



# Full wwPDB X-ray Structure Validation Report

Nov 4, 2014 – 05:24 PM EST

PDB ID : 4RC1  
Title : Structure of the methanofuran/methanopterinbiosynthetic enzyme MJ1099 from Methanocaldococcus jannaschii with PRPP  
Authors : Bobik, T.A.; Morales, E.J.; Cascio, D.; Sawaya, M.R.; Yeates, T.O.; Rasche, M.E.  
Deposited on : 2014-09-14  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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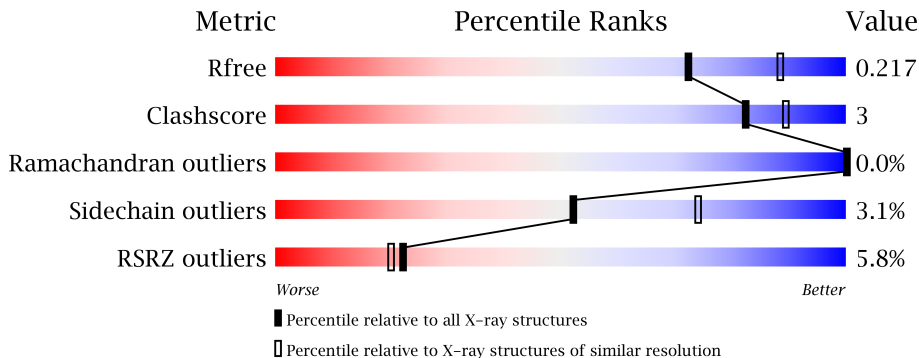
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	
1	F	242	
1	G	242	
1	H	242	
1	I	242	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	F	301	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16231 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 UPF0264 protein MJ1099.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1814	1155	310	341	8			
1	B	242	Total	C	N	O	S	0	0	0
			1827	1162	315	342	8			
1	C	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			
1	D	242	Total	C	N	O	S	0	0	0
			1827	1162	315	342	8			
1	E	236	Total	C	N	O	S	0	0	0
			1763	1125	296	334	8			
1	F	238	Total	C	N	O	S	0	0	0
			1784	1137	303	336	8			
1	G	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			
1	H	229	Total	C	N	O	S	0	0	0
			1720	1101	286	325	8			
1	I	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q58499
A	-5	HIS	-	EXPRESSION TAG	UNP Q58499
A	-4	HIS	-	EXPRESSION TAG	UNP Q58499
A	-3	HIS	-	EXPRESSION TAG	UNP Q58499
A	-2	HIS	-	EXPRESSION TAG	UNP Q58499
A	-1	HIS	-	EXPRESSION TAG	UNP Q58499
A	0	HIS	-	EXPRESSION TAG	UNP Q58499
B	-6	MET	-	EXPRESSION TAG	UNP Q58499
B	-5	HIS	-	EXPRESSION TAG	UNP Q58499
B	-4	HIS	-	EXPRESSION TAG	UNP Q58499
B	-3	HIS	-	EXPRESSION TAG	UNP Q58499

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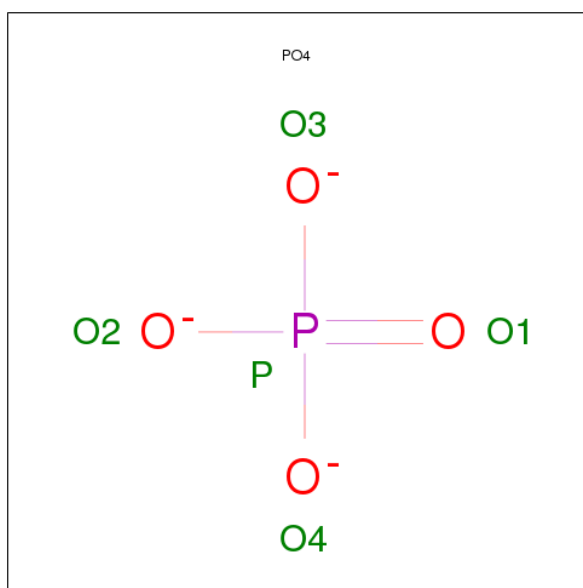
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q58499
B	-1	HIS	-	EXPRESSION TAG	UNP Q58499
B	0	HIS	-	EXPRESSION TAG	UNP Q58499
C	-6	MET	-	EXPRESSION TAG	UNP Q58499
C	-5	HIS	-	EXPRESSION TAG	UNP Q58499
C	-4	HIS	-	EXPRESSION TAG	UNP Q58499
C	-3	HIS	-	EXPRESSION TAG	UNP Q58499
C	-2	HIS	-	EXPRESSION TAG	UNP Q58499
C	-1	HIS	-	EXPRESSION TAG	UNP Q58499
C	0	HIS	-	EXPRESSION TAG	UNP Q58499
D	-6	MET	-	EXPRESSION TAG	UNP Q58499
D	-5	HIS	-	EXPRESSION TAG	UNP Q58499
D	-4	HIS	-	EXPRESSION TAG	UNP Q58499
D	-3	HIS	-	EXPRESSION TAG	UNP Q58499
D	-2	HIS	-	EXPRESSION TAG	UNP Q58499
D	-1	HIS	-	EXPRESSION TAG	UNP Q58499
D	0	HIS	-	EXPRESSION TAG	UNP Q58499
E	-6	MET	-	EXPRESSION TAG	UNP Q58499
E	-5	HIS	-	EXPRESSION TAG	UNP Q58499
E	-4	HIS	-	EXPRESSION TAG	UNP Q58499
E	-3	HIS	-	EXPRESSION TAG	UNP Q58499
E	-2	HIS	-	EXPRESSION TAG	UNP Q58499
E	-1	HIS	-	EXPRESSION TAG	UNP Q58499
E	0	HIS	-	EXPRESSION TAG	UNP Q58499
F	-6	MET	-	EXPRESSION TAG	UNP Q58499
F	-5	HIS	-	EXPRESSION TAG	UNP Q58499
F	-4	HIS	-	EXPRESSION TAG	UNP Q58499
F	-3	HIS	-	EXPRESSION TAG	UNP Q58499
F	-2	HIS	-	EXPRESSION TAG	UNP Q58499
F	-1	HIS	-	EXPRESSION TAG	UNP Q58499
F	0	HIS	-	EXPRESSION TAG	UNP Q58499
G	-6	MET	-	EXPRESSION TAG	UNP Q58499
G	-5	HIS	-	EXPRESSION TAG	UNP Q58499
G	-4	HIS	-	EXPRESSION TAG	UNP Q58499
G	-3	HIS	-	EXPRESSION TAG	UNP Q58499
G	-2	HIS	-	EXPRESSION TAG	UNP Q58499
G	-1	HIS	-	EXPRESSION TAG	UNP Q58499
G	0	HIS	-	EXPRESSION TAG	UNP Q58499
H	-6	MET	-	EXPRESSION TAG	UNP Q58499
H	-5	HIS	-	EXPRESSION TAG	UNP Q58499
H	-4	HIS	-	EXPRESSION TAG	UNP Q58499
H	-3	HIS	-	EXPRESSION TAG	UNP Q58499

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	HIS	-	EXPRESSION TAG	UNP Q58499
H	-1	HIS	-	EXPRESSION TAG	UNP Q58499
H	0	HIS	-	EXPRESSION TAG	UNP Q58499
I	-6	MET	-	EXPRESSION TAG	UNP Q58499
I	-5	HIS	-	EXPRESSION TAG	UNP Q58499
I	-4	HIS	-	EXPRESSION TAG	UNP Q58499
I	-3	HIS	-	EXPRESSION TAG	UNP Q58499
I	-2	HIS	-	EXPRESSION TAG	UNP Q58499
I	-1	HIS	-	EXPRESSION TAG	UNP Q58499
I	0	HIS	-	EXPRESSION TAG	UNP Q58499

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	38	Total 38	O 38	0	0
3	C	17	Total 17	O 17	0	0
3	D	17	Total 17	O 17	0	0
3	E	16	Total 16	O 16	0	0
3	F	11	Total 11	O 11	0	0
3	G	4	Total 4	O 4	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.

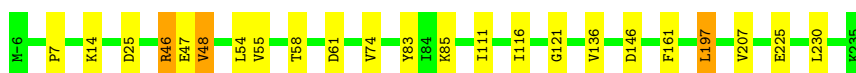
- Molecule 1: UPF0264 protein MJ1099

Chain A: 



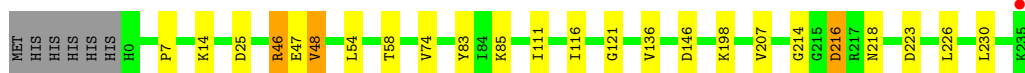
- Molecule 1: UPF0264 protein MJ1099

Chain B: 



- Molecule 1: UPF0264 protein MJ1099

Chain C: 



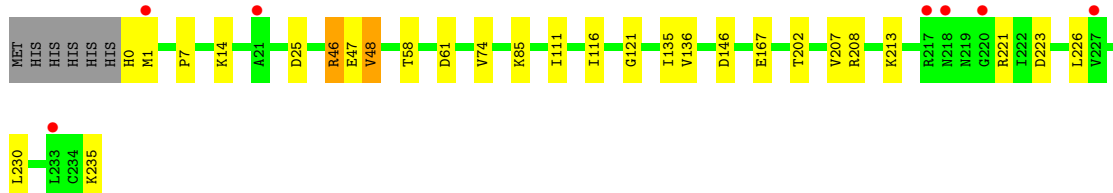
- Molecule 1: UPF0264 protein MJ1099

Chain D: 



- Molecule 1: UPF0264 protein MJ1099

Chain E: 



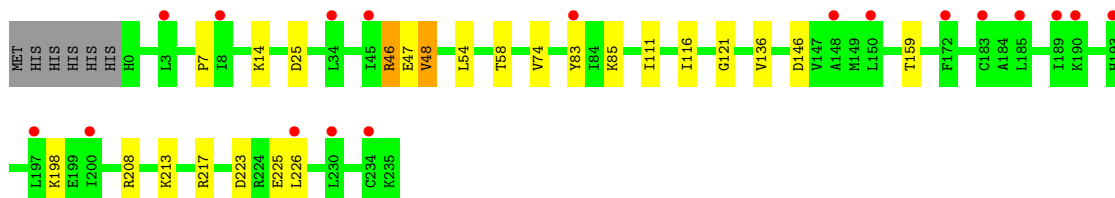
- Molecule 1: UPF0264 protein MJ1099

Chain F: 



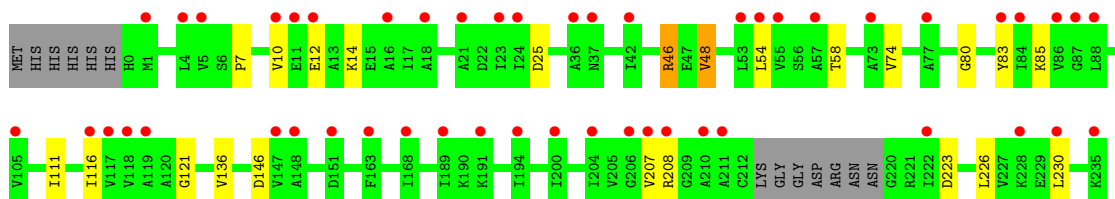
- Molecule 1: UPF0264 protein MJ1099

Chain G:



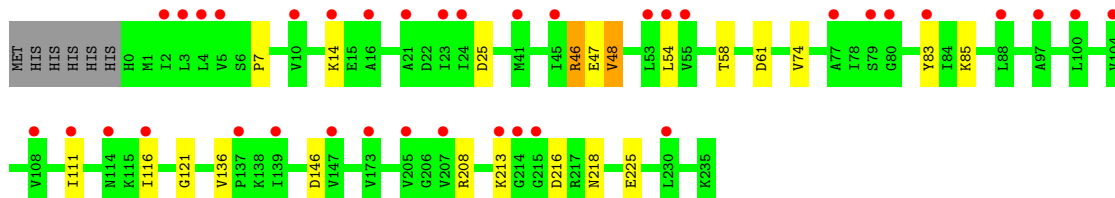
- Molecule 1: UPF0264 protein MJ1099

Chain H:



- Molecule 1: UPF0264 protein MJ1099

Chain I:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.87Å 153.03Å 132.84Å 90.00° 111.97° 90.00°	Depositor
Resolution (Å)	65.00 – 2.40 65.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (65.00-2.40) 98.4 (65.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.193 , 0.210 0.197 , 0.217	Depositor DCC
$R_{free}$ test set	5118 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102608 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PO4

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	0.59	0/1844	0.75	0/2492
1	B	0.53	0/1857	0.71	1/2508 (0.0%)
1	C	0.50	0/1797	0.68	0/2426
1	D	0.50	0/1857	0.70	1/2508 (0.0%)
1	E	0.49	0/1788	0.71	1/2415 (0.0%)
1	F	0.50	0/1810	0.71	0/2444
1	G	0.47	0/1797	0.66	0/2426
1	H	0.46	0/1744	0.67	0/2355
1	I	0.44	0/1797	0.67	1/2426 (0.0%)
All	All	0.50	0/16291	0.70	4/22000 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	61	ASP	N-CA-C	-5.14	97.12	111.00
1	I	61	ASP	N-CA-C	-5.07	97.32	111.00
1	D	61	ASP	N-CA-C	-5.04	97.39	111.00
1	B	61	ASP	N-CA-C	-5.03	97.41	111.00

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	1814	0	1855	12	0
1	B	1827	0	1875	11	0
1	C	1772	0	1838	12	0
1	D	1827	0	1875	12	0
1	E	1763	0	1825	16	0
1	F	1784	0	1845	11	0
1	G	1772	0	1838	10	0
1	H	1720	0	1789	12	0
1	I	1772	0	1838	8	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	I	5	0	0	0	0
3	A	47	0	0	0	0
3	B	38	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
3	E	16	0	0	1	0
3	F	11	0	0	0	0
3	G	4	0	0	0	0
All	All	16231	0	16578	101	0

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 3.

All (101) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:83:TYR:CE1	1:F:118:VAL:HG21	2.37	0.60
1:G:7:PRO:HD2	1:G:25:ASP:O	2.02	0.59
1:A:46:ARG:O	1:A:46:ARG:HD3	2.04	0.57
1:C:214:GLY:C	1:C:216:ASP:H	2.06	0.57
1:E:213:LYS:HG2	1:E:221:ARG:H	1.70	0.57
1:E:223:ASP:HB3	1:E:226:LEU:HD12	1.85	0.57
1:I:7:PRO:HD2	1:I:25:ASP:O	2.05	0.57
1:G:14:LYS:HE2	1:G:48:VAL:HG21	1.88	0.54
1:I:116:ILE:HG23	1:I:146:ASP:HB2	1.89	0.53
1:D:74:VAL:HG13	1:D:111:ILE:HD11	1.91	0.53
1:A:14:LYS:HE2	1:A:48:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:58:THR:HG22	1:D:85:LYS:HD2	1.91	0.53
1:A:7:PRO:HD2	1:A:25:ASP:O	2.09	0.52
1:B:46:ARG:O	1:B:46:ARG:HD3	2.10	0.52
1:E:0:HIS:ND1	1:E:235:LYS:HA	2.24	0.52
1:E:14:LYS:HE2	1:E:48:VAL:HG21	1.90	0.52
1:H:46:ARG:HG3	1:H:80:GLY:O	2.10	0.52
1:D:14:LYS:HE2	1:D:48:VAL:HG21	1.92	0.52
1:F:46:ARG:HD3	1:F:46:ARG:O	2.09	0.52
1:C:46:ARG:HD3	1:C:46:ARG:O	2.09	0.52
1:G:46:ARG:O	1:G:46:ARG:HD3	2.10	0.52
1:E:46:ARG:HD3	1:E:46:ARG:O	2.10	0.51
1:E:7:PRO:HD2	1:E:25:ASP:O	2.11	0.51
1:G:74:VAL:HG13	1:G:111:ILE:HD11	1.91	0.51
1:B:58:THR:HG22	1:B:85:LYS:HD2	1.92	0.50
1:F:194:ILE:HD11	1:F:230:LEU:HD22	1.94	0.50
1:G:58:THR:HG22	1:G:85:LYS:HD2	1.93	0.50
1:E:58:THR:HG22	1:E:85:LYS:HD2	1.94	0.50
1:C:74:VAL:HG13	1:C:111:ILE:HD11	1.94	0.50
1:C:207:VAL:HG21	1:C:230:LEU:HD13	1.93	0.50
1:H:58:THR:HG22	1:H:85:LYS:HD2	1.93	0.50
1:D:46:ARG:O	1:D:46:ARG:HD3	2.12	0.50
1:I:121:GLY:HA3	1:I:136:VAL:HG21	1.94	0.49
1:C:14:LYS:HE2	1:C:48:VAL:HG21	1.93	0.49
1:I:14:LYS:HE2	1:I:48:VAL:HG21	1.93	0.49
1:E:74:VAL:HG13	1:E:111:ILE:HD11	1.95	0.49
1:I:46:ARG:O	1:I:46:ARG:HD3	2.12	0.49
1:A:207:VAL:HG21	1:A:230:LEU:HD13	1.95	0.48
1:F:74:VAL:HG13	1:F:111:ILE:HD11	1.95	0.48
1:I:74:VAL:HG13	1:I:111:ILE:HD11	1.94	0.48
1:G:116:ILE:HG23	1:G:146:ASP:HB2	1.94	0.48
1:D:83:TYR:CE1	1:D:118:VAL:HG21	2.49	0.48
1:E:116:ILE:HG23	1:E:146:ASP:HB2	1.95	0.48
1:D:121:GLY:HA3	1:D:136:VAL:HG21	1.96	0.48
1:C:58:THR:HG22	1:C:85:LYS:HD2	1.95	0.48
1:D:-1:HIS:O	1:D:198:LYS:HG2	2.14	0.48
1:B:14:LYS:HE2	1:B:48:VAL:HG21	1.95	0.48
1:G:54:LEU:HD13	1:G:83:TYR:CE1	2.48	0.48
1:H:14:LYS:HE2	1:H:48:VAL:HG21	1.95	0.47
1:G:121:GLY:HA3	1:G:136:VAL:HG21	1.96	0.47
1:H:116:ILE:HG23	1:H:146:ASP:HB2	1.96	0.47
1:H:121:GLY:HA3	1:H:136:VAL:HG21	1.96	0.47
1:E:207:VAL:HG21	1:E:230:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:58:THR:HG22	1:I:85:LYS:HD2	1.96	0.47
1:C:54:LEU:HD13	1:C:83:TYR:CE1	2.50	0.47
1:H:207:VAL:HG21	1:H:230:LEU:HD13	1.96	0.47
1:A:74:VAL:HG13	1:A:111:ILE:HD11	1.97	0.47
1:E:1:MET:HG2	1:E:202:THR:O	2.14	0.46
1:E:121:GLY:HA3	1:E:136:VAL:HG21	1.98	0.46
1:E:0:HIS:CE1	1:E:235:LYS:HG2	2.50	0.46
1:F:116:ILE:HG23	1:F:146:ASP:HB2	1.97	0.46
1:A:121:GLY:HA3	1:A:136:VAL:HG21	1.97	0.46
1:C:121:GLY:HA3	1:C:136:VAL:HG21	1.96	0.46
1:E:0:HIS:HE1	1:E:235:LYS:HG2	1.81	0.46
1:F:121:GLY:HA3	1:F:136:VAL:HG21	1.97	0.46
1:B:74:VAL:HG13	1:B:111:ILE:HD11	1.97	0.46
1:B:121:GLY:HA3	1:B:136:VAL:HG21	1.97	0.46
1:F:221:ARG:HG2	1:F:221:ARG:HH11	1.81	0.46
1:C:7:PRO:HD2	1:C:25:ASP:O	2.16	0.46
1:C:116:ILE:HG23	1:C:146:ASP:HB2	1.96	0.45
1:H:74:VAL:HG13	1:H:111:ILE:HD11	1.98	0.45
1:D:116:ILE:HG23	1:D:146:ASP:HB2	1.99	0.45
1:H:7:PRO:HD2	1:H:25:ASP:O	2.16	0.45
1:B:7:PRO:HD2	1:B:25:ASP:O	2.18	0.44
1:B:46:ARG:HA	1:B:55:VAL:HG21	2.00	0.44
1:A:78:ILE:HG21	1:D:78:ILE:HG13	1.99	0.44
1:D:7:PRO:HD2	1:D:25:ASP:O	2.17	0.44
1:G:223:ASP:HB3	1:G:226:LEU:HD12	2.00	0.43
1:H:54:LEU:HD13	1:H:83:TYR:CE1	2.52	0.43
1:H:12:GLU:OE1	1:H:208:ARG:NH2	2.51	0.43
1:H:223:ASP:HB3	1:H:226:LEU:HD12	2.01	0.43
1:G:208:ARG:NH1	1:G:217:ARG:O	2.52	0.43
1:B:54:LEU:HD13	1:B:83:TYR:CE1	2.54	0.42
1:E:135:ILE:HA	3:E:409:HOH:O	2.19	0.42
1:H:10:VAL:HG13	1:H:48:VAL:HG11	2.01	0.42
1:B:116:ILE:HG23	1:B:146:ASP:HB2	2.01	0.42
1:F:46:ARG:HD3	1:F:46:ARG:C	2.39	0.42
1:B:207:VAL:HG21	1:B:230:LEU:HD13	2.02	0.42
1:I:54:LEU:HD13	1:I:83:TYR:CE1	2.54	0.42
1:D:46:ARG:HA	1:D:55:VAL:HG21	2.02	0.42
1:F:10:VAL:HG13	1:F:48:VAL:HG11	2.02	0.42
1:C:223:ASP:HB3	1:C:226:LEU:HD12	2.03	0.41
1:E:46:ARG:HD3	1:E:46:ARG:C	2.39	0.41
1:A:194:ILE:HD11	1:A:230:LEU:HD22	2.03	0.41
1:A:78:ILE:HG13	1:D:78:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:PHE:HZ	1:B:197:LEU:HD13	1.85	0.41
1:A:2:ILE:HG23	1:A:22:ASP:HB2	2.03	0.41
1:F:11:GLU:HG3	1:F:221:ARG:HH21	1.85	0.41
1:A:113:GLU:HG3	1:F:218:ASN:HB2	2.03	0.40
1:A:46:ARG:HA	1:A:55:VAL:HG21	2.02	0.40
1:C:46:ARG:HD3	1:C:46:ARG:C	2.40	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	239/242 (99%)	235 (98%)	4 (2%)	0	100	100
1	B	240/242 (99%)	235 (98%)	5 (2%)	0	100	100
1	C	234/242 (97%)	230 (98%)	4 (2%)	0	100	100
1	D	240/242 (99%)	236 (98%)	4 (2%)	0	100	100
1	E	234/242 (97%)	230 (98%)	4 (2%)	0	100	100
1	F	236/242 (98%)	233 (99%)	3 (1%)	0	100	100
1	G	234/242 (97%)	231 (99%)	3 (1%)	0	100	100
1	H	225/242 (93%)	223 (99%)	2 (1%)	0	100	100
1	I	234/242 (97%)	230 (98%)	3 (1%)	1 (0%)	43	61
All	All	2116/2178 (97%)	2083 (98%)	32 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	213	LYS

### 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	188/191 (98%)	183 (97%)	5 (3%)	57	78
1	B	190/191 (100%)	185 (97%)	5 (3%)	59	79
1	C	185/191 (97%)	179 (97%)	6 (3%)	51	72
1	D	190/191 (100%)	183 (96%)	7 (4%)	45	66
1	E	183/191 (96%)	178 (97%)	5 (3%)	57	78
1	F	185/191 (97%)	178 (96%)	7 (4%)	44	65
1	G	185/191 (97%)	178 (96%)	7 (4%)	44	65
1	H	180/191 (94%)	178 (99%)	2 (1%)	84	94
1	I	185/191 (97%)	178 (96%)	7 (4%)	44	65
All	All	1671/1719 (97%)	1620 (97%)	51 (3%)	52	74

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	48	VAL
1	A	51	LYS
1	A	213	LYS
1	A	216	ASP
1	B	46	ARG
1	B	47	GLU
1	B	48	VAL
1	B	197	LEU
1	B	225	GLU
1	C	46	ARG
1	C	47	GLU
1	C	48	VAL
1	C	198	LYS
1	C	216	ASP
1	C	218	ASN
1	D	46	ARG
1	D	47	GLU
1	D	48	VAL

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Mol	Chain	Res	Type
1	D	217	ARG
1	D	218	ASN
1	D	219	ASN
1	D	225	GLU
1	E	46	ARG
1	E	47	GLU
1	E	48	VAL
1	E	167	GLU
1	E	208	ARG
1	F	0	HIS
1	F	11	GLU
1	F	46	ARG
1	F	47	GLU
1	F	48	VAL
1	F	198	LYS
1	F	225	GLU
1	G	46	ARG
1	G	47	GLU
1	G	48	VAL
1	G	159	THR
1	G	198	LYS
1	G	213	LYS
1	G	225	GLU
1	H	46	ARG
1	H	48	VAL
1	I	46	ARG
1	I	47	GLU
1	I	48	VAL
1	I	208	ARG
1	I	216	ASP
1	I	218	ASN
1	I	225	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	C	219	ASN
1	D	-4	HIS
1	D	-1	HIS
1	F	218	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 ⓘ

6 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	PO4	B	301	-	4,4,4	2.18	1 (25%)	6,6,6	0.33	0
2	PO4	C	301	-	4,4,4	1.11	0	6,6,6	0.31	0
2	PO4	D	301	-	4,4,4	1.27	1 (25%)	6,6,6	0.31	0
2	PO4	E	301	-	4,4,4	0.93	0	6,6,6	0.28	0
2	PO4	F	301	-	4,4,4	0.98	0	6,6,6	0.28	0
2	PO4	I	301	-	4,4,4	0.87	0	6,6,6	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	301	-	-	0/0/0/0	0/0/0/0
2	PO4	C	301	-	-	0/0/0/0	0/0/0/0
2	PO4	D	301	-	-	0/0/0/0	0/0/0/0
2	PO4	E	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	F	301	-	-	0/0/0/0	0/0/0/0
2	PO4	I	301	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PO4	P-O4	4.12	1.69	1.52
2	D	301	PO4	P-O4	2.14	1.61	1.52

There are no bond angle outliers.

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	241/242 (99%)	0.16	3 (1%) 75 75	49, 61, 102, 158	0
1	B	242/242 (100%)	0.02	0 100 100	55, 73, 99, 122	0
1	C	236/242 (97%)	0.11	1 (0%) 90 90	52, 83, 139, 160	0
1	D	242/242 (100%)	-0.02	5 (2%) 60 58	52, 85, 145, 167	0
1	E	236/242 (97%)	0.27	7 (2%) 48 45	62, 96, 163, 189	0
1	F	238/242 (98%)	0.18	3 (1%) 74 73	63, 95, 137, 163	0
1	G	236/242 (97%)	0.37	18 (7%) 14 12	76, 113, 164, 179	0
1	H	229/242 (94%)	1.18	49 (21%) 1 1	102, 140, 187, 201	0
1	I	236/242 (97%)	0.98	37 (15%) 3 2	102, 147, 185, 206	0
All	All	2136/2178 (98%)	0.35	123 (5%) 22 20	49, 96, 167, 206	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	230	LEU	7.6
1	H	211	ALA	7.1
1	H	191	LYS	6.8
1	I	24	ILE	6.5
1	H	210	ALA	6.4
1	I	83	TYR	6.2
1	G	230	LEU	6.0
1	H	189	ILE	5.8
1	I	214	GLY	5.7
1	I	54	LEU	5.5
1	H	84	ILE	5.5
1	I	108	VAL	5.2
1	H	222	ILE	5.2
1	H	11	GLU	5.1
1	H	53	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	H	10	VAL	5.0
1	A	218	ASN	4.7
1	I	5	VAL	4.4
1	I	55	VAL	4.4
1	I	53	LEU	4.2
1	H	36	ALA	4.2
1	G	226	LEU	4.2
1	I	3	LEU	4.2
1	I	215	GLY	4.1
1	E	217	ARG	4.1
1	H	54	LEU	4.1
1	H	55	VAL	4.1
1	I	2	ILE	4.0
1	G	83	TYR	4.0
1	I	45	ILE	4.0
1	E	218	ASN	3.9
1	I	230	LEU	3.9
1	H	4	LEU	3.8
1	I	116	ILE	3.8
1	G	234	CYS	3.8
1	G	197	LEU	3.7
1	A	219	ASN	3.7
1	H	24	ILE	3.5
1	H	148	ALA	3.5
1	I	79	SER	3.4
1	H	37	ASN	3.4
1	H	207	VAL	3.4
1	F	214	GLY	3.3
1	H	200	ILE	3.3
1	F	216	ASP	3.2
1	H	206	GLY	3.2
1	G	189	ILE	3.2
1	H	118	VAL	3.2
1	F	215	GLY	3.1
1	I	139	ILE	3.1
1	G	3	LEU	3.1
1	H	83	TYR	3.0
1	I	4	LEU	3.0
1	H	18	ALA	3.0
1	H	23	ILE	3.0
1	I	100	LEU	3.0
1	G	200	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	116	ILE	2.9
1	H	117	VAL	2.9
1	H	194	ILE	2.9
1	H	12	GLU	2.9
1	I	14	LYS	2.9
1	G	183	CYS	2.9
1	G	193	HIS	2.8
1	H	16	ALA	2.8
1	H	21	ALA	2.8
1	H	88	LEU	2.8
1	I	77	ALA	2.8
1	I	23	ILE	2.8
1	I	104	VAL	2.8
1	I	16	ALA	2.7
1	H	87	GLY	2.7
1	D	218	ASN	2.7
1	A	211	ALA	2.6
1	H	86	VAL	2.6
1	H	119	ALA	2.6
1	H	228	LYS	2.6
1	E	21	ALA	2.5
1	D	213	LYS	2.5
1	H	57	ALA	2.5
1	H	105	VAL	2.5
1	G	172	PHE	2.5
1	I	114	ASN	2.5
1	G	8	ILE	2.5
1	I	88	LEU	2.5
1	I	41	MET	2.5
1	H	168	ILE	2.4
1	I	147	VAL	2.4
1	E	233	LEU	2.4
1	D	83	TYR	2.3
1	D	54	LEU	2.3
1	E	220	GLY	2.3
1	G	185	LEU	2.3
1	H	77	ALA	2.2
1	I	205	VAL	2.2
1	H	42	ILE	2.2
1	H	235	LYS	2.2
1	C	235	LYS	2.2
1	G	190	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	163	PHE	2.2
1	H	208	ARG	2.2
1	I	111	ILE	2.2
1	I	10	VAL	2.2
1	H	1	MET	2.1
1	H	147	VAL	2.1
1	E	227	VAL	2.1
1	H	73	ALA	2.1
1	I	213	LYS	2.1
1	H	151	ASP	2.1
1	I	21	ALA	2.1
1	G	34	LEU	2.1
1	G	150	LEU	2.1
1	I	207	VAL	2.1
1	I	80	GLY	2.1
1	E	1	MET	2.1
1	I	97	ALA	2.0
1	D	217	ARG	2.0
1	G	148	ALA	2.0
1	G	45	ILE	2.0
1	H	204	ILE	2.0
1	I	137	PRO	2.0
1	H	5	VAL	2.0
1	I	173	VAL	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	F	301	5/5	0.22	3.93	149,152,153,154	0
2	PO4	C	301	5/5	0.15	0.03	115,115,117,122	0
2	PO4	D	301	5/5	0.15	-0.12	110,112,113,115	0
2	PO4	I	301	5/5	0.13	-0.64	168,169,169,170	0
2	PO4	E	301	5/5	0.14	-0.83	142,143,144,145	0
2	PO4	B	301	5/5	0.12	-1.34	60,79,83,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.