



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:17 PM UTC

PDB ID : 7OJS / pdb\_00007ojs  
Title : Complex structure 2 of the Bacillus subtilis CdaA c-di-AMP cyclase domain (CdaACD) and the phosphoglucomutase GlmM short variant (GlmMF369)  
Authors : Pathania, M.; Grundling, A.G.; Freemont, P.  
Deposited on : 2021-05-17  
Resolution : 4.20 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

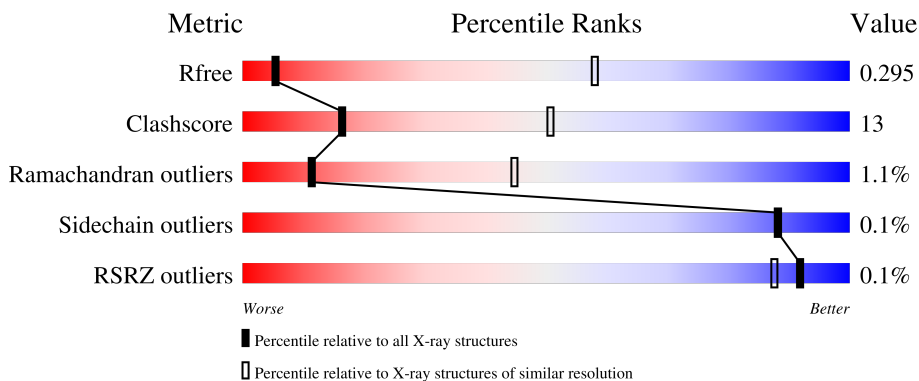
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	369	
1	B	369	
1	C	369	
1	F	369	
1	G	369	

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Mol	Chain	Length	Quality of chain
1	J	369	 77% 23%
2	D	167	 65% 22% • 13%
2	E	167	 65% 21% • 13%
2	H	167	 59% 27% • 13%
2	I	167	 60% 26% • 13%
2	K	167	 62% 24% • 13%
2	L	167	 60% 25% • 13%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23208 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 Phosphoglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	368	2762	1731	464	553	14	0	1	0
1	F	368	2762	1731	464	553	14	0	1	0
1	A	368	2762	1731	464	553	14	3	1	0
1	B	368	2762	1731	464	553	14	0	1	0
1	G	368	2762	1731	464	553	14	0	1	0
1	J	368	2762	1731	464	553	14	3	1	0

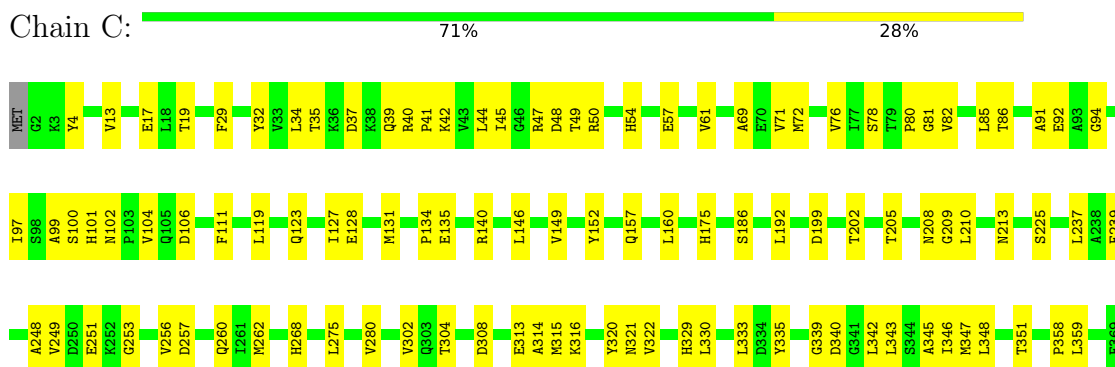
- Molecule 2 is a protein called Cyclic di-AMP synthase CdaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	146	1106	692	187	222	5	121	0	0
2	I	146	1106	692	187	222	5	121	0	0
2	D	146	1106	692	187	222	5	121	0	0
2	E	146	1106	692	187	222	5	121	0	0
2	K	146	1106	692	187	222	5	121	0	0
2	L	146	1106	692	187	222	5	121	0	0

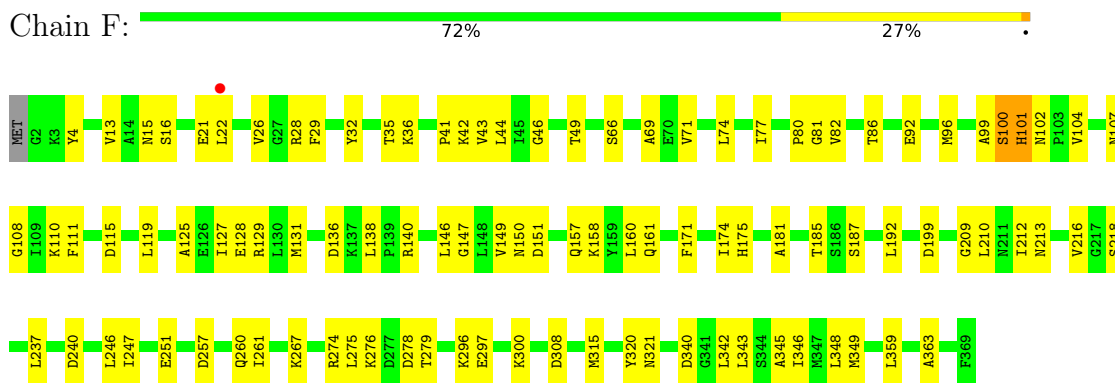
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

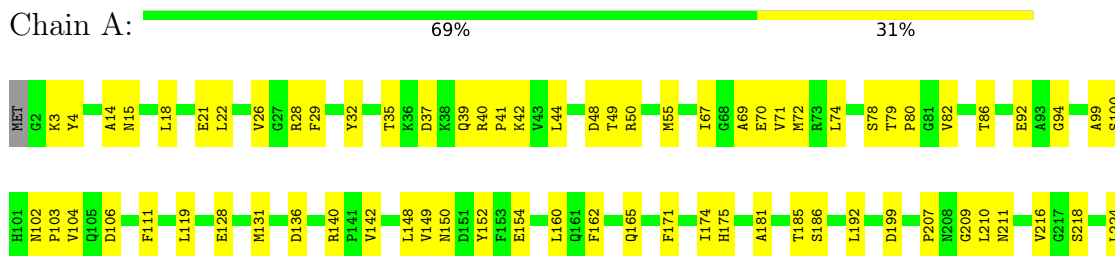
- Molecule 1: Phosphoglucosamine mutase

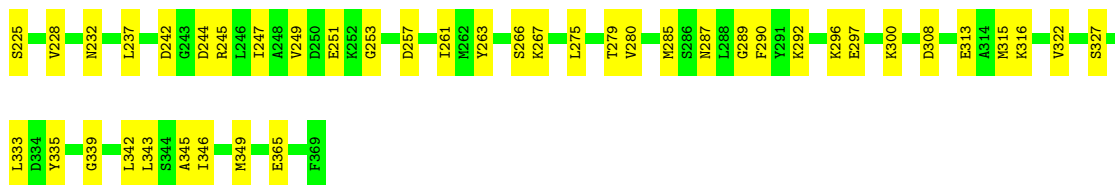


- Molecule 1: Phosphoglucosamine mutase



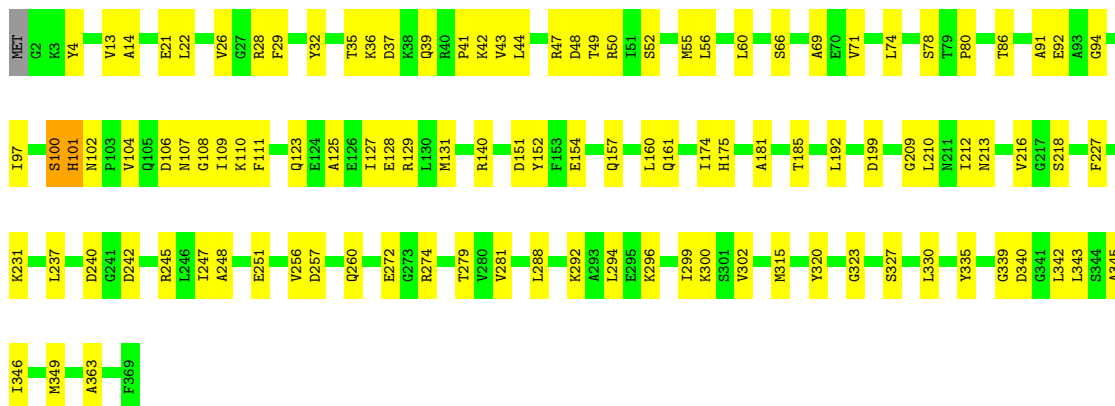
- Molecule 1: Phosphoglucosamine mutase





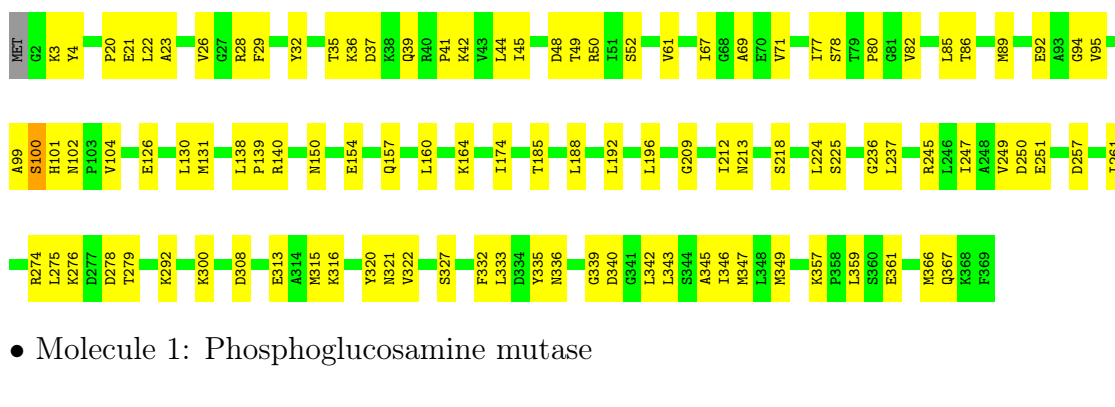
- Molecule 1: Phosphoglucosamine mutase

Chain B: 70% 29%



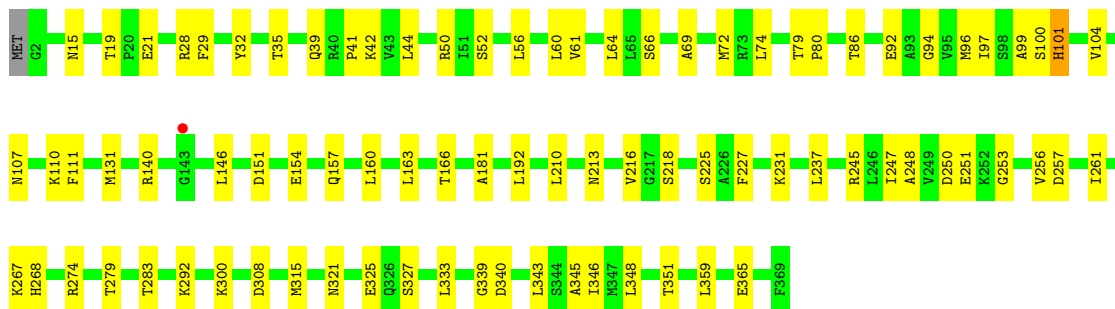
- Molecule 1: Phosphoglucosamine mutase

Chain G: 72% 28%

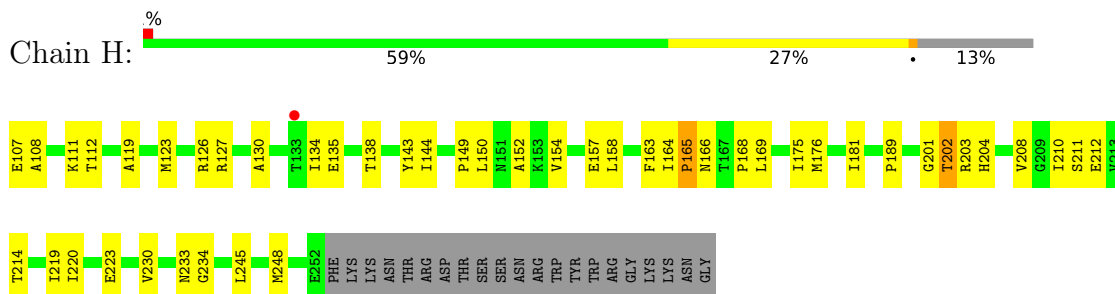


- Molecule 1: Phosphoglucosamine mutase

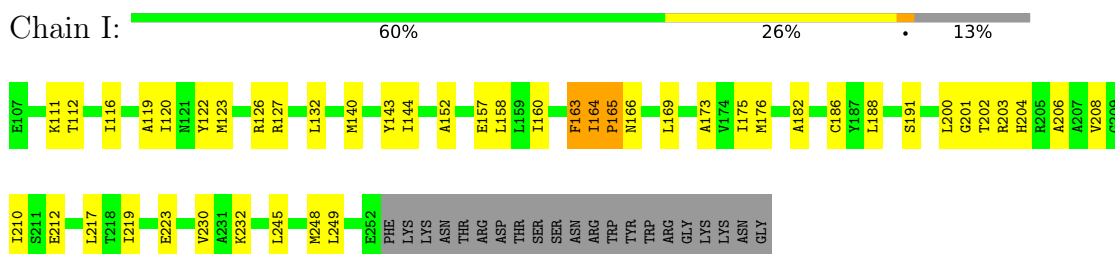
Chain J: 77% 23%



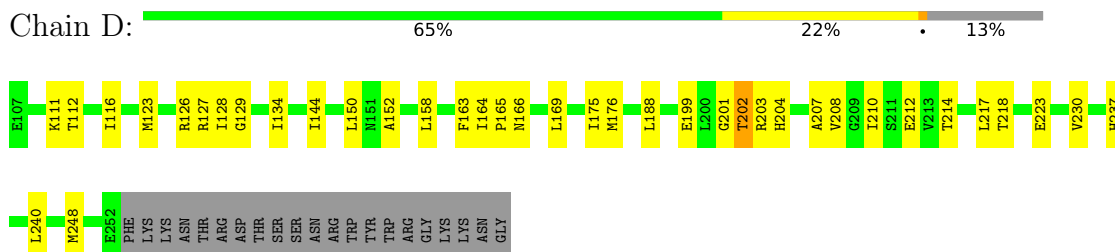
- Molecule 2: Cyclic di-AMP synthase CdaA



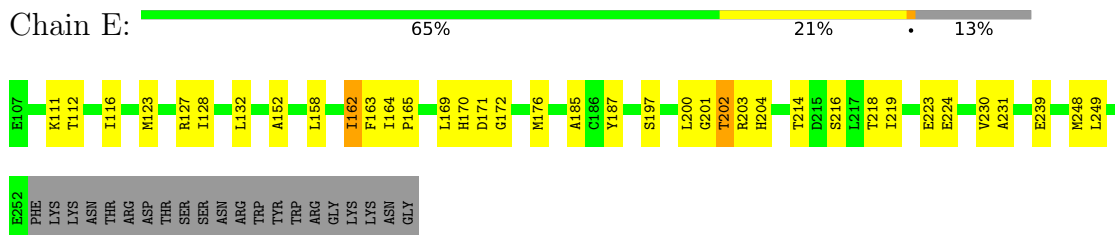
- Molecule 2: Cyclic di-AMP synthase CdaA



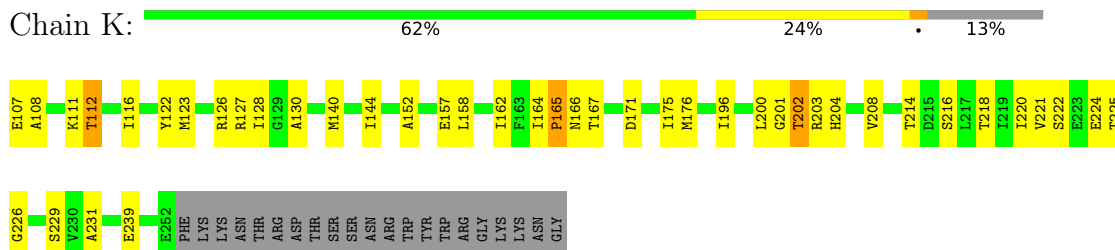
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- Molecule 2: Cyclic di-AMP synthase CdaA

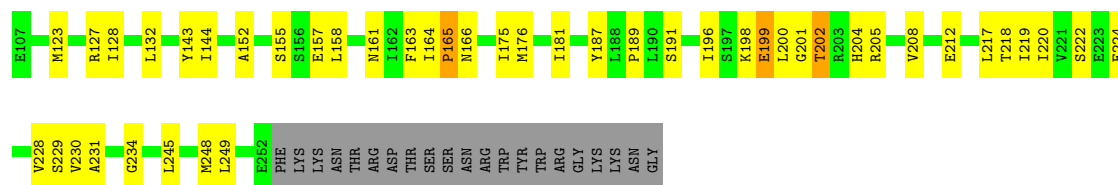


- Molecule 2: Cyclic di-AMP synthase CdaA



- Molecule 2: Cyclic di-AMP synthase CdaA

Chain L:  60% 25% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.80Å 228.54Å 153.19Å 90.00° 99.86° 90.00°	Depositor
Resolution (Å)	75.47 – 4.20 75.47 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (75.47-4.20) 99.2 (75.47-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 4.15Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.226 , 0.295 0.230 , 0.295	Depositor DCC
$R_{free}$ test set	1506 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.1	Xtrriage
Anisotropy	0.957	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 78.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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](#)

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	0.14	0/2806	0.38	0/3781
1	B	0.14	0/2806	0.36	0/3781
1	C	0.15	0/2806	0.39	0/3781
1	F	0.14	0/2806	0.38	0/3781
1	G	0.15	0/2806	0.39	0/3781
1	J	0.14	0/2806	0.36	0/3781
2	D	0.16	0/1118	0.47	0/1512
2	E	0.17	0/1118	0.47	0/1512
2	H	0.17	0/1118	0.48	0/1512
2	I	0.21	0/1118	0.56	3/1512 (0.2%)
2	K	0.22	0/1118	0.55	0/1512
2	L	0.18	0/1118	0.53	0/1512
All	All	0.16	0/23544	0.42	3/31758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	163	PHE	CA-C-N	-5.82	118.27	123.33
2	I	163	PHE	C-N-CA	-5.82	118.27	123.33
2	I	164	ILE	CB-CA-C	5.65	115.61	110.13

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	2762	0	2732	74	0
1	B	2762	0	2732	74	0
1	C	2762	0	2732	68	0
1	F	2762	0	2732	71	0
1	G	2762	0	2732	74	0
1	J	2762	0	2732	53	0
2	D	1106	0	1128	36	0
2	E	1106	0	1128	28	0
2	H	1106	0	1128	38	0
2	I	1106	0	1128	34	0
2	K	1106	0	1128	31	0
2	L	1106	0	1128	33	0
All	All	23208	0	23160	582	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 13.

The worst 5 of 582 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)
2:L:123:MET:HE1	2:L:163:PHE:HB2	1.58	0.85
2:D:123:MET:HE1	2:D:163:PHE:HB2	1.60	0.84
1:J:42:LYS:H	1:J:92:GLU:HG2	1.41	0.84
2:H:123:MET:HE1	2:H:163:PHE:HB2	1.60	0.83
1:J:41:PRO:HD2	1:J:69:ALA:HA	1.60	0.81

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	367/369 (100%)	342 (93%)	22 (6%)	3 (1%)	<b>16</b> 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	367/369 (100%)	347 (95%)	17 (5%)	3 (1%)	16	52
1	C	367/369 (100%)	339 (92%)	25 (7%)	3 (1%)	16	52
1	F	367/369 (100%)	343 (94%)	22 (6%)	2 (0%)	24	62
1	G	367/369 (100%)	340 (93%)	24 (6%)	3 (1%)	16	52
1	J	367/369 (100%)	344 (94%)	21 (6%)	2 (0%)	24	62
2	D	144/167 (86%)	128 (89%)	14 (10%)	2 (1%)	9	39
2	E	144/167 (86%)	122 (85%)	18 (12%)	4 (3%)	4	25
2	H	144/167 (86%)	128 (89%)	14 (10%)	2 (1%)	9	39
2	I	144/167 (86%)	129 (90%)	13 (9%)	2 (1%)	9	39
2	K	144/167 (86%)	126 (88%)	13 (9%)	5 (4%)	3	21
2	L	144/167 (86%)	127 (88%)	14 (10%)	3 (2%)	5	30
All	All	3066/3216 (95%)	2815 (92%)	217 (7%)	34 (1%)	11	45

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	100	SER
1	A	100	SER
1	B	100	SER
2	K	165	PRO
2	L	202	THR

### 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	294/294 (100%)	294 (100%)	0	100	100
1	B	294/294 (100%)	293 (100%)	1 (0%)	86	84
1	C	294/294 (100%)	294 (100%)	0	100	100
1	F	294/294 (100%)	294 (100%)	0	100	100
1	G	294/294 (100%)	294 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	294/294 (100%)	294 (100%)	0	100	100
2	D	120/139 (86%)	120 (100%)	0	100	100
2	E	120/139 (86%)	120 (100%)	0	100	100
2	H	120/139 (86%)	120 (100%)	0	100	100
2	I	120/139 (86%)	119 (99%)	1 (1%)	73	77
2	K	120/139 (86%)	120 (100%)	0	100	100
2	L	120/139 (86%)	120 (100%)	0	100	100
All	All	2484/2598 (96%)	2482 (100%)	2 (0%)	88	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	232	LYS
1	B	36	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	157	GLN
1	G	260	GLN
1	J	326	GLN
1	G	326	GLN
1	B	220	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	368/369 (99%)	-0.38	0 <a href="#">100</a> <a href="#">100</a>	64, 119, 150, 176	1 (0%)
1	B	368/369 (99%)	-0.40	0 <a href="#">100</a> <a href="#">100</a>	86, 135, 174, 192	1 (0%)
1	C	368/369 (99%)	-0.33	0 <a href="#">100</a> <a href="#">100</a>	68, 113, 149, 169	1 (0%)
1	F	368/369 (99%)	-0.38	1 (0%) <a href="#">90</a> <a href="#">80</a>	59, 102, 134, 158	1 (0%)
1	G	368/369 (99%)	-0.41	0 <a href="#">100</a> <a href="#">100</a>	83, 129, 156, 176	1 (0%)
1	J	368/369 (99%)	-0.38	1 (0%) <a href="#">90</a> <a href="#">80</a>	67, 118, 145, 164	1 (0%)
2	D	146/167 (87%)	-0.31	0 <a href="#">100</a> <a href="#">100</a>	38, 96, 134, 173	27 (18%)
2	E	146/167 (87%)	-0.18	0 <a href="#">100</a> <a href="#">100</a>	37, 96, 119, 150	27 (18%)
2	H	146/167 (87%)	-0.22	1 (0%) <a href="#">84</a> <a href="#">70</a>	36, 98, 133, 150	27 (18%)
2	I	146/167 (87%)	-0.24	0 <a href="#">100</a> <a href="#">100</a>	41, 104, 126, 144	27 (18%)
2	K	146/167 (87%)	-0.26	0 <a href="#">100</a> <a href="#">100</a>	32, 90, 111, 137	27 (18%)
2	L	146/167 (87%)	-0.30	0 <a href="#">100</a> <a href="#">100</a>	39, 91, 128, 147	27 (18%)
All	All	3084/3216 (95%)	-0.34	3 (0%) <a href="#">92</a> <a href="#">87</a>	32, 112, 153, 192	168 (5%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	143	GLY	2.6
2	H	133	THR	2.3
1	F	22	LEU	2.1

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.