



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 09:07 pm GMT

PDB ID : 4RC1
Title : Structure of the methanofuran/methanopterin biosynthetic 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

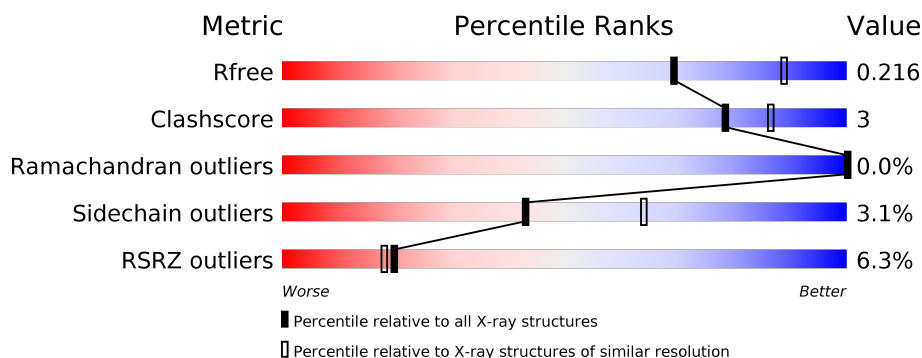
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (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 ≥ 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	242	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	242	<div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	C	242	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	D	242	<div> <div></div> <div>90%</div> <div>10%</div> <div>•</div> </div>
1	E	242	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>
1	F	242	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	242	<div><div></div><div>11%</div><div>88%</div><div>9% • •</div></div>
1	H	242	<div><div></div><div>22%</div><div>85%</div><div>9% • 5%</div></div>
1	I	242	<div><div></div><div>18%</div><div>88%</div><div>8% • •</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16231 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 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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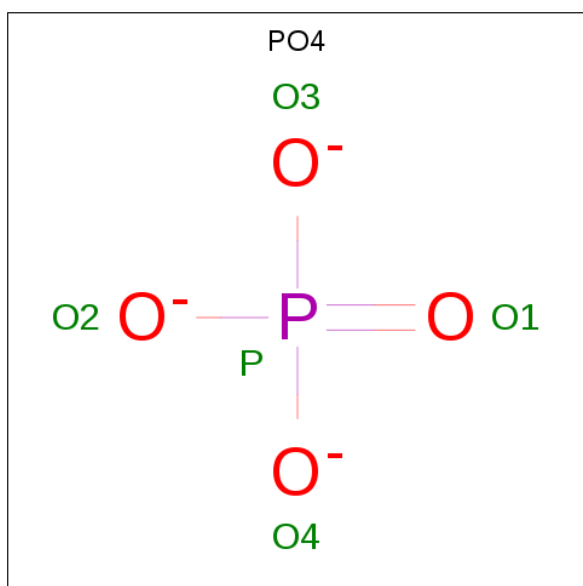
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q58499
B	-1	HIS	-	EXPRESSION TAG	UNP Q58499
B	0	HIS	-	EXPRESSION TAG	UNP Q58499
C	-6	MET	-	EXPRESSION TAG	UNP Q58499
C	-5	HIS	-	EXPRESSION TAG	UNP Q58499
C	-4	HIS	-	EXPRESSION TAG	UNP Q58499
C	-3	HIS	-	EXPRESSION TAG	UNP Q58499
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: O₄P).



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

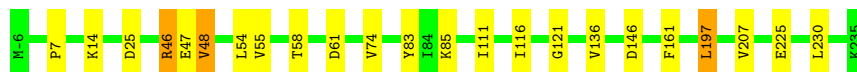
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



- Molecule 1: UPF0264 protein MJ1099



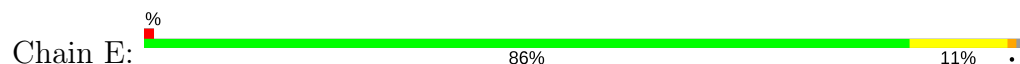
- Molecule 1: UPF0264 protein MJ1099



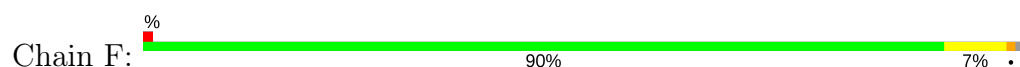
- Molecule 1: UPF0264 protein MJ1099



- Molecule 1: UPF0264 protein MJ1099



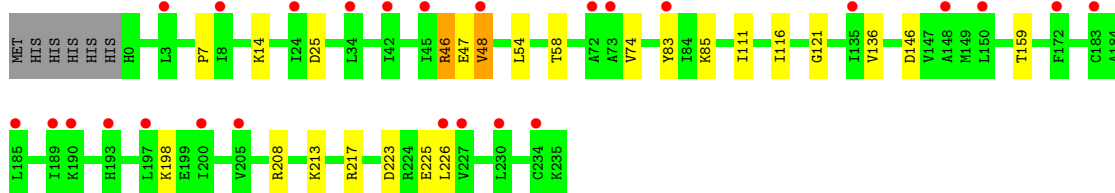
- Molecule 1: UPF0264 protein MJ1099





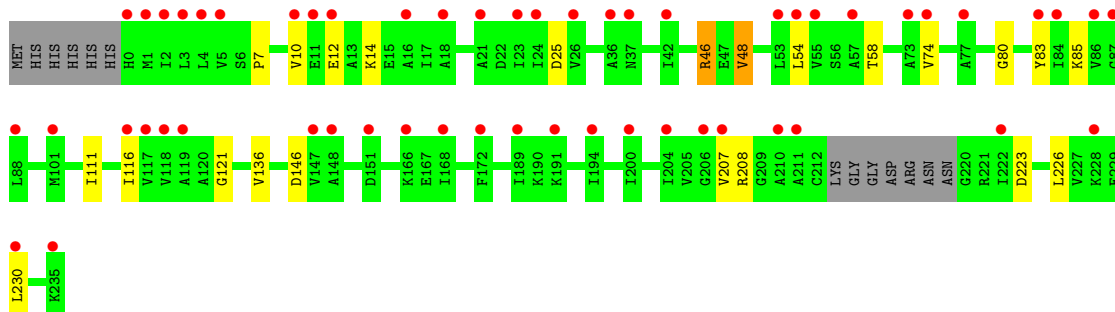
- Molecule 1: UPF0264 protein MJ1099

Chain G: 11% 88% 9% ..



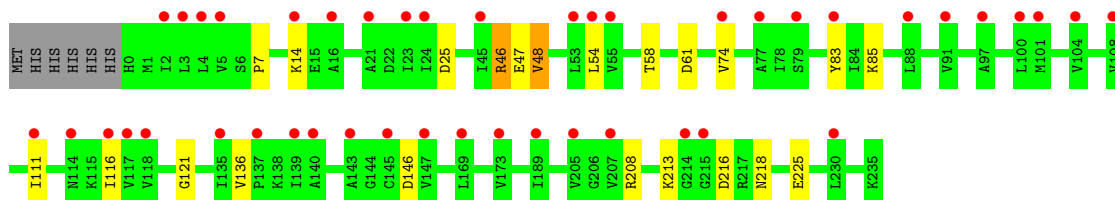
- Molecule 1: UPF0264 protein MJ1099

Chain H: 22% 85% 9% • 5%



- Molecule 1: UPF0264 protein MJ1099

Chain I: 18% 88% 8% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.5 (65.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.40Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.193 , 0.210 0.197 , 0.216	Depositor DCC
R_{free} test set	5118 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16231	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 (101) 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: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
1:D:58:THR:HG22	1:D:85:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG13	1:D:78:ILE:HG21	2.01	0.41
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 [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	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%)	36	51
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%)	48	68
1	B	190/191 (100%)	185 (97%)	5 (3%)	49	70
1	C	185/191 (97%)	179 (97%)	6 (3%)	42	62
1	D	190/191 (100%)	183 (96%)	7 (4%)	37	56
1	E	183/191 (96%)	178 (97%)	5 (3%)	48	68
1	F	185/191 (97%)	178 (96%)	7 (4%)	36	55
1	G	185/191 (97%)	178 (96%)	7 (4%)	36	55
1	H	180/191 (94%)	178 (99%)	2 (1%)	76	88
1	I	185/191 (97%)	178 (96%)	7 (4%)	36	55
All	All	1671/1719 (97%)	1620 (97%)	51 (3%)	43	64

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

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Mol	Chain	Res	Type
1	D	48	VAL
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	2.49	2 (50%)	6,6,6	1.21	0
2	PO4	C	301	-	4,4,4	1.38	1 (25%)	6,6,6	0.98	0
2	PO4	D	301	-	4,4,4	1.54	1 (25%)	6,6,6	0.94	0
2	PO4	E	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.39	0
2	PO4	F	301	-	4,4,4	1.48	1 (25%)	6,6,6	0.42	0
2	PO4	I	301	-	4,4,4	1.36	1 (25%)	6,6,6	0.39	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	E	301	-	-	0/0/0/0	0/0/0/0
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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	PO4	P-O1	2.22	1.55	1.50
2	D	301	PO4	P-O1	2.29	1.55	1.50
2	I	301	PO4	P-O1	2.53	1.56	1.50
2	B	301	PO4	P-O1	2.69	1.56	1.50
2	F	301	PO4	P-O1	2.73	1.56	1.50
2	E	301	PO4	P-O1	2.96	1.57	1.50
2	B	301	PO4	P-O4	4.15	1.69	1.54

There are no bond angle outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/242 (99%)	0.39	3 (1%) 79 77	49, 61, 102, 158	0
1	B	242/242 (100%)	-0.01	0 100 100	55, 73, 99, 122	0
1	C	236/242 (97%)	0.13	2 (0%) 86 84	52, 83, 139, 160	0
1	D	242/242 (100%)	0.03	1 (0%) 92 91	52, 85, 145, 167	0
1	E	236/242 (97%)	0.21	3 (1%) 77 75	62, 96, 163, 189	0
1	F	238/242 (98%)	0.20	2 (0%) 86 84	63, 95, 137, 163	0
1	G	236/242 (97%)	0.54	26 (11%) 5 5	76, 113, 164, 179	0
1	H	229/242 (94%)	1.25	54 (23%) 0 0	102, 140, 187, 201	0
1	I	236/242 (97%)	0.97	44 (18%) 1 1	102, 147, 185, 206	0
All	All	2136/2178 (98%)	0.41	135 (6%) 20 18	49, 96, 167, 206	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	191	LYS	7.2
1	H	211	ALA	7.0
1	H	230	LEU	6.7
1	H	210	ALA	6.6
1	I	24	ILE	6.4
1	I	83	TYR	6.2
1	I	54	LEU	6.1
1	H	84	ILE	6.1
1	H	10	VAL	5.9
1	I	108	VAL	5.8
1	H	189	ILE	5.8
1	I	214	GLY	5.7
1	G	230	LEU	5.5
1	H	36	ALA	5.5
1	H	53	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	189	ILE	5.2
1	I	215	GLY	4.9
1	H	11	GLU	4.7
1	I	55	VAL	4.7
1	H	200	ILE	4.7
1	H	55	VAL	4.6
1	A	218	ASN	4.6
1	H	37	ASN	4.6
1	G	197	LEU	4.6
1	G	200	ILE	4.5
1	H	4	LEU	4.4
1	G	226	LEU	4.4
1	I	116	ILE	4.3
1	I	3	LEU	4.1
1	H	54	LEU	4.1
1	H	21	ALA	4.1
1	H	222	ILE	4.0
1	I	2	ILE	4.0
1	I	5	VAL	4.0
1	G	83	TYR	3.9
1	H	24	ILE	3.9
1	I	53	LEU	3.8
1	G	185	LEU	3.8
1	H	116	ILE	3.8
1	G	172	PHE	3.7
1	G	193	HIS	3.7
1	I	139	ILE	3.7
1	A	219	ASN	3.7
1	G	3	LEU	3.6
1	H	148	ALA	3.6
1	G	234	CYS	3.5
1	G	150	LEU	3.5
1	H	23	ILE	3.4
1	H	88	LEU	3.4
1	H	207	VAL	3.4
1	H	118	VAL	3.3
1	I	230	LEU	3.3
1	I	79	SER	3.3
1	H	16	ALA	3.2
1	I	104	VAL	3.2
1	E	217	ARG	3.1
1	A	211	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	87	GLY	3.1
1	H	42	ILE	3.1
1	G	72	ALA	3.1
1	G	190	LYS	3.0
1	G	183	CYS	3.0
1	G	135	ILE	3.0
1	H	117	VAL	2.9
1	I	117	VAL	2.9
1	G	73	ALA	2.9
1	I	88	LEU	2.9
1	H	83	TYR	2.9
1	I	97	ALA	2.8
1	H	168	ILE	2.8
1	I	140	ALA	2.8
1	C	235	LYS	2.7
1	I	100	LEU	2.7
1	G	8	ILE	2.7
1	I	23	ILE	2.7
1	I	143	ALA	2.7
1	G	148	ALA	2.6
1	I	114	ASN	2.6
1	I	147	VAL	2.6
1	H	1	MET	2.6
1	I	135	ILE	2.6
1	H	57	ALA	2.6
1	H	204	ILE	2.6
1	H	119	ALA	2.5
1	I	16	ALA	2.5
1	G	42	ILE	2.5
1	H	12	GLU	2.5
1	I	4	LEU	2.5
1	H	2	ILE	2.5
1	H	77	ALA	2.5
1	I	45	ILE	2.5
1	I	21	ALA	2.5
1	G	45	ILE	2.5
1	I	137	PRO	2.5
1	I	74	VAL	2.5
1	H	228	LYS	2.5
1	F	215	GLY	2.4
1	H	0	HIS	2.4
1	H	26	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	206	GLY	2.4
1	H	18	ALA	2.4
1	H	73	ALA	2.4
1	I	77	ALA	2.3
1	H	235	LYS	2.3
1	E	227	VAL	2.3
1	I	118	VAL	2.3
1	I	169	LEU	2.3
1	G	24	ILE	2.3
1	H	5	VAL	2.3
1	E	218	ASN	2.3
1	I	189	ILE	2.3
1	F	140	ALA	2.3
1	G	48	VAL	2.3
1	I	205	VAL	2.3
1	I	111	ILE	2.2
1	H	74	VAL	2.2
1	H	172	PHE	2.2
1	G	34	LEU	2.2
1	C	217	ARG	2.2
1	G	205	VAL	2.2
1	H	166	LYS	2.2
1	H	194	ILE	2.2
1	H	86	VAL	2.1
1	I	91	VAL	2.1
1	H	3	LEU	2.1
1	H	147	VAL	2.1
1	H	151	ASP	2.1
1	I	101	MET	2.1
1	I	14	LYS	2.1
1	D	54	LEU	2.1
1	I	207	VAL	2.0
1	G	227	VAL	2.0
1	H	101	MET	2.0
1	I	145	CYS	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 [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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	F	301	5/5	0.74	0.22	149,152,153,154	0
2	PO4	I	301	5/5	0.81	0.15	168,169,169,170	0
2	PO4	D	301	5/5	0.83	0.16	110,112,113,115	0
2	PO4	C	301	5/5	0.83	0.16	115,115,117,122	0
2	PO4	E	301	5/5	0.87	0.12	142,143,144,145	0
2	PO4	B	301	5/5	0.95	0.11	60,79,83,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.