



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 07:11 AM EDT

PDB ID : 4XVZ  
Title : MycF mycinamicin III 3'-O-methyltransferase in complex with Mg  
Authors : Akey, D.L.; Smith, J.L.  
Deposited on : 2015-01-28  
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

<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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

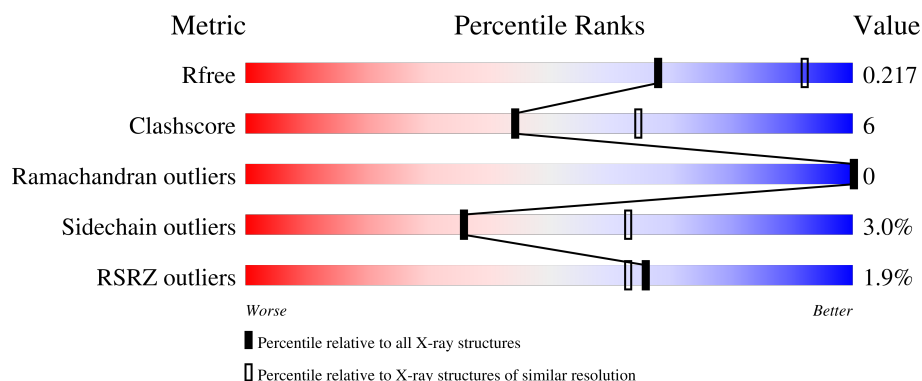
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	283	<div> <div>0%</div> <div> <div>59%</div> <div>11%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	283	<div> <div>0%</div> <div> <div>58%</div> <div>11%</div> <div>•</div> <div>30%</div> </div> </div>
1	C	283	<div> <div>0%</div> <div> <div>59%</div> <div>11%</div> <div>•</div> <div>28%</div> </div> </div>
1	D	283	<div> <div>2%</div> <div> <div>60%</div> <div>10%</div> <div>30%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	301	-	-	X	-
2	CL	C	301	-	-	X	-
2	CL	D	301	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6458 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 Mycinamicin III 3''-O-methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	Se	0	0	0
			1591	1005	285	291	5	5			
1	B	197	Total	C	N	O	S	Se	0	0	0
			1563	989	278	287	4	5			
1	C	203	Total	C	N	O	S	Se	0	0	0
			1600	1011	284	295	5	5			
1	D	199	Total	C	N	O	S	Se	0	0	0
			1561	989	272	291	4	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	initiating methionine	UNP Q49492
A	-21	HIS	-	expression tag	UNP Q49492
A	-20	HIS	-	expression tag	UNP Q49492
A	-19	HIS	-	expression tag	UNP Q49492
A	-18	HIS	-	expression tag	UNP Q49492
A	-17	HIS	-	expression tag	UNP Q49492
A	-16	HIS	-	expression tag	UNP Q49492
A	-15	SER	-	expression tag	UNP Q49492
A	-14	SER	-	expression tag	UNP Q49492
A	-13	GLY	-	expression tag	UNP Q49492
A	-12	VAL	-	expression tag	UNP Q49492
A	-11	ASP	-	expression tag	UNP Q49492
A	-10	LEU	-	expression tag	UNP Q49492
A	-9	GLY	-	expression tag	UNP Q49492
A	-8	THR	-	expression tag	UNP Q49492
A	-7	GLU	-	expression tag	UNP Q49492
A	-6	ASN	-	expression tag	UNP Q49492
A	-5	LEU	-	expression tag	UNP Q49492
A	-4	TYR	-	expression tag	UNP Q49492
A	-3	PHE	-	expression tag	UNP Q49492
A	-2	GLN	-	expression tag	UNP Q49492

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q49492
A	0	ASN	-	expression tag	UNP Q49492
A	1	ALA	-	expression tag	UNP Q49492
A	255	CYS	-	expression tag	UNP Q49492
A	256	ASN	-	expression tag	UNP Q49492
A	257	ILE	-	expression tag	UNP Q49492
A	258	GLY	-	expression tag	UNP Q49492
A	259	SER	-	expression tag	UNP Q49492
A	260	GLY	-	expression tag	UNP Q49492
B	-22	MSE	-	initiating methionine	UNP Q49492
B	-21	HIS	-	expression tag	UNP Q49492
B	-20	HIS	-	expression tag	UNP Q49492
B	-19	HIS	-	expression tag	UNP Q49492
B	-18	HIS	-	expression tag	UNP Q49492
B	-17	HIS	-	expression tag	UNP Q49492
B	-16	HIS	-	expression tag	UNP Q49492
B	-15	SER	-	expression tag	UNP Q49492
B	-14	SER	-	expression tag	UNP Q49492
B	-13	GLY	-	expression tag	UNP Q49492
B	-12	VAL	-	expression tag	UNP Q49492
B	-11	ASP	-	expression tag	UNP Q49492
B	-10	LEU	-	expression tag	UNP Q49492
B	-9	GLY	-	expression tag	UNP Q49492
B	-8	THR	-	expression tag	UNP Q49492
B	-7	GLU	-	expression tag	UNP Q49492
B	-6	ASN	-	expression tag	UNP Q49492
B	-5	LEU	-	expression tag	UNP Q49492
B	-4	TYR	-	expression tag	UNP Q49492
B	-3	PHE	-	expression tag	UNP Q49492
B	-2	GLN	-	expression tag	UNP Q49492
B	-1	SER	-	expression tag	UNP Q49492
B	0	ASN	-	expression tag	UNP Q49492
B	1	ALA	-	expression tag	UNP Q49492
B	255	CYS	-	expression tag	UNP Q49492
B	256	ASN	-	expression tag	UNP Q49492
B	257	ILE	-	expression tag	UNP Q49492
B	258	GLY	-	expression tag	UNP Q49492
B	259	SER	-	expression tag	UNP Q49492
B	260	GLY	-	expression tag	UNP Q49492
C	-22	MSE	-	initiating methionine	UNP Q49492
C	-21	HIS	-	expression tag	UNP Q49492
C	-20	HIS	-	expression tag	UNP Q49492

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	HIS	-	expression tag	UNP Q49492
C	-18	HIS	-	expression tag	UNP Q49492
C	-17	HIS	-	expression tag	UNP Q49492
C	-16	HIS	-	expression tag	UNP Q49492
C	-15	SER	-	expression tag	UNP Q49492
C	-14	SER	-	expression tag	UNP Q49492
C	-13	GLY	-	expression tag	UNP Q49492
C	-12	VAL	-	expression tag	UNP Q49492
C	-11	ASP	-	expression tag	UNP Q49492
C	-10	LEU	-	expression tag	UNP Q49492
C	-9	GLY	-	expression tag	UNP Q49492
C	-8	THR	-	expression tag	UNP Q49492
C	-7	GLU	-	expression tag	UNP Q49492
C	-6	ASN	-	expression tag	UNP Q49492
C	-5	LEU	-	expression tag	UNP Q49492
C	-4	TYR	-	expression tag	UNP Q49492
C	-3	PHE	-	expression tag	UNP Q49492
C	-2	GLN	-	expression tag	UNP Q49492
C	-1	SER	-	expression tag	UNP Q49492
C	0	ASN	-	expression tag	UNP Q49492
C	1	ALA	-	expression tag	UNP Q49492
C	255	CYS	-	expression tag	UNP Q49492
C	256	ASN	-	expression tag	UNP Q49492
C	257	ILE	-	expression tag	UNP Q49492
C	258	GLY	-	expression tag	UNP Q49492
C	259	SER	-	expression tag	UNP Q49492
C	260	GLY	-	expression tag	UNP Q49492
D	-22	MSE	-	initiating methionine	UNP Q49492
D	-21	HIS	-	expression tag	UNP Q49492
D	-20	HIS	-	expression tag	UNP Q49492
D	-19	HIS	-	expression tag	UNP Q49492
D	-18	HIS	-	expression tag	UNP Q49492
D	-17	HIS	-	expression tag	UNP Q49492
D	-16	HIS	-	expression tag	UNP Q49492
D	-15	SER	-	expression tag	UNP Q49492
D	-14	SER	-	expression tag	UNP Q49492
D	-13	GLY	-	expression tag	UNP Q49492
D	-12	VAL	-	expression tag	UNP Q49492
D	-11	ASP	-	expression tag	UNP Q49492
D	-10	LEU	-	expression tag	UNP Q49492
D	-9	GLY	-	expression tag	UNP Q49492
D	-8	THR	-	expression tag	UNP Q49492

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	GLU	-	expression tag	UNP Q49492
D	-6	ASN	-	expression tag	UNP Q49492
D	-5	LEU	-	expression tag	UNP Q49492
D	-4	TYR	-	expression tag	UNP Q49492
D	-3	PHE	-	expression tag	UNP Q49492
D	-2	GLN	-	expression tag	UNP Q49492
D	-1	SER	-	expression tag	UNP Q49492
D	0	ASN	-	expression tag	UNP Q49492
D	1	ALA	-	expression tag	UNP Q49492
D	255	CYS	-	expression tag	UNP Q49492
D	256	ASN	-	expression tag	UNP Q49492
D	257	ILE	-	expression tag	UNP Q49492
D	258	GLY	-	expression tag	UNP Q49492
D	259	SER	-	expression tag	UNP Q49492
D	260	GLY	-	expression tag	UNP Q49492

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is water.

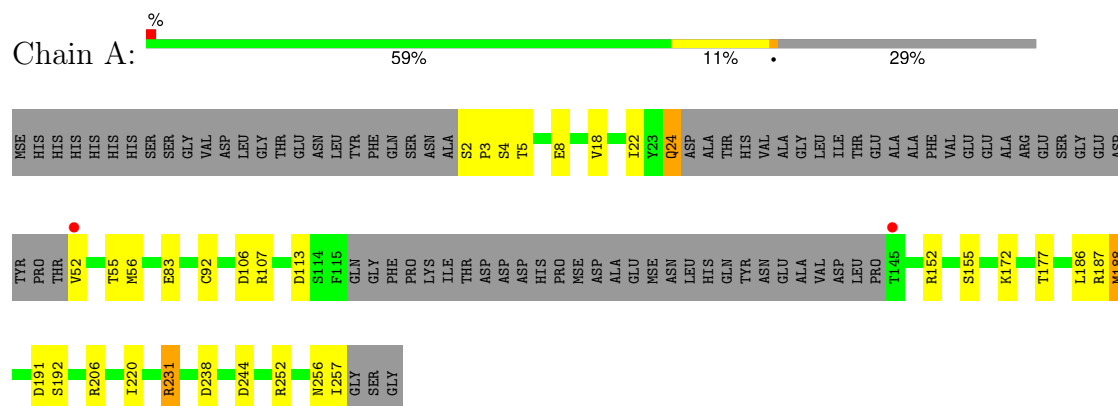
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	9	Total 9	O 9	0	0
4	C	53	Total 53	O 53	0	0
4	D	18	Total 18	O 18	0	0



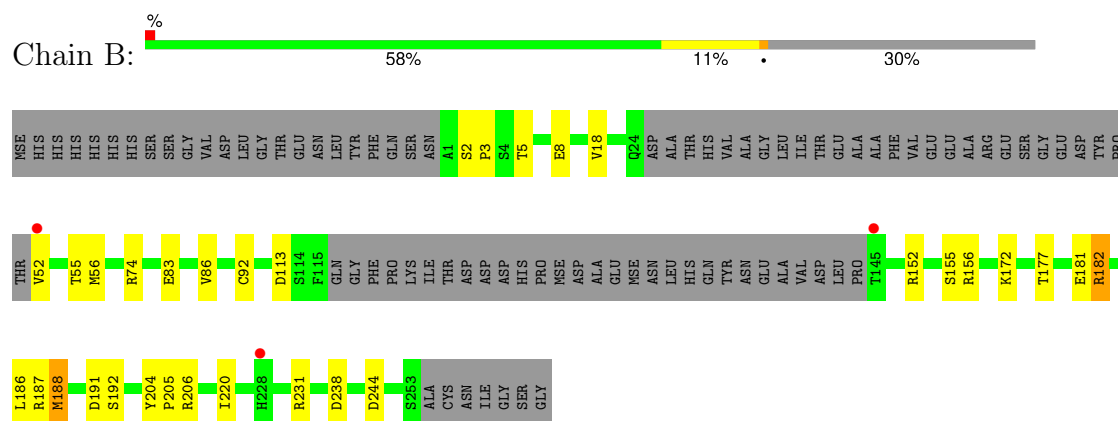
### 3 Residue-property plots [i](#)

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.

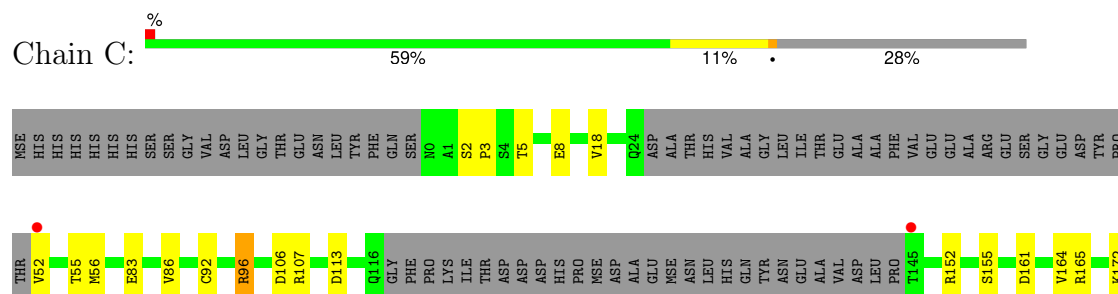
#### • Molecule 1: Mycinamicin III 3''-O-methyltransferase

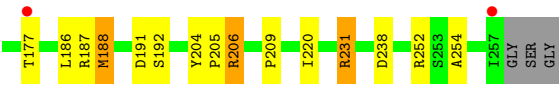


#### • Molecule 1: Mycinamicin III 3''-O-methyltransferase

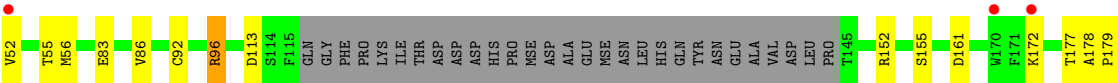


#### • Molecule 1: Mycinamicin III 3''-O-methyltransferase





● Molecule 1: Mycinamicin III 3''-O-methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.86Å 148.59Å 66.86Å 90.00° 120.23° 90.00°	Depositor
Resolution (Å)	45.60 – 2.49 45.60 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.60-2.49) 99.3 (45.60-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.178 , 0.217 0.178 , 0.217	Depositor DCC
$R_{free}$ test set	1811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.108 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

### 5.1 Standard geometry

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

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	0.86	0/1621	0.95	10/2188 (0.5%)
1	B	0.68	0/1593	0.89	5/2151 (0.2%)
1	C	0.94	0/1630	1.20	12/2202 (0.5%)
1	D	0.70	0/1591	0.95	6/2151 (0.3%)
All	All	0.80	0/6435	1.00	33/8692 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ARG	NE-CZ-NH2	-22.45	109.07	120.30
1	C	206	ARG	NE-CZ-NH1	21.93	131.26	120.30
1	C	96	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	D	96	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	D	96	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	C	96	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	C	231	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	C	231	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	A	231	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	C	188	MSE	CA-CB-CG	-6.62	102.05	113.30
1	D	206	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	56	MSE	CA-CB-CG	-6.25	102.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	188	MSE	CA-CB-CG	-5.87	103.32	113.30
1	B	206	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	206	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	188	MSE	CA-CB-CG	-5.75	103.53	113.30
1	B	56	MSE	CA-CB-CG	-5.66	103.68	113.30
1	D	56	MSE	CA-CB-CG	-5.56	103.85	113.30
1	D	206	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	C	107	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	206	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	A	231	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	56	MSE	CA-CB-CG	-5.41	104.11	113.30
1	A	107	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	106	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	188	MSE	CA-CB-CG	-5.12	104.60	113.30
1	B	244	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	244	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	206	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	C	106	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	252	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	96	ARG	CD-NE-CZ	5.02	130.62	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	25	ASP	Peptide

## 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	1591	0	1552	19	0
1	B	1563	0	1522	16	0
1	C	1600	0	1552	24	0
1	D	1561	0	1501	15	0
2	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	2	0
2	C	1	0	0	2	0
2	D	1	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	55	0	0	2	0
4	B	9	0	0	0	0
4	C	53	0	0	5	0
4	D	18	0	0	2	0
All	All	6458	0	6127	73	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 6.

All (73) 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:A:113:ASP:OD2	2:A:301:CL:CL	2.33	0.83
1:B:113:ASP:OD2	2:B:301:CL:CL	2.43	0.72
1:A:83:GLU:OE2	1:A:187:ARG:NH1	2.23	0.70
1:C:83:GLU:OE2	1:C:187:ARG:NH1	2.24	0.70
1:B:86:VAL:O	2:B:301:CL:CL	2.46	0.70
1:C:113:ASP:OD2	2:C:301:CL:CL	2.47	0.70
1:D:83:GLU:OE2	1:D:187:ARG:NH1	2.22	0.69
1:C:206:ARG:HD3	4:C:420:HOH:O	1.94	0.68
1:B:83:GLU:OE2	1:B:187:ARG:NH1	2.23	0.66
1:D:86:VAL:O	2:D:301:CL:CL	2.51	0.65
1:C:231:ARG:NH1	1:C:238:ASP:O	2.30	0.65
1:B:231:ARG:NH1	1:B:238:ASP:O	2.30	0.65
1:C:206:ARG:CD	4:C:420:HOH:O	2.45	0.64
1:D:231:ARG:NH1	1:D:238:ASP:O	2.30	0.64
1:A:5:THR:HG23	1:A:8:GLU:H	1.63	0.63
1:B:5:THR:HG23	1:B:8:GLU:H	1.64	0.62
1:A:231:ARG:NH1	1:A:238:ASP:O	2.32	0.62
1:C:5:THR:HG23	1:C:8:GLU:H	1.66	0.61
1:A:24:GLN:CA	1:A:24:GLN:OE1	2.49	0.61
1:C:231:ARG:HD3	4:C:405:HOH:O	2.01	0.60
1:C:86:VAL:HG13	1:C:113:ASP:HB2	1.85	0.59
1:C:164:VAL:C	1:C:165:ARG:HG2	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:THR:HG23	4:D:409:HOH:O	2.03	0.58
1:A:18:VAL:HG13	1:A:55:THR:HG22	1.89	0.55
1:D:5:THR:HG22	1:D:7:VAL:N	2.22	0.55
1:A:256:ASN:O	1:A:257:ILE:HD13	2.07	0.54
1:B:18:VAL:HG13	1:B:55:THR:HG22	1.90	0.54
1:A:24:GLN:OE1	1:A:24:GLN:HA	2.09	0.53
1:C:18:VAL:HG13	1:C:55:THR:HG22	1.91	0.53
1:D:96:ARG:NH1	4:D:413:HOH:O	2.27	0.52
1:D:18:VAL:HG13	1:D:55:THR:HG22	1.91	0.52
1:C:86:VAL:O	2:C:301:CL:CL	2.66	0.51
1:B:181:GLU:O	1:B:182:ARG:HD2	2.10	0.51
1:C:164:VAL:O	1:C:165:ARG:HG2	2.12	0.50
1:C:96:ARG:NH1	4:C:413:HOH:O	2.24	0.49
1:A:231:ARG:HD3	4:A:405:HOH:O	2.12	0.49
1:B:5:THR:HG22	1:B:8:GLU:CG	2.43	0.48
1:A:22:ILE:HB	4:A:441:HOH:O	2.14	0.47
1:D:96:ARG:NH2	1:D:161:ASP:OD2	2.47	0.47
1:D:191:ASP:HB2	1:D:220:ILE:HG21	1.97	0.47
1:C:96:ARG:NH2	1:C:161:ASP:OD2	2.48	0.46
1:A:83:GLU:HG2	1:A:92:CYS:SG	2.55	0.46
1:B:204:TYR:N	1:B:205:PRO:CD	2.79	0.46
1:B:191:ASP:HB2	1:B:220:ILE:HG21	1.98	0.46
1:D:113:ASP:OD2	2:D:301:CL:CL	2.71	0.45
1:B:83:GLU:HG2	1:B:92:CYS:SG	2.56	0.45
1:D:5:THR:HG22	1:D:7:VAL:H	1.81	0.45
1:D:83:GLU:HG2	1:D:92:CYS:SG	2.56	0.45
1:A:5:THR:HG22	1:A:8:GLU:CG	2.47	0.45
1:A:24:GLN:OE1	1:A:24:GLN:N	2.49	0.45
1:B:5:THR:CG2	1:B:8:GLU:H	2.28	0.45
1:A:191:ASP:HB2	1:A:220:ILE:HG21	1.99	0.45
1:C:83:GLU:HG2	1:C:92:CYS:SG	2.57	0.45
1:A:24:GLN:HB2	1:B:156:ARG:NH2	2.32	0.44
1:C:5:THR:HG22	1:C:8:GLU:CG	2.47	0.44
1:C:206:ARG:HD2	4:C:420:HOH:O	2.11	0.44
1:A:5:THR:CG2	1:A:8:GLU:H	2.30	0.44
1:A:152:ARG:O	1:A:155:SER:HB3	2.18	0.43
1:D:2:SER:HA	1:D:3:PRO:HD2	1.87	0.43
1:B:2:SER:HA	1:B:3:PRO:HD2	1.87	0.43
1:C:2:SER:HA	1:C:3:PRO:HD2	1.88	0.43
1:C:191:ASP:HB2	1:C:220:ILE:HG21	2.00	0.43
1:C:152:ARG:O	1:C:155:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HG	1:A:188:MSE:HE2	2.00	0.42
1:C:209:PRO:HB3	1:C:254:ALA:HA	2.01	0.42
1:A:2:SER:HA	1:A:3:PRO:HD2	1.87	0.42
1:D:152:ARG:O	1:D:155:SER:HB3	2.19	0.42
1:C:186:LEU:HG	1:C:188:MSE:HE2	2.01	0.42
1:B:152:ARG:O	1:B:155:SER:HB3	2.20	0.41
1:C:204:TYR:N	1:C:205:PRO:CD	2.84	0.41
1:D:178:ALA:HA	1:D:179:PRO:HD3	1.96	0.41
1:C:5:THR:CG2	1:C:8:GLU:H	2.31	0.41
1:B:186:LEU:HG	1:B:188:MSE:HE2	2.03	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	194/283 (69%)	190 (98%)	4 (2%)	0	100	100
1	B	191/283 (68%)	187 (98%)	4 (2%)	0	100	100
1	C	197/283 (70%)	192 (98%)	5 (2%)	0	100	100
1	D	193/283 (68%)	188 (97%)	5 (3%)	0	100	100
All	All	775/1132 (68%)	757 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	169/229 (74%)	163 (96%)	6 (4%)	30	56
1	B	165/229 (72%)	159 (96%)	6 (4%)	30	56
1	C	168/229 (73%)	164 (98%)	4 (2%)	44	70
1	D	163/229 (71%)	159 (98%)	4 (2%)	42	69
All	All	665/916 (73%)	645 (97%)	20 (3%)	36	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	GLN
1	A	52	VAL
1	A	172	LYS
1	A	177	THR
1	A	192	SER
1	B	52	VAL
1	B	74	ARG
1	B	172	LYS
1	B	177	THR
1	B	182	ARG
1	B	192	SER
1	C	52	VAL
1	C	172	LYS
1	C	177	THR
1	C	192	SER
1	D	52	VAL
1	D	172	LYS
1	D	177	THR
1	D	192	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	151	GLN
1	C	151	GLN
1	D	151	GLN

### 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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 [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	195/283 (68%)	-0.41	2 (1%) 79 76	29, 46, 79, 110	0
1	B	192/283 (67%)	0.07	3 (1%) 70 67	46, 73, 105, 119	0
1	C	198/283 (69%)	-0.40	4 (2%) 64 62	29, 45, 80, 107	0
1	D	194/283 (68%)	-0.06	6 (3%) 51 48	42, 65, 97, 117	0
All	All	779/1132 (68%)	-0.20	15 (1%) 66 63	29, 58, 97, 119	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	ALA	4.9
1	C	257	ILE	4.5
1	D	52	VAL	4.1
1	B	52	VAL	3.7
1	C	52	VAL	3.5
1	A	52	VAL	3.1
1	D	254	ALA	2.8
1	C	145	THR	2.8
1	A	145	THR	2.4
1	B	145	THR	2.3
1	C	177	THR	2.3
1	D	228	HIS	2.3
1	B	228	HIS	2.2
1	D	172	LYS	2.1
1	D	170	TRP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	C	301	1/1	0.83	0.14	82,82,82,82	0
2	CL	D	301	1/1	0.86	0.08	86,86,86,86	0
2	CL	A	301	1/1	0.87	0.10	90,90,90,90	0
2	CL	B	301	1/1	0.92	0.07	83,83,83,83	0
3	MG	B	302	1/1	0.99	0.04	43,43,43,43	0
3	MG	A	302	1/1	1.00	0.01	27,27,27,27	0
3	MG	C	302	1/1	1.00	0.01	25,25,25,25	0
3	MG	D	302	1/1	1.00	0.01	36,36,36,36	0

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

There are no such residues in this entry.