	G	307	22/22	0.23	-0.55	6,8,12,13	0
2	BMP	I	309	22/22	0.20	-0.59	6,8,12,13	0
2	BMP	J	310	22/22	0.21	-0.78	6,8,12,13	0
2	BMP	L	312	22/22	0.21	-0.81	6,8,12,13	0
2	BMP	C	303	22/22	0.17	-0.92	6,8,12,13	0
2	BMP	F	306	22/22	0.20	-0.94	6,8,12,13	0
2	BMP	P	316	22/22	0.20	-0.99	6,8,12,13	0
2	BMP	D	304	22/22	0.18	-1.14	6,8,12,13	0
2	BMP	K	311	22/22	0.17	-1.54	6,8,12,13	0
2	BMP	H	308	22/22	0.15	-1.59	6,8,12,13	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.