



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2017 – 02:58 PM EDT

PDB ID : 5JJP  
Title : Crystal structure of CmiS6  
Authors : Cieslak, J.; Miyanaga, A.; Kudo, F.; Eguchi, T.  
Deposited on : 2016-04-25  
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

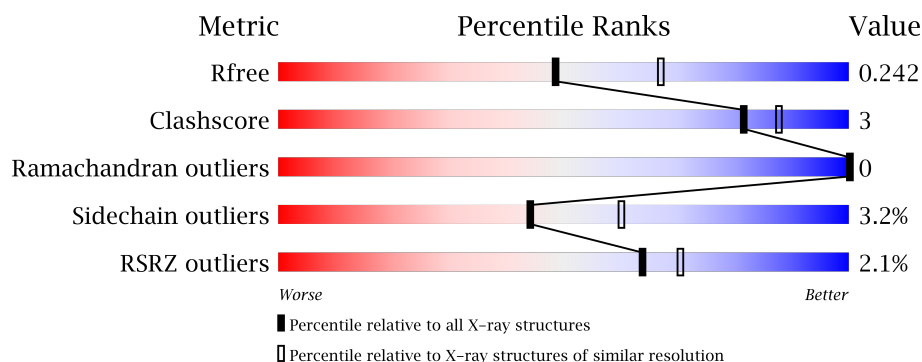
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. 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	543	<div> <div> <div></div> <div>69%</div> <div>6%</div> <div>24%</div> </div> </div>
1	B	543	<div> <div> <div></div> <div>70%</div> <div>6%</div> <div>23%</div> </div> </div>
1	C	543	<div> <div> <div>3%</div> <div>68%</div> <div>28%</div> </div> </div>
1	D	543	<div> <div> <div></div> <div>70%</div> <div>6%</div> <div>23%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12947 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 Nonribosomal peptide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3140	2006	555	571	8			
1	B	418	Total	C	N	O	S	0	0	0
			3174	2024	562	580	8			
1	C	392	Total	C	N	O	S	0	0	0
			2967	1892	528	539	8			
1	D	416	Total	C	N	O	S	0	0	0
			3157	2015	557	577	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP X5IJ97
A	-14	ASN	-	expression tag	UNP X5IJ97
A	-13	HIS	-	expression tag	UNP X5IJ97
A	-12	LYS	-	expression tag	UNP X5IJ97
A	-11	VAL	-	expression tag	UNP X5IJ97
A	-10	HIS	-	expression tag	UNP X5IJ97
A	-9	HIS	-	expression tag	UNP X5IJ97
A	-8	HIS	-	expression tag	UNP X5IJ97
A	-7	HIS	-	expression tag	UNP X5IJ97
A	-6	HIS	-	expression tag	UNP X5IJ97
A	-5	HIS	-	expression tag	UNP X5IJ97
A	-4	ILE	-	expression tag	UNP X5IJ97
A	-3	GLU	-	expression tag	UNP X5IJ97
A	-2	GLY	-	expression tag	UNP X5IJ97
A	-1	ARG	-	expression tag	UNP X5IJ97
A	0	HIS	-	expression tag	UNP X5IJ97
B	-15	MET	-	initiating methionine	UNP X5IJ97
B	-14	ASN	-	expression tag	UNP X5IJ97
B	-13	HIS	-	expression tag	UNP X5IJ97
B	-12	LYS	-	expression tag	UNP X5IJ97
B	-11	VAL	-	expression tag	UNP X5IJ97

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP X5IJ97
B	-9	HIS	-	expression tag	UNP X5IJ97
B	-8	HIS	-	expression tag	UNP X5IJ97
B	-7	HIS	-	expression tag	UNP X5IJ97
B	-6	HIS	-	expression tag	UNP X5IJ97
B	-5	HIS	-	expression tag	UNP X5IJ97
B	-4	ILE	-	expression tag	UNP X5IJ97
B	-3	GLU	-	expression tag	UNP X5IJ97
B	-2	GLY	-	expression tag	UNP X5IJ97
B	-1	ARG	-	expression tag	UNP X5IJ97
B	0	HIS	-	expression tag	UNP X5IJ97
C	-15	MET	-	initiating methionine	UNP X5IJ97
C	-14	ASN	-	expression tag	UNP X5IJ97
C	-13	HIS	-	expression tag	UNP X5IJ97
C	-12	LYS	-	expression tag	UNP X5IJ97
C	-11	VAL	-	expression tag	UNP X5IJ97
C	-10	HIS	-	expression tag	UNP X5IJ97
C	-9	HIS	-	expression tag	UNP X5IJ97
C	-8	HIS	-	expression tag	UNP X5IJ97
C	-7	HIS	-	expression tag	UNP X5IJ97
C	-6	HIS	-	expression tag	UNP X5IJ97
C	-5	HIS	-	expression tag	UNP X5IJ97
C	-4	ILE	-	expression tag	UNP X5IJ97
C	-3	GLU	-	expression tag	UNP X5IJ97
C	-2	GLY	-	expression tag	UNP X5IJ97
C	-1	ARG	-	expression tag	UNP X5IJ97
C	0	HIS	-	expression tag	UNP X5IJ97
D	-15	MET	-	initiating methionine	UNP X5IJ97
D	-14	ASN	-	expression tag	UNP X5IJ97
D	-13	HIS	-	expression tag	UNP X5IJ97
D	-12	LYS	-	expression tag	UNP X5IJ97
D	-11	VAL	-	expression tag	UNP X5IJ97
D	-10	HIS	-	expression tag	UNP X5IJ97
D	-9	HIS	-	expression tag	UNP X5IJ97
D	-8	HIS	-	expression tag	UNP X5IJ97
D	-7	HIS	-	expression tag	UNP X5IJ97
D	-6	HIS	-	expression tag	UNP X5IJ97
D	-5	HIS	-	expression tag	UNP X5IJ97
D	-4	ILE	-	expression tag	UNP X5IJ97
D	-3	GLU	-	expression tag	UNP X5IJ97
D	-2	GLY	-	expression tag	UNP X5IJ97
D	-1	ARG	-	expression tag	UNP X5IJ97

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP X5IJ97

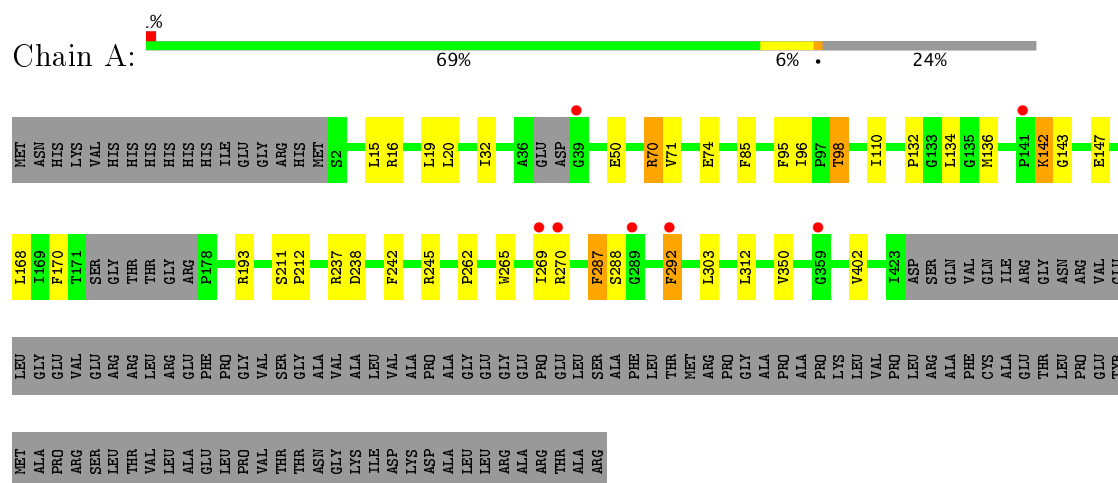
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total 148	O 148	0	0
2	B	151	Total 151	O 151	0	0
2	C	59	Total 59	O 59	0	0
2	D	151	Total 151	O 151	0	0

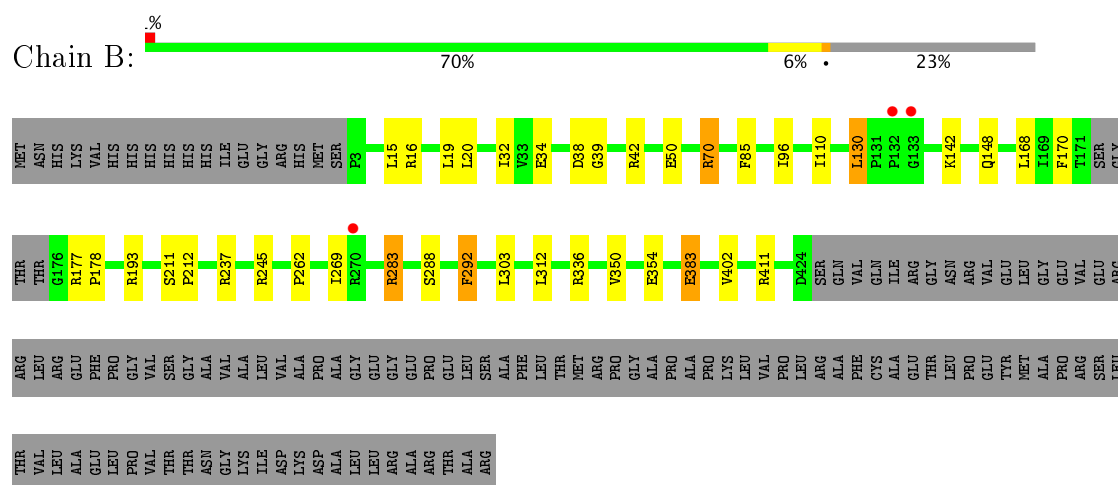
### 3 Residue-property plots [i](#)

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.

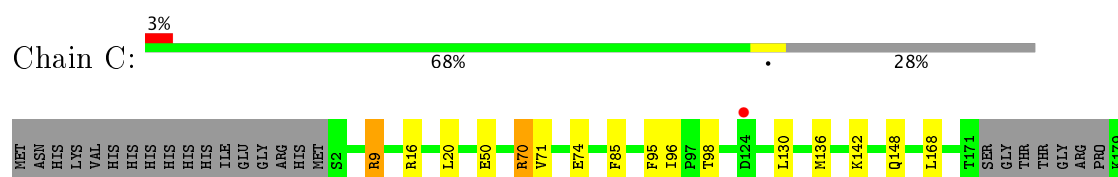
#### • Molecule 1: Nonribosomal peptide synthase



#### • Molecule 1: Nonribosomal peptide synthase



#### • Molecule 1: Nonribosomal peptide synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.29Å 109.21Å 198.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.43 – 2.30 55.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (55.43-2.30) 98.9 (55.37-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.206 , 0.244 0.210 , 0.242	Depositor DCC
$R_{free}$ test set	4062 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

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	0.74	0/3221	0.89	8/4394 (0.2%)
1	B	0.76	0/3256	0.89	7/4442 (0.2%)
1	C	0.63	0/3036	0.82	5/4132 (0.1%)
1	D	0.72	0/3239	0.87	7/4420 (0.2%)
All	All	0.71	0/12752	0.87	27/17388 (0.2%)

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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	C	193	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	D	193	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	32	ILE	CG1-CB-CG2	-9.37	90.79	111.40
1	A	193	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	193	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	C	193	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	283	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	193	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	193	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	193	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	70	ARG	NE-CZ-NH2	-8.46	116.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	287	PHE	CB-CA-C	-7.66	95.07	110.40
1	C	287	PHE	CB-CA-C	-7.60	95.19	110.40
1	C	70	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	D	287	PHE	CB-CA-C	-7.16	96.08	110.40
1	D	70	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	70	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	B	70	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	70	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	C	70	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	298	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	134	LEU	CA-CB-CG	5.38	127.68	115.30
1	D	298	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	336	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	238	ASP	CB-CG-OD2	5.11	122.90	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	PRO	Peptide
1	D	291	ASP	Peptide

## 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	3140	0	3123	23	0
1	B	3174	0	3149	21	0
1	C	2967	0	2956	12	0
1	D	3157	0	3134	18	0
2	A	148	0	0	0	0
2	B	151	0	0	2	0
2	C	59	0	0	1	0
2	D	151	0	0	1	0
All	All	12947	0	12362	74	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 (74) 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:B:177:ARG:HG2	1:B:178:PRO:HD2	1.61	0.81
1:D:287:PHE:CD2	1:D:292:PHE:HE2	2.09	0.71
1:B:411:ARG:HD2	2:B:631:HOH:O	1.92	0.69
1:A:287:PHE:CZ	1:A:292:PHE:HE1	2.11	0.69
1:A:287:PHE:CE1	1:A:292:PHE:HE1	2.12	0.65
1:D:16:ARG:NH1	1:D:20:LEU:HD12	2.13	0.63
1:A:16:ARG:NH1	1:A:20:LEU:HD12	2.13	0.62
1:A:287:PHE:CZ	1:A:292:PHE:CE1	2.89	0.61
1:B:34:GLU:OE2	1:B:42:ARG:NH1	2.34	0.61
1:B:16:ARG:NH1	1:B:20:LEU:HD12	2.16	0.61
1:B:130:LEU:HD23	1:B:130:LEU:H	1.66	0.60
1:C:16:ARG:NH1	1:C:20:LEU:HD12	2.17	0.59
1:A:20:LEU:HD13	1:A:50:GLU:HG2	1.83	0.59
1:B:38:ASP:OD1	1:B:39:GLY:N	2.36	0.59
1:B:20:LEU:HD13	1:B:50:GLU:HG2	1.85	0.59
1:D:266:ARG:HB2	1:D:267:PRO:HD3	1.84	0.59
1:D:20:LEU:HD13	1:D:50:GLU:HG2	1.85	0.58
1:C:20:LEU:HD13	1:C:50:GLU:HG2	1.87	0.57
1:C:186:ARG:HG2	2:C:620:HOH:O	2.06	0.55
1:B:177:ARG:HG2	1:B:178:PRO:CD	2.35	0.55
1:B:96:ILE:CD1	1:B:168:LEU:HB2	2.38	0.53
1:A:16:ARG:HH11	1:A:20:LEU:HD12	1.72	0.53
1:D:96:ILE:CD1	1:D:168:LEU:HB2	2.39	0.53
1:C:96:ILE:CD1	1:C:168:LEU:HB2	2.39	0.53
1:A:242:PHE:CD2	1:A:242:PHE:N	2.77	0.53
1:D:16:ARG:HH11	1:D:20:LEU:HD12	1.74	0.52
1:A:288:SER:HB3	1:A:312:LEU:HB3	1.92	0.52
1:C:130:LEU:HD13	1:C:136:MET:SD	2.50	0.52
1:A:96:ILE:CD1	1:A:168:LEU:HB2	2.41	0.51
1:A:74:GLU:OE1	1:A:98:THR:CG2	2.58	0.51
1:D:288:SER:HB3	1:D:312:LEU:HB3	1.93	0.51
1:C:288:SER:HB3	1:C:312:LEU:HB3	1.93	0.51
1:D:287:PHE:CD2	1:D:292:PHE:CE2	2.96	0.50
1:D:179:LYS:NZ	2:D:603:HOH:O	2.44	0.49
1:C:9:ARG:HG3	1:C:9:ARG:HH11	1.76	0.49
1:A:16:ARG:NH1	1:A:20:LEU:CD1	2.76	0.49
1:B:16:ARG:HH11	1:B:20:LEU:HD12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:SER:HB3	1:B:312:LEU:HB3	1.95	0.48
1:C:16:ARG:HH11	1:C:20:LEU:HD12	1.78	0.48
1:D:16:ARG:NH1	1:D:20:LEU:CD1	2.77	0.47
1:B:16:ARG:NH1	1:B:20:LEU:CD1	2.79	0.46
1:D:74:GLU:OE2	1:D:98:THR:CG2	2.64	0.45
1:C:74:GLU:OE2	1:C:98:THR:CG2	2.65	0.45
1:D:130:LEU:HD13	1:D:136:MET:SD	2.56	0.45
1:D:269:ILE:HD12	1:D:303:LEU:HD12	1.98	0.45
1:A:262:PRO:HB3	1:A:292:PHE:CD1	2.51	0.45
1:D:265:TRP:O	1:D:269:ILE:HG12	2.16	0.45
1:A:136:MET:HE1	1:A:147:GLU:HG3	2.00	0.44
1:B:283:ARG:NH2	2:B:602:HOH:O	2.36	0.44
1:D:211:SER:HA	1:D:212:PRO:HD3	1.91	0.44
1:D:110:ILE:HD12	1:D:170:PHE:CG	2.53	0.44
1:B:383:GLU:HG3	1:B:383:GLU:H	1.61	0.44
1:A:262:PRO:HB3	1:A:292:PHE:CG	2.53	0.43
1:C:16:ARG:NH1	1:C:20:LEU:CD1	2.80	0.43
1:B:177:ARG:CG	1:B:178:PRO:HD2	2.42	0.43
1:A:74:GLU:OE1	1:A:98:THR:HG21	2.19	0.43
1:A:110:ILE:HD12	1:A:170:PHE:CG	2.54	0.42
1:B:96:ILE:HD13	1:B:168:LEU:HB2	2.01	0.42
1:A:142:LYS:HD3	1:A:143:GLY:N	2.35	0.42
1:B:269:ILE:HD12	1:B:303:LEU:HD12	2.01	0.42
1:A:15:LEU:O	1:A:19:LEU:HG	2.20	0.41
1:A:269:ILE:HD12	1:A:303:LEU:HD12	2.01	0.41
1:A:71:VAL:O	1:A:95:PHE:HA	2.21	0.41
1:B:110:ILE:HD12	1:B:170:PHE:CG	2.55	0.41
1:D:71:VAL:O	1:D:95:PHE:HA	2.20	0.41
1:B:211:SER:HA	1:B:212:PRO:HD3	1.90	0.41
1:A:242:PHE:HB2	1:A:245:ARG:HB2	2.02	0.41
1:A:211:SER:HA	1:A:212:PRO:HD3	1.89	0.41
1:B:262:PRO:HB3	1:B:292:PHE:CG	2.56	0.41
1:D:15:LEU:O	1:D:19:LEU:HG	2.20	0.41
1:C:71:VAL:O	1:C:95:PHE:HA	2.21	0.40
1:B:15:LEU:O	1:B:19:LEU:HG	2.21	0.40
1:C:96:ILE:HD13	1:C:168:LEU:HB2	2.04	0.40
1:A:265:TRP:O	1:A:269:ILE:HG12	2.21	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	408/543 (75%)	395 (97%)	13 (3%)	0	100	100
1	B	414/543 (76%)	402 (97%)	12 (3%)	0	100	100
1	C	378/543 (70%)	369 (98%)	9 (2%)	0	100	100
1	D	412/543 (76%)	398 (97%)	14 (3%)	0	100	100
All	All	1612/2172 (74%)	1564 (97%)	48 (3%)	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	320/424 (76%)	311 (97%)	9 (3%)	49	65
1	B	323/424 (76%)	310 (96%)	13 (4%)	36	50
1	C	301/424 (71%)	292 (97%)	9 (3%)	46	63
1	D	322/424 (76%)	313 (97%)	9 (3%)	49	65
All	All	1266/1696 (75%)	1226 (97%)	40 (3%)	44	60

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	85	PHE

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Mol	Chain	Res	Type
1	A	98	THR
1	A	142	LYS
1	A	237	ARG
1	A	270	ARG
1	A	292	PHE
1	A	350	VAL
1	A	402	VAL
1	B	32	ILE
1	B	70	ARG
1	B	85	PHE
1	B	130	LEU
1	B	142	LYS
1	B	148	GLN
1	B	237	ARG
1	B	245	ARG
1	B	292	PHE
1	B	350	VAL
1	B	354	GLU
1	B	383	GLU
1	B	402	VAL
1	C	9	ARG
1	C	70	ARG
1	C	85	PHE
1	C	142	LYS
1	C	148	GLN
1	C	245	ARG
1	C	350	VAL
1	C	354	GLU
1	C	402	VAL
1	D	32	ILE
1	D	70	ARG
1	D	85	PHE
1	D	134	LEU
1	D	142	LYS
1	D	270	ARG
1	D	292	PHE
1	D	350	VAL
1	D	354	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	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 carbohydrates 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 ⓘ

### 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	414/543 (76%)	-0.08	7 (1%) 70 76	12, 24, 57, 94	0
1	B	418/543 (76%)	-0.09	3 (0%) 87 90	12, 22, 50, 77	0
1	C	392/543 (72%)	0.23	18 (4%) 33 40	15, 34, 67, 85	0
1	D	416/543 (76%)	-0.09	6 (1%) 75 80	13, 26, 50, 74	0
All	All	1640/2172 (75%)	-0.01	34 (2%) 64 70	12, 26, 58, 94	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	PHE	3.7
1	C	276	VAL	3.5
1	B	270	ARG	3.4
1	D	292	PHE	3.4
1	C	237	ARG	3.4
1	C	273	PRO	3.4
1	D	142	LYS	3.2
1	C	279	LEU	3.1
1	A	359	GLY	3.1
1	C	418	TYR	3.0
1	C	302	GLY	3.0
1	A	292	PHE	3.0
1	B	132	PRO	2.9
1	A	289	GLY	2.9
1	C	246	PHE	2.8
1	C	265	TRP	2.6
1	A	270	ARG	2.6
1	C	282	LEU	2.5
1	B	133	GLY	2.4
1	D	36	ALA	2.4
1	C	244	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	37	GLU	2.2
1	D	147	GLU	2.2
1	C	297	LEU	2.2
1	A	141	PRO	2.2
1	C	261	VAL	2.2
1	C	249	PHE	2.2
1	A	39	GLY	2.2
1	D	287	PHE	2.1
1	C	361	PRO	2.1
1	A	269	ILE	2.1
1	C	240	LEU	2.1
1	C	296	ASP	2.1
1	C	124	ASP	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 carbohydrates 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.