



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 03:20 PM EST

PDB ID : 5KKU  
Title : Crystal structure of an N-terminal dehydratase from difficidin assembly line  
Authors : Keatinge-Clay, A.T.; Zeng, J.  
Deposited on : 2016-06-22  
Resolution : 2.22 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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028442

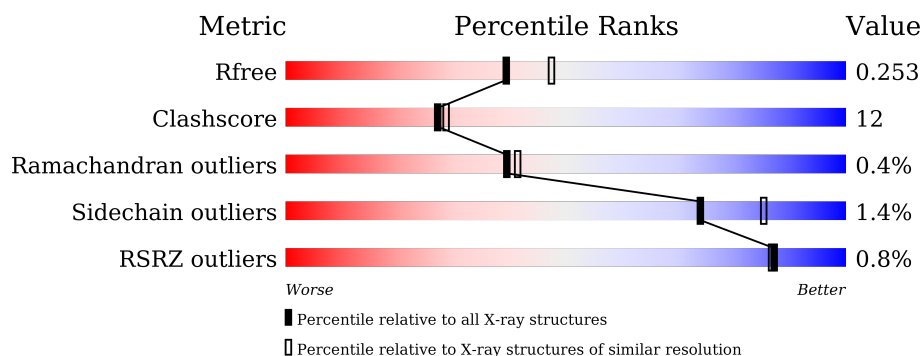
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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))
$R_{free}$	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	300	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div> </div>
1	B	300	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	C	300	<div> <div></div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	300	<div> <div></div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9353 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 Polyketide synthase type I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2333	1478	409	434	12			
1	B	289	Total	C	N	O	S	0	0	0
			2351	1488	412	439	12			
1	C	289	Total	C	N	O	S	0	0	0
			2351	1488	412	439	12			
1	D	284	Total	C	N	O	S	0	0	0
			2316	1468	407	429	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLU	-	expression tag	UNP Q1RS44
A	295	HIS	-	expression tag	UNP Q1RS44
A	296	HIS	-	expression tag	UNP Q1RS44
A	297	HIS	-	expression tag	UNP Q1RS44
A	298	HIS	-	expression tag	UNP Q1RS44
A	299	HIS	-	expression tag	UNP Q1RS44
A	300	HIS	-	expression tag	UNP Q1RS44
B	294	GLU	-	expression tag	UNP Q1RS44
B	295	HIS	-	expression tag	UNP Q1RS44
B	296	HIS	-	expression tag	UNP Q1RS44
B	297	HIS	-	expression tag	UNP Q1RS44
B	298	HIS	-	expression tag	UNP Q1RS44
B	299	HIS	-	expression tag	UNP Q1RS44
B	300	HIS	-	expression tag	UNP Q1RS44
C	294	GLU	-	expression tag	UNP Q1RS44
C	295	HIS	-	expression tag	UNP Q1RS44
C	296	HIS	-	expression tag	UNP Q1RS44
C	297	HIS	-	expression tag	UNP Q1RS44
C	298	HIS	-	expression tag	UNP Q1RS44
C	299	HIS	-	expression tag	UNP Q1RS44
C	300	HIS	-	expression tag	UNP Q1RS44

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	GLU	-	expression tag	UNP Q1RS44
D	295	HIS	-	expression tag	UNP Q1RS44
D	296	HIS	-	expression tag	UNP Q1RS44
D	297	HIS	-	expression tag	UNP Q1RS44
D	298	HIS	-	expression tag	UNP Q1RS44
D	299	HIS	-	expression tag	UNP Q1RS44
D	300	HIS	-	expression tag	UNP Q1RS44

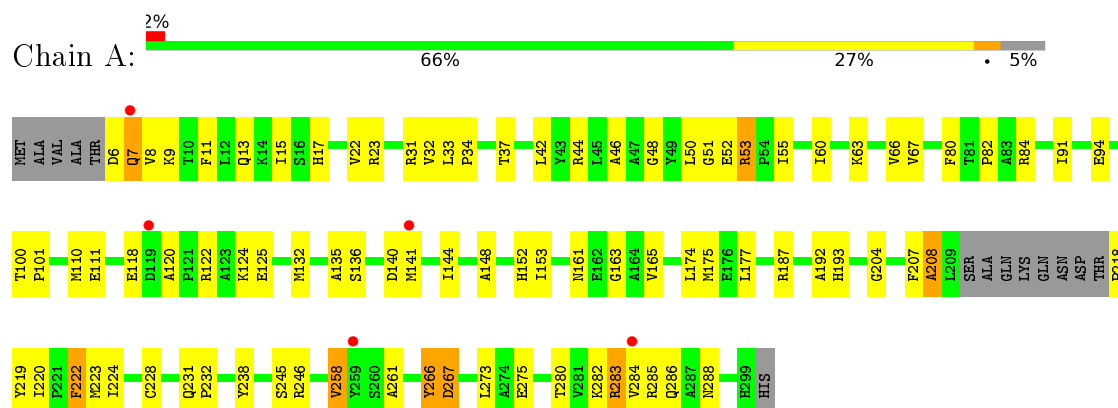
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0

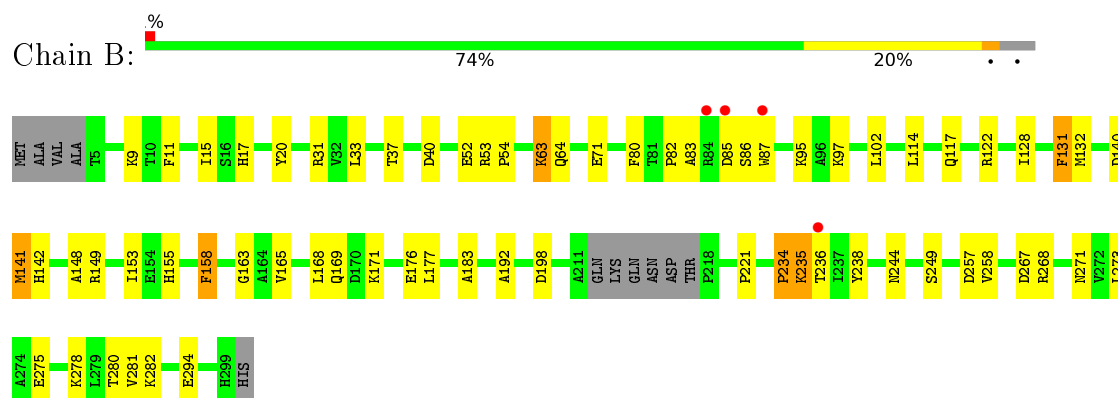
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

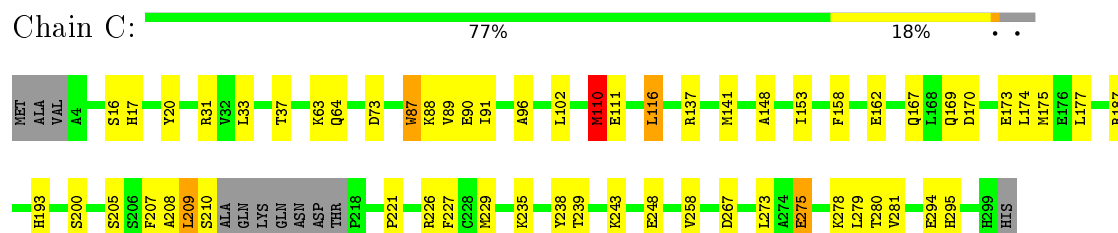
#### • Molecule 1: Polyketide synthase type I



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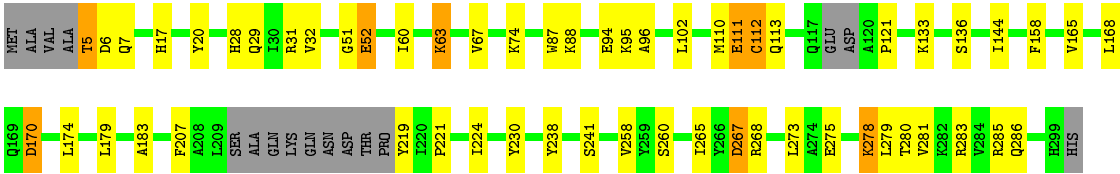
#### • Molecule 1: Polyketide synthase type I

Chain D: 

76%

16%

• 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.35Å 73.98Å 94.18Å 90.20° 90.08° 90.66°	Depositor
Resolution (Å)	39.79 – 2.22 41.35 – 2.22	Depositor EDS
% Data completeness (in resolution range)	89.0 (39.79-2.22) 87.3 (41.35-2.22)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.217 , 0.248 0.225 , 0.253	Depositor DCC
$R_{free}$ test set	2513 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 9.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.269 for h,-k,-l 0.012 for -h,k,-l 0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	1.45	5/2388 (0.2%)	1.10	25/3222 (0.8%)
1	B	1.44	5/2406 (0.2%)	0.92	5/3247 (0.2%)
1	C	1.45	6/2406 (0.2%)	1.03	11/3247 (0.3%)
1	D	1.40	7/2369 (0.3%)	0.93	8/3195 (0.3%)
All	All	1.44	23/9569 (0.2%)	1.00	49/12911 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	3
All	All	0	6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	GLU	CD-OE1	-7.61	1.17	1.25
1	A	267	ASP	N-CA	-7.30	1.31	1.46
1	B	275	GLU	CD-OE1	-6.77	1.18	1.25
1	B	275	GLU	CD-OE2	-6.66	1.18	1.25
1	D	136	SER	CB-OG	-6.53	1.33	1.42
1	D	267	ASP	N-CA	-6.47	1.33	1.46
1	B	294	GLU	CD-OE2	-6.16	1.18	1.25
1	C	294	GLU	CD-OE1	-6.13	1.19	1.25
1	A	136	SER	CB-OG	-6.07	1.34	1.42
1	C	248	GLU	CD-OE1	-5.93	1.19	1.25
1	A	261	ALA	C-N	-5.85	1.20	1.34
1	D	87	TRP	CB-CG	-5.73	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	PHE	C-N	-5.66	1.21	1.34
1	D	267	ASP	C-N	-5.51	1.21	1.34
1	C	110	MET	C-N	-5.51	1.21	1.34
1	D	241	SER	CB-OG	-5.47	1.35	1.42
1	A	275	GLU	CD-OE1	-5.41	1.19	1.25
1	C	275	GLU	CD-OE2	-5.40	1.19	1.25
1	A	288	ASN	C-N	-5.37	1.21	1.34
1	C	87	TRP	CB-CG	-5.24	1.40	1.50
1	C	173	GLU	CD-OE1	-5.19	1.20	1.25
1	D	94	GLU	CD-OE2	-5.06	1.20	1.25
1	D	275	GLU	CD-OE1	-5.01	1.20	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	MET	C-N-CA	16.91	163.98	121.70
1	C	110	MET	O-C-N	-16.63	96.09	122.70
1	C	64	GLN	N-CA-CB	12.72	133.50	110.60
1	A	63	LYS	CB-CA-C	-12.26	85.88	110.40
1	C	110	MET	CA-C-N	11.27	142.00	117.20
1	A	63	LYS	N-CA-C	9.79	137.42	111.00
1	D	63	LYS	N-CA-C	-9.56	85.19	111.00
1	A	135	ALA	CA-C-N	-8.21	99.14	117.20
1	A	51	GLY	N-CA-C	-8.18	92.64	113.10
1	A	208	ALA	N-CA-C	7.95	132.47	111.00
1	D	51	GLY	C-N-CA	-7.95	101.83	121.70
1	C	111	GLU	O-C-N	7.82	135.21	122.70
1	C	116	LEU	O-C-N	-7.76	110.28	122.70
1	A	222	PHE	CB-CA-C	-7.57	95.27	110.40
1	B	131	PHE	CA-C-N	-7.47	100.77	117.20
1	A	261	ALA	C-N-CA	7.27	139.88	121.70
1	A	267	ASP	CA-C-N	-7.20	101.37	117.20
1	A	135	ALA	CA-C-O	7.01	134.82	120.10
1	A	23	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	258	VAL	N-CA-C	-6.92	92.31	111.00
1	B	158	PHE	C-N-CA	6.85	138.83	121.70
1	C	111	GLU	CA-C-N	-6.85	102.13	117.20
1	A	52	GLU	N-CA-C	-6.83	92.57	111.00
1	D	268	ARG	O-C-N	6.74	133.49	122.70
1	A	52	GLU	CB-CA-C	6.67	123.73	110.40
1	A	228	CYS	C-N-CA	6.58	138.15	121.70
1	A	208	ALA	C-N-CA	6.56	138.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ARG	N-CA-C	-6.34	93.88	111.00
1	A	228	CYS	O-C-N	-6.11	112.93	122.70
1	B	131	PHE	CA-C-O	5.98	132.66	120.10
1	D	52	GLU	CA-C-N	-5.86	104.30	117.20
1	C	63	LYS	N-CA-C	5.84	126.78	111.00
1	B	53	ARG	C-N-CD	5.84	140.66	128.40
1	A	267	ASP	CA-C-O	5.79	132.27	120.10
1	A	261	ALA	O-C-N	-5.78	113.45	122.70
1	C	116	LEU	CA-C-N	5.63	129.60	117.20
1	A	100	THR	C-N-CD	5.61	140.17	128.40
1	A	220	ILE	C-N-CD	5.59	140.14	128.40
1	A	222	PHE	N-CA-C	5.59	126.09	111.00
1	B	244	ASN	N-CA-CB	-5.51	100.68	110.60
1	A	192	ALA	CB-CA-C	5.44	118.26	110.10
1	C	64	GLN	N-CA-C	-5.43	96.34	111.00
1	D	267	ASP	CA-C-N	-5.42	105.27	117.20
1	A	120	ALA	C-N-CD	5.40	139.74	128.40
1	D	267	ASP	C-N-CA	5.34	135.05	121.70
1	C	209	LEU	N-CA-C	-5.26	96.80	111.00
1	D	63	LYS	C-N-CA	5.14	134.55	121.70
1	D	63	LYS	CB-CA-C	-5.10	100.20	110.40
1	A	135	ALA	C-N-CA	5.04	134.30	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	TYR	Peptide
1	B	131	PHE	Peptide
1	C	110	MET	Mainchain
1	D	278	LYS	Mainchain
1	D	52	GLU	Mainchain
1	D	63	LYS	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	2333	0	2277	90	0
1	B	2351	0	2293	51	0
1	C	2351	0	2295	46	0
1	D	2316	0	2266	36	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	9353	0	9131	222	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 12.

All (222) 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:7:GLN:HA	1:A:82:PRO:CG	1.23	1.44
1:A:7:GLN:CA	1:A:82:PRO:HG2	1.52	1.30
1:A:6:ASP:O	1:A:7:GLN:HG2	1.12	1.23
1:C:88:LYS:NZ	1:C:90:GLU:OE1	1.70	1.22
1:A:7:GLN:CA	1:A:82:PRO:CG	2.04	1.18
1:A:141:MET:HB2	1:A:163:GLY:O	1.40	1.17
1:A:141:MET:HB2	1:A:163:GLY:C	1.67	1.14
1:A:7:GLN:HA	1:A:82:PRO:HG3	1.32	1.11
1:A:6:ASP:O	1:A:7:GLN:CG	2.01	1.09
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.10	1.08
1:C:88:LYS:NZ	1:C:90:GLU:CD	2.11	1.04
1:D:278:LYS:O	1:D:278:LYS:HG3	1.54	1.02
1:B:82:PRO:HA	1:B:87:TRP:CD1	2.01	0.96
1:D:260:SER:HB2	1:D:279:LEU:O	1.66	0.95
1:A:219:TYR:CZ	1:A:283:ARG:HB2	2.01	0.95
1:B:82:PRO:HA	1:B:87:TRP:HD1	1.30	0.95
1:B:86:SER:HB2	1:B:114:LEU:O	1.65	0.94
1:B:168:LEU:HG	1:B:169:GLN:HG2	1.50	0.94
1:A:141:MET:CB	1:A:163:GLY:O	2.18	0.91
1:C:88:LYS:HZ2	1:C:90:GLU:CD	1.73	0.91
1:A:246:ARG:NH1	1:A:246:ARG:HB2	1.85	0.90
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.36	0.89
1:C:87:TRP:HZ3	1:C:116:LEU:CD1	1.86	0.89
1:B:141:MET:HE3	1:B:177:LEU:HD21	1.55	0.88
1:C:87:TRP:HZ3	1:C:116:LEU:HD11	1.40	0.87
1:A:32:VAL:HG22	1:A:67:VAL:HG22	1.56	0.86
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.90	0.85
1:A:246:ARG:HH11	1:A:246:ARG:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG22	1:A:282:LYS:HG3	1.59	0.83
1:A:218:PRO:O	1:A:283:ARG:HA	1.78	0.83
1:A:285:ARG:CZ	1:A:285:ARG:HA	2.09	0.83
1:A:7:GLN:CA	1:A:82:PRO:HG3	1.95	0.82
1:C:137:ARG:NH1	1:C:137:ARG:HG3	1.94	0.81
1:B:33:LEU:HD11	1:B:37:THR:HG21	1.64	0.79
1:D:278:LYS:O	1:D:278:LYS:CG	2.30	0.79
1:C:141:MET:HE1	1:C:177:LEU:HD21	1.64	0.79
1:A:6:ASP:C	1:A:7:GLN:HG2	2.03	0.78
1:C:87:TRP:CZ3	1:C:116:LEU:HD11	2.18	0.77
1:B:142:HIS:O	1:B:149:ARG:NH1	2.17	0.76
1:A:33:LEU:HB3	1:A:66:VAL:HB	1.68	0.75
1:A:140:ASP:OD1	1:A:141:MET:N	2.20	0.75
1:A:33:LEU:HD11	1:A:37:THR:HG21	1.69	0.75
1:B:267:ASP:HB3	1:B:273:LEU:HD21	1.69	0.73
1:A:219:TYR:CE2	1:A:283:ARG:HB2	2.23	0.73
1:A:222:PHE:O	1:A:222:PHE:CD1	2.42	0.72
1:C:88:LYS:HZ1	1:C:90:GLU:CD	1.84	0.72
1:D:260:SER:CB	1:D:279:LEU:O	2.38	0.71
1:A:122:ARG:NH1	1:A:122:ARG:HG2	1.89	0.71
1:A:231:GLN:HG3	1:A:232:PRO:HD2	1.73	0.70
1:A:222:PHE:O	1:A:223:MET:HG3	1.90	0.70
1:A:141:MET:HB3	1:A:163:GLY:H	1.55	0.70
1:A:219:TYR:CE1	1:A:283:ARG:HB2	2.27	0.69
1:D:60:ILE:HG23	1:D:110:MET:HE2	1.73	0.69
1:A:165:VAL:HG22	1:A:175:MET:HG2	1.73	0.69
1:D:144:ILE:HG13	1:D:165:VAL:HG21	1.74	0.69
1:A:7:GLN:HA	1:A:82:PRO:HG2	0.70	0.69
1:A:161:ASN:HD22	1:A:177:LEU:HB3	1.58	0.69
1:B:177:LEU:O	1:B:236:THR:HA	1.92	0.69
1:D:170:ASP:O	1:D:207:PHE:CE1	2.46	0.69
1:D:219:TYR:CE2	1:D:283:ARG:HB2	2.28	0.68
1:A:267:ASP:HB3	1:A:273:LEU:HD21	1.73	0.68
1:C:200:SER:OG	1:C:239:THR:HG21	1.93	0.68
1:A:285:ARG:NE	1:A:285:ARG:HA	2.08	0.67
1:A:222:PHE:O	1:A:222:PHE:CG	2.44	0.67
1:C:227:PHE:HE1	1:C:229:MET:CE	2.07	0.67
1:B:54:PRO:HB2	1:B:117:GLN:OE1	1.95	0.67
1:A:141:MET:CB	1:A:163:GLY:H	2.07	0.67
1:A:32:VAL:HG12	1:A:33:LEU:N	2.09	0.67
1:D:111:GLU:O	1:D:112:CYS:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:PHE:O	1:B:183:ALA:HB2	1.95	0.67
1:C:88:LYS:HE3	1:C:90:GLU:HG3	1.76	0.67
1:A:55:ILE:C	1:A:55:ILE:HD12	2.16	0.66
1:D:5:THR:HG23	1:D:7:GLN:H	1.59	0.66
1:B:128:ILE:O	1:B:132:MET:HB2	1.96	0.66
1:C:208:ALA:O	1:C:210:SER:N	2.28	0.66
1:A:9:LYS:HG2	1:A:11:PHE:CZ	2.32	0.64
1:B:141:MET:HE3	1:B:177:LEU:CD2	2.25	0.64
1:A:144:ILE:HG13	1:A:165:VAL:HG21	1.79	0.64
1:C:226:ARG:NH2	1:C:275:GLU:OE1	2.31	0.64
1:D:174:LEU:HD11	1:D:238:TYR:HB3	1.80	0.64
1:D:60:ILE:HG23	1:D:110:MET:CE	2.28	0.63
1:A:13:GLN:OE1	1:A:44:ARG:NH2	2.32	0.62
1:B:258:VAL:CG2	1:B:282:LYS:HG3	2.28	0.62
1:A:258:VAL:CG1	1:A:280:THR:CG2	2.78	0.62
1:A:141:MET:CB	1:A:163:GLY:N	2.62	0.62
1:A:258:VAL:CG1	1:A:280:THR:HG23	2.30	0.61
1:C:209:LEU:N	1:C:209:LEU:HD12	2.16	0.61
1:D:168:LEU:HD13	1:D:168:LEU:C	2.21	0.60
1:A:7:GLN:CB	1:A:82:PRO:HG2	2.30	0.60
1:B:258:VAL:HG13	1:B:280:THR:HG23	1.82	0.60
1:A:94:GLU:OE2	1:A:101:PRO:HB2	2.01	0.59
1:A:246:ARG:CB	1:A:246:ARG:HH11	2.12	0.59
1:B:258:VAL:HG23	1:B:282:LYS:HG3	1.85	0.58
1:D:265:ILE:HG22	1:D:273:LEU:HD12	1.86	0.58
1:A:141:MET:HE1	1:A:177:LEU:HD21	1.85	0.57
1:A:204:GLY:HA3	1:A:246:ARG:NH2	2.20	0.57
1:C:258:VAL:HG13	1:C:280:THR:HG23	1.86	0.57
1:B:128:ILE:O	1:B:132:MET:CB	2.53	0.56
1:A:207:PHE:O	1:A:208:ALA:HB3	2.06	0.56
1:A:266:TYR:HB3	1:A:267:ASP:O	2.06	0.55
1:B:267:ASP:OD2	1:B:271:ASN:ND2	2.29	0.55
1:C:170:ASP:O	1:C:243:LYS:HD3	2.06	0.55
1:A:141:MET:HB2	1:A:163:GLY:CA	2.37	0.54
1:C:187:ARG:HA	1:C:193:HIS:HD2	1.72	0.53
1:D:96:ALA:HA	1:D:102:LEU:HD13	1.89	0.53
1:A:122:ARG:NH1	1:A:122:ARG:CG	2.53	0.53
1:C:167:GLN:OE1	1:C:170:ASP:OD1	2.27	0.53
1:A:32:VAL:HG12	1:A:33:LEU:H	1.74	0.53
1:B:95:LYS:HB3	1:B:102:LEU:HD12	1.91	0.52
1:C:221:PRO:HA	1:C:281:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:PHE:HE1	1:C:229:MET:HE1	1.73	0.52
1:C:209:LEU:CD1	1:C:209:LEU:N	2.72	0.52
1:C:267:ASP:HB3	1:C:273:LEU:HD21	1.92	0.52
1:C:20:TYR:HB3	1:C:158:PHE:CG	2.44	0.51
1:B:163:GLY:HA3	1:B:176:GLU:O	2.09	0.51
1:D:95:LYS:HB3	1:D:102:LEU:HD22	1.90	0.51
1:A:174:LEU:HD11	1:A:238:TYR:HB3	1.93	0.51
1:D:17:HIS:CE1	1:D:31:ARG:HD2	2.45	0.51
1:B:15:ILE:CD1	1:B:33:LEU:HD22	2.41	0.50
1:A:187:ARG:HA	1:A:193:HIS:HD2	1.75	0.50
1:B:221:PRO:HA	1:B:281:VAL:HG12	1.94	0.50
1:C:137:ARG:HH11	1:C:137:ARG:CG	2.14	0.50
1:A:283:ARG:HG2	1:A:284:VAL:N	2.26	0.50
1:A:17:HIS:CE1	1:A:31:ARG:HD2	2.47	0.50
1:A:8:VAL:HA	1:A:80:PHE:O	2.12	0.50
1:A:152:HIS:CE1	1:A:286:GLN:HE22	2.29	0.50
1:C:87:TRP:CZ3	1:C:116:LEU:CD1	2.77	0.49
1:A:222:PHE:O	1:A:223:MET:CG	2.59	0.49
1:A:22:VAL:HB	1:A:31:ARG:HB3	1.94	0.49
1:A:32:VAL:CG1	1:A:33:LEU:N	2.73	0.49
1:B:258:VAL:HG22	1:B:282:LYS:HG3	1.95	0.49
1:A:110:MET:HG2	1:A:111:GLU:N	2.28	0.49
1:D:32:VAL:HG22	1:D:67:VAL:HG22	1.95	0.48
1:B:155:HIS:NE2	1:B:198:ASP:OD2	2.46	0.48
1:A:219:TYR:CE2	1:A:283:ARG:CB	2.93	0.48
1:B:83:ALA:HB3	1:B:86:SER:O	2.14	0.48
1:B:9:LYS:HE2	1:B:11:PHE:CZ	2.48	0.48
1:D:258:VAL:HG13	1:D:280:THR:HG23	1.97	0.47
1:D:219:TYR:CZ	1:D:283:ARG:HB2	2.49	0.47
1:B:52:GLU:HG2	1:B:52:GLU:O	2.14	0.47
1:D:121:PRO:HB3	1:D:230:TYR:CE2	2.49	0.47
1:A:55:ILE:O	1:A:55:ILE:HD12	2.14	0.47
1:D:88:LYS:HG3	1:D:113:GLN:OE1	2.13	0.47
1:A:33:LEU:CB	1:A:66:VAL:HB	2.39	0.47
1:A:42:LEU:HD11	1:A:91:ILE:HD11	1.97	0.47
1:B:141:MET:HB2	1:B:163:GLY:O	2.15	0.47
1:B:168:LEU:HG	1:B:169:GLN:CG	2.32	0.47
1:D:224:ILE:HG12	1:D:279:LEU:HD13	1.96	0.47
1:D:221:PRO:HA	1:D:281:VAL:HG12	1.97	0.47
1:C:148:ALA:HB1	1:C:153:ILE:HB	1.97	0.46
1:B:278:LYS:HG2	1:B:278:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PRO:CA	1:B:87:TRP:HD1	2.15	0.46
1:A:141:MET:N	1:A:163:GLY:O	2.49	0.46
1:B:267:ASP:OD2	1:B:271:ASN:HB2	2.15	0.46
1:B:141:MET:HE1	1:B:165:VAL:CG2	2.45	0.46
1:A:148:ALA:HB1	1:A:153:ILE:HB	1.97	0.46
1:A:204:GLY:HA3	1:A:246:ARG:HH21	1.77	0.46
1:B:80:PHE:HE2	1:B:114:LEU:HD13	1.80	0.45
1:D:110:MET:HG2	1:D:111:GLU:N	2.31	0.45
1:A:46:ALA:C	1:A:48:GLY:N	2.70	0.45
1:A:50:LEU:HD12	1:A:55:ILE:HG21	1.98	0.45
1:C:170:ASP:O	1:C:243:LYS:CD	2.65	0.45
1:A:9:LYS:HG2	1:A:11:PHE:CE2	2.51	0.45
1:B:71:GLU:O	1:B:97:LYS:HD2	2.17	0.45
1:B:40:ASP:HB2	1:B:192:ALA:O	2.17	0.45
1:A:132:MET:HE1	1:A:238:TYR:HE2	1.81	0.44
1:C:205:SER:O	1:C:209:LEU:HD13	2.16	0.44
1:D:28:HIS:O	1:D:29:GLN:HB2	2.16	0.44
1:A:42:LEU:CD1	1:A:91:ILE:HD11	2.47	0.44
1:B:17:HIS:CE1	1:B:31:ARG:HD2	2.53	0.44
1:C:162:GLU:OE1	1:C:162:GLU:HA	2.17	0.44
1:D:267:ASP:HB3	1:D:273:LEU:HD21	1.99	0.44
1:B:140:ASP:O	1:B:142:HIS:N	2.50	0.44
1:C:295:HIS:NE2	1:D:133:LYS:HD3	2.33	0.44
1:B:148:ALA:HB1	1:B:153:ILE:HB	2.00	0.44
1:B:169:GLN:HE21	1:B:171:LYS:HE2	1.83	0.44
1:B:141:MET:HE1	1:B:165:VAL:HG23	2.00	0.43
1:B:9:LYS:HE2	1:B:11:PHE:CE2	2.53	0.43
1:C:169:GLN:O	1:C:170:ASP:HB2	2.17	0.43
1:C:33:LEU:HD11	1:C:37:THR:HG21	2.00	0.43
1:C:16:SER:HA	1:C:73:ASP:HB3	2.00	0.43
1:A:219:TYR:HA	1:A:283:ARG:HA	2.00	0.43
1:B:63:LYS:HB2	1:B:64:GLN:H	1.60	0.43
1:A:32:VAL:CG1	1:A:33:LEU:H	2.30	0.43
1:C:207:PHE:CE2	1:C:243:LYS:HG3	2.53	0.43
1:C:235:LYS:HE2	1:C:235:LYS:HB3	1.83	0.43
1:D:20:TYR:HB3	1:D:158:PHE:CG	2.54	0.43
1:D:285:ARG:NH1	1:D:286:GLN:HB2	2.34	0.43
1:D:60:ILE:HA	1:D:112:CYS:HB3	2.00	0.43
1:B:282:LYS:HB3	1:B:282:LYS:HE3	1.52	0.42
1:A:15:ILE:HG13	1:A:33:LEU:HD22	2.01	0.42
1:A:285:ARG:CA	1:A:285:ARG:NE	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LYS:HG2	1:C:89:VAL:N	2.34	0.42
1:A:50:LEU:O	1:A:53:ARG:NH2	2.36	0.42
1:B:249:SER:OG	1:B:257:ASP:OD1	2.24	0.42
1:A:34:PRO:O	1:A:37:THR:HB	2.19	0.42
1:B:20:TYR:HB3	1:B:158:PHE:CG	2.55	0.42
1:B:236:THR:O	1:B:238:TYR:CE1	2.73	0.42
1:C:174:LEU:HD11	1:C:238:TYR:HB3	2.01	0.42
1:C:91:ILE:HD12	1:C:110:MET:CE	2.50	0.42
1:A:7:GLN:N	1:A:82:PRO:HG3	2.35	0.41
1:C:96:ALA:HA	1:C:102:LEU:HD13	2.01	0.41
1:C:227:PHE:CE1	1:C:229:MET:HE1	2.55	0.41
1:B:176:GLU:HG3	1:B:238:TYR:CE2	2.55	0.41
1:B:234:PRO:HB2	1:B:235:LYS:H	1.61	0.41
1:C:141:MET:CE	1:C:175:MET:CE	2.98	0.41
1:C:278:LYS:O	1:C:279:LEU:C	2.59	0.41
1:C:91:ILE:CD1	1:C:110:MET:HE1	2.50	0.41
1:D:67:VAL:O	1:D:74:LYS:NZ	2.53	0.41
1:A:258:VAL:HG13	1:A:280:THR:CG2	2.50	0.41
1:A:285:ARG:HA	1:A:285:ARG:NH1	2.34	0.41
1:D:60:ILE:CG2	1:D:110:MET:CE	2.99	0.41
1:A:219:TYR:CZ	1:A:283:ARG:CB	2.89	0.41
1:A:60:ILE:HB	1:A:224:ILE:HB	2.03	0.41
1:C:17:HIS:CE1	1:C:31:ARG:HD2	2.55	0.40
1:D:60:ILE:CG2	1:D:110:MET:HE3	2.51	0.40
1:D:179:LEU:HB3	1:D:183:ALA:HB3	2.03	0.40
1:B:236:THR:HG22	1:B:236:THR:O	2.21	0.40
1:A:144:ILE:HG13	1:A:165:VAL:CG2	2.49	0.40
1:D:144:ILE:HG13	1:D:165:VAL:CG2	2.47	0.40
1:A:141:MET:HE3	1:A:177:LEU:HD23	2.04	0.40
1:B:9:LYS:HG2	1:B:11:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/300 (94%)	266 (94%)	14 (5%)	2 (1%)	26	25
1	B	285/300 (95%)	272 (95%)	11 (4%)	2 (1%)	26	25
1	C	285/300 (95%)	277 (97%)	8 (3%)	0	100	100
1	D	278/300 (93%)	268 (96%)	9 (3%)	1 (0%)	39	41
All	All	1130/1200 (94%)	1083 (96%)	42 (4%)	5 (0%)	39	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	B	141	MET
1	B	234	PRO
1	A	125	GLU
1	D	112	CYS

### 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	252/263 (96%)	247 (98%)	5 (2%)	63	75
1	B	254/263 (97%)	249 (98%)	5 (2%)	63	75
1	C	254/263 (97%)	254 (100%)	0	100	100
1	D	250/263 (95%)	246 (98%)	4 (2%)	70	82
All	All	1010/1052 (96%)	996 (99%)	14 (1%)	74	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	118	GLU
1	A	124	LYS

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Mol	Chain	Res	Type
1	A	245	SER
1	A	283	ARG
1	B	63	LYS
1	B	85	ASP
1	B	122	ARG
1	B	235	LYS
1	B	268	ARG
1	D	5	THR
1	D	6	ASP
1	D	111	GLU
1	D	170	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	167	GLN
1	A	286	GLN
1	B	169	GLN
1	B	286	GLN
1	C	286	GLN
1	D	296	HIS

### 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 ⓘ

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	286/300 (95%)	-0.26	5 (1%) 73 72	20, 28, 48, 61	0
1	B	289/300 (96%)	-0.40	4 (1%) 78 77	17, 27, 40, 59	0
1	C	289/300 (96%)	-0.47	0 100 100	16, 26, 43, 55	0
1	D	284/300 (94%)	-0.44	0 100 100	19, 27, 43, 52	0
All	All	1148/1200 (95%)	-0.39	9 (0%) 87 87	16, 27, 44, 61	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	MET	8.8
1	B	85	ASP	5.2
1	A	7	GLN	4.0
1	A	284	VAL	3.5
1	B	84	ARG	2.6
1	B	236	THR	2.6
1	A	119	ASP	2.5
1	B	87	TRP	2.4
1	A	259	TYR	2.3

### 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.