



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:35 AM GMT

PDB ID : 3FBQ  
Title : The crystal structure of the conserved domain protein from Bacillus anthracis  
Authors : Zhang, R.; Joachimiak, G.; Kim, Y.; Gornicki, P.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-11-19  
Resolution : 2.71 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

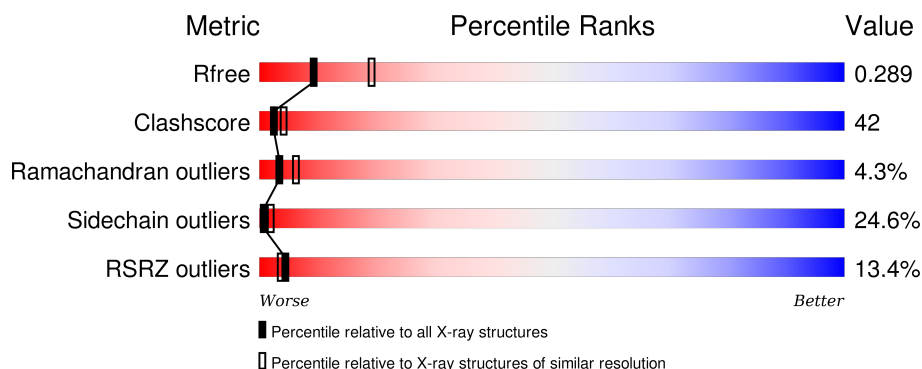
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	292	<div> <div>13%</div> <div>41%</div> <div>37%</div> <div>15%</div> <div>• •</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2249 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 Conserved domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2222	1387	384	444	7			

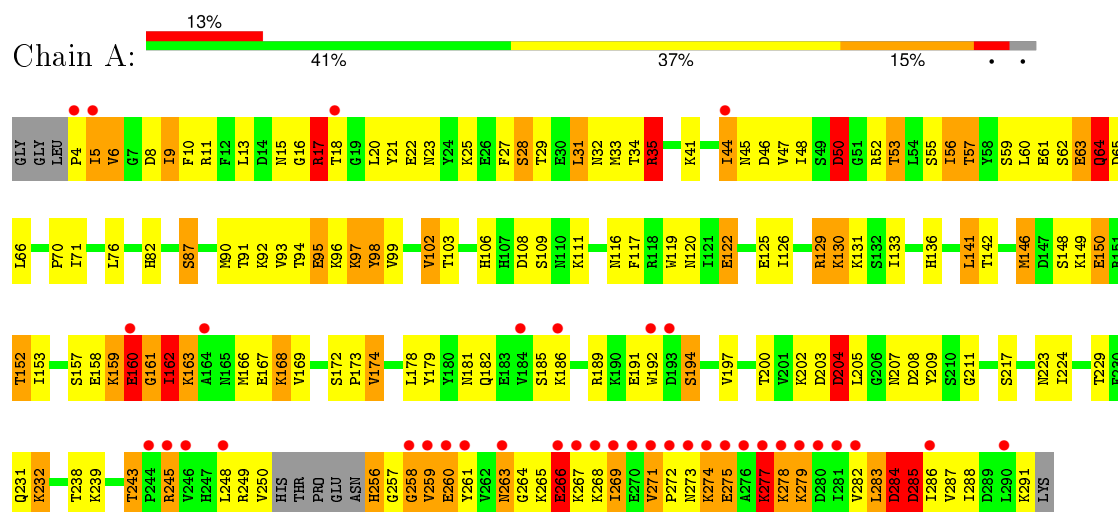
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		

### 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: Conserved domain protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.41Å 101.41Å 101.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.80 – 2.71 45.35 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.6 (71.80-2.71) 99.6 (45.35-2.71)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, $R_{free}$	0.206 , 0.283 0.224 , 0.289	Depositor DCC
$R_{free}$ test set	463 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.8	EDS
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 9691 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.01	1/2257 (0.0%)	1.12	11/3035 (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	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	GLU	CD-OE2	5.78	1.32	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	VAL	C-N-CD	-15.62	86.24	120.60
1	A	82	HIS	CB-CA-C	6.48	123.36	110.40
1	A	31	LEU	CA-CB-CG	6.08	129.30	115.30
1	A	285	ASP	N-CA-C	5.91	126.95	111.00
1	A	146	MET	CG-SD-CE	-5.76	90.98	100.20
1	A	17	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	82	HIS	C-N-CA	-5.30	111.17	122.30
1	A	98	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	11	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	17	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	35	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	LYS	Peptide
1	A	15	ASN	Peptide
1	A	16	GLY	Peptide
1	A	161	GLY	Peptide
1	A	162	ILE	Peptide
1	A	204	ASP	Peptide
1	A	256	HIS	Peptide
1	A	257	GLY	Peptide
1	A	258	GLY	Peptide
1	A	263	ASN	Peptide
1	A	264	GLY	Peptide
1	A	277	LYS	Peptide
1	A	4	PRO	Peptide
1	A	50	ASP	Peptide
1	A	63	GLU	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	2222	0	2202	187	1
2	A	27	0	0	7	0
All	All	2249	0	2202	187	1

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 42.

All (187) 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:191:GLU:HG3	1:A:192:TRP:CD1	1.74	1.23
1:A:283:LEU:HD22	1:A:283:LEU:N	1.55	1.14
1:A:269:ILE:H	1:A:269:ILE:HD12	1.00	1.10
1:A:162:ILE:HG22	1:A:162:ILE:O	1.54	1.08
1:A:274:LYS:HB3	1:A:277:LYS:HB2	1.34	1.06
1:A:282:VAL:C	1:A:283:LEU:HD22	1.77	1.04
1:A:265:LYS:O	1:A:266:GLU:HB3	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:O	1:A:285:ASP:HB2	1.59	1.02
1:A:94:THR:HG22	1:A:96:LYS:H	1.22	1.02
1:A:90:MET:HE2	1:A:98:TYR:CD2	1.98	0.98
1:A:269:ILE:N	1:A:269:ILE:HD12	1.79	0.97
1:A:260:GLU:O	1:A:271:VAL:HG13	1.66	0.93
1:A:283:LEU:CD2	1:A:283:LEU:N	2.30	0.92
1:A:5:ILE:HG22	1:A:6:VAL:H	1.35	0.92
1:A:269:ILE:H	1:A:269:ILE:CD1	1.83	0.92
1:A:45:ASN:HB2	1:A:57:THR:HG22	1.51	0.91
1:A:271:VAL:HG11	1:A:275:GLU:HG2	1.56	0.88
1:A:5:ILE:HG21	1:A:99:VAL:CG1	2.04	0.87
1:A:5:ILE:HG22	1:A:6:VAL:N	1.87	0.85
1:A:44:ILE:HG22	1:A:44:ILE:O	1.76	0.85
1:A:50:ASP:HB2	1:A:53:THR:H	1.41	0.85
1:A:9:ILE:HD11	1:A:13:LEU:HD12	1.58	0.85
1:A:50:ASP:HB3	1:A:52:ARG:H	1.43	0.84
1:A:106:HIS:CD2	1:A:108:ASP:HB3	2.14	0.82
1:A:90:MET:HE2	1:A:98:TYR:CG	2.14	0.82
1:A:191:GLU:HG3	1:A:192:TRP:NE1	1.97	0.80
1:A:29:THR:O	1:A:47:VAL:HG12	1.82	0.79
1:A:29:THR:HB	1:A:47:VAL:CG1	2.13	0.79
1:A:259:VAL:HG13	1:A:260:GLU:H	1.47	0.79
1:A:25:LYS:HG3	1:A:46:ASP:OD1	1.83	0.78
1:A:182:GLN:NE2	1:A:197:VAL:HG23	1.97	0.78
1:A:9:ILE:HD11	1:A:13:LEU:CD1	2.13	0.78
1:A:256:HIS:HD2	1:A:279:LYS:NZ	1.81	0.77
1:A:66:LEU:HB3	1:A:70:PRO:HG3	1.67	0.77
1:A:259:VAL:CG1	1:A:260:GLU:N	2.48	0.76
1:A:9:ILE:CD1	1:A:13:LEU:CD1	2.67	0.72
1:A:259:VAL:CG1	1:A:260:GLU:H	2.03	0.72
1:A:283:LEU:C	1:A:284:ASP:OD2	2.29	0.71
1:A:265:LYS:O	1:A:266:GLU:CB	2.38	0.71
1:A:5:ILE:HG21	1:A:99:VAL:HG11	1.72	0.71
1:A:44:ILE:CG2	1:A:44:ILE:O	2.39	0.70
1:A:92:LYS:HZ2	1:A:95:GLU:HA	1.57	0.70
1:A:245:ARG:HH11	1:A:245:ARG:CG	2.05	0.69
1:A:278:LYS:O	1:A:279:LYS:HG2	1.92	0.69
1:A:106:HIS:HD2	1:A:108:ASP:H	1.42	0.68
1:A:249:ARG:HG3	1:A:279:LYS:HB3	1.76	0.68
1:A:274:LYS:HB3	1:A:277:LYS:CB	2.19	0.67
1:A:90:MET:CE	1:A:98:TYR:HB3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HG22	1:A:6:VAL:HG13	1.78	0.66
1:A:9:ILE:CD1	1:A:13:LEU:HD12	2.26	0.66
1:A:159:LYS:O	1:A:161:GLY:N	2.29	0.65
1:A:203:ASP:O	1:A:205:LEU:N	2.30	0.65
1:A:284:ASP:OD2	1:A:284:ASP:N	2.29	0.65
1:A:9:ILE:HD12	1:A:13:LEU:HG	1.78	0.65
1:A:168:LYS:HB3	1:A:179:TYR:CD2	2.33	0.64
1:A:163:LYS:HG3	1:A:163:LYS:O	1.97	0.64
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.63	0.64
1:A:258:GLY:O	1:A:259:VAL:HG23	1.99	0.63
1:A:76:LEU:HD22	1:A:102:VAL:HG22	1.80	0.63
1:A:256:HIS:CD2	1:A:279:LYS:NZ	2.65	0.62
1:A:185:SER:O	1:A:189:ARG:HG3	1.99	0.62
1:A:90:MET:HE2	1:A:98:TYR:HB3	1.81	0.62
1:A:259:VAL:HG13	1:A:271:VAL:CG1	2.30	0.61
1:A:245:ARG:HG2	1:A:245:ARG:HH11	1.64	0.60
1:A:117:PHE:CZ	1:A:141:LEU:HD11	2.37	0.60
1:A:62:SER:OG	1:A:63:GLU:N	2.35	0.60
1:A:191:GLU:CD	1:A:192:TRP:HE1	2.06	0.59
1:A:10:PHE:HB3	1:A:21:TYR:HB3	1.82	0.59
1:A:90:MET:CE	1:A:98:TYR:CG	2.86	0.59
1:A:259:VAL:HG12	1:A:260:GLU:N	2.17	0.59
1:A:90:MET:HE2	1:A:98:TYR:CB	2.32	0.59
1:A:5:ILE:CG2	1:A:6:VAL:H	2.03	0.58
1:A:256:HIS:HD2	1:A:279:LYS:HZ1	1.50	0.58
1:A:50:ASP:CB	1:A:52:ARG:H	2.15	0.58
1:A:191:GLU:CG	1:A:192:TRP:NE1	2.66	0.57
1:A:29:THR:HB	1:A:47:VAL:HG13	1.84	0.56
1:A:34:THR:HG21	1:A:41:LYS:CE	2.34	0.56
1:A:256:HIS:CD2	1:A:279:LYS:HZ2	2.22	0.56
1:A:152:THR:HG23	2:A:297:HOH:O	2.04	0.56
1:A:243:THR:HG23	2:A:300:HOH:O	2.06	0.56
1:A:106:HIS:HD2	1:A:108:ASP:HB3	1.64	0.56
1:A:243:THR:HG22	1:A:285:ASP:OD1	2.06	0.56
1:A:29:THR:HB	1:A:47:VAL:HG12	1.88	0.55
1:A:94:THR:HG22	1:A:96:LYS:N	2.07	0.55
1:A:282:VAL:CA	1:A:283:LEU:HD22	2.37	0.55
1:A:50:ASP:OD2	1:A:53:THR:HG23	2.07	0.54
1:A:44:ILE:CD1	1:A:56:ILE:HD13	2.37	0.54
1:A:90:MET:CE	1:A:98:TYR:CB	2.86	0.54
1:A:116:ASN:OD1	1:A:142:THR:CG2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:CZ	1:A:141:LEU:CD1	2.91	0.54
1:A:158:GLU:HG3	1:A:163:LYS:HB2	1.90	0.53
1:A:27:PHE:CD1	1:A:146:MET:HE1	2.44	0.52
1:A:211:GLY:HA2	1:A:229:THR:O	2.09	0.52
1:A:136:HIS:HD2	2:A:306:HOH:O	1.91	0.52
1:A:5:ILE:CG2	1:A:6:VAL:N	2.58	0.52
1:A:117:PHE:HZ	1:A:141:LEU:HD11	1.74	0.52
1:A:5:ILE:CG2	1:A:99:VAL:HG11	2.40	0.52
1:A:238:THR:HG22	1:A:239:LYS:HG3	1.90	0.52
1:A:61:GLU:HA	1:A:96:LYS:O	2.09	0.51
1:A:44:ILE:HD13	1:A:56:ILE:HD13	1.91	0.51
1:A:60:LEU:HD23	1:A:90:MET:CE	2.41	0.51
1:A:34:THR:HG21	1:A:41:LYS:HE2	1.92	0.51
1:A:271:VAL:CG1	1:A:275:GLU:HG2	2.35	0.51
1:A:71:ILE:HB	1:A:125:GLU:HB2	1.93	0.51
1:A:111:LYS:NZ	1:A:148:SER:OG	2.36	0.50
1:A:284:ASP:O	1:A:285:ASP:CB	2.43	0.50
1:A:62:SER:CB	1:A:66:LEU:HD21	2.41	0.50
1:A:95:GLU:N	1:A:95:GLU:OE2	2.44	0.50
1:A:271:VAL:HG21	1:A:275:GLU:HG2	1.93	0.50
1:A:17:ARG:NH1	1:A:17:ARG:HG3	2.27	0.50
1:A:92:LYS:NZ	1:A:95:GLU:HA	2.26	0.50
1:A:116:ASN:OD1	1:A:142:THR:HG21	2.12	0.50
1:A:167:GLU:OE1	1:A:181:ASN:ND2	2.43	0.50
1:A:166:MET:HG3	1:A:288:ILE:HD11	1.93	0.49
1:A:191:GLU:OE1	1:A:192:TRP:NE1	2.45	0.49
1:A:191:GLU:CD	1:A:192:TRP:NE1	2.66	0.49
1:A:243:THR:CG2	2:A:300:HOH:O	2.61	0.48
1:A:9:ILE:HD12	1:A:13:LEU:CG	2.43	0.48
1:A:90:MET:HE3	1:A:98:TYR:HB3	1.95	0.48
1:A:259:VAL:HG13	1:A:271:VAL:HG12	1.96	0.48
1:A:17:ARG:CG	1:A:17:ARG:HH11	2.27	0.48
1:A:23:ASN:HB2	1:A:174:VAL:HG22	1.97	0.47
1:A:31:LEU:O	1:A:32:ASN:C	2.52	0.47
1:A:5:ILE:CG2	1:A:99:VAL:CG1	2.87	0.47
1:A:159:LYS:HB3	1:A:160:GLU:H	1.48	0.47
1:A:64:GLN:HE21	1:A:133:ILE:HD11	1.79	0.47
1:A:64:GLN:H	1:A:96:LYS:HD2	1.79	0.47
1:A:126:ILE:HG22	1:A:129:ARG:H	1.78	0.47
1:A:159:LYS:C	1:A:161:GLY:H	2.18	0.47
1:A:34:THR:HG21	1:A:41:LYS:HE3	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HB3	1:A:197:VAL:HG21	1.97	0.46
1:A:64:GLN:NE2	1:A:133:ILE:HD11	2.30	0.46
1:A:169:VAL:HG23	1:A:178:LEU:HD23	1.97	0.46
1:A:194:SER:O	1:A:194:SER:OG	2.31	0.46
1:A:129:ARG:O	1:A:131:LYS:HB2	2.16	0.46
1:A:103:THR:HG22	2:A:298:HOH:O	2.15	0.46
1:A:192:TRP:CE3	1:A:248:LEU:HB3	2.50	0.46
1:A:245:ARG:NH1	1:A:245:ARG:CG	2.69	0.46
1:A:44:ILE:HG13	1:A:119:TRP:CE3	2.51	0.46
1:A:44:ILE:HG13	1:A:119:TRP:CZ3	2.51	0.46
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.73	0.45
1:A:266:GLU:CG	1:A:266:GLU:O	2.65	0.45
1:A:50:ASP:CB	1:A:53:THR:H	2.20	0.45
1:A:266:GLU:HA	1:A:267:LYS:HA	1.54	0.45
1:A:146:MET:HB2	1:A:146:MET:HE2	1.47	0.44
1:A:28:SER:OG	1:A:48:ILE:HB	2.18	0.44
1:A:8:ASP:C	1:A:8:ASP:OD1	2.55	0.44
1:A:45:ASN:N	1:A:57:THR:O	2.49	0.44
1:A:34:THR:O	1:A:35:ARG:HD3	2.18	0.44
1:A:209:TYR:HD2	1:A:231:GLN:HB2	1.82	0.44
1:A:120:ASN:HB3	2:A:317:HOH:O	2.18	0.44
1:A:106:HIS:HD2	1:A:108:ASP:CB	2.30	0.44
1:A:266:GLU:HG3	1:A:266:GLU:O	2.17	0.43
1:A:95:GLU:CA	1:A:95:GLU:OE2	2.66	0.43
1:A:203:ASP:C	1:A:205:LEU:N	2.68	0.43
1:A:282:VAL:HA	1:A:283:LEU:HD22	2.00	0.43
1:A:161:GLY:O	1:A:185:SER:N	2.51	0.43
1:A:52:ARG:HG3	1:A:53:THR:HG22	2.00	0.43
1:A:256:HIS:HD2	1:A:279:LYS:HZ2	1.54	0.43
1:A:191:GLU:HG3	1:A:192:TRP:HD1	1.60	0.43
1:A:60:LEU:HD23	1:A:90:MET:HE3	2.01	0.43
1:A:282:VAL:O	1:A:283:LEU:HD13	2.18	0.43
1:A:62:SER:HB3	1:A:66:LEU:HD21	2.01	0.43
1:A:271:VAL:HG11	1:A:275:GLU:CG	2.39	0.43
1:A:278:LYS:HD2	1:A:278:LYS:HA	1.37	0.43
1:A:94:THR:HB	1:A:97:LYS:HB2	2.01	0.42
1:A:62:SER:HB2	1:A:66:LEU:HD21	1.99	0.42
1:A:70:PRO:HG2	1:A:90:MET:HE1	2.01	0.42
1:A:202:LYS:HA	1:A:207:ASN:O	2.19	0.42
1:A:106:HIS:CD2	1:A:108:ASP:H	2.30	0.42
1:A:9:ILE:CD1	1:A:13:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.89	0.42
1:A:60:LEU:HD23	1:A:90:MET:HE1	2.02	0.41
1:A:203:ASP:OD1	1:A:205:LEU:HB3	2.20	0.41
1:A:286:ILE:HG22	1:A:287:VAL:N	2.34	0.41
1:A:265:LYS:HG2	1:A:265:LYS:H	1.66	0.41
1:A:111:LYS:HE2	1:A:150:GLU:OE2	2.20	0.41
1:A:217:SER:O	1:A:224:ILE:HA	2.21	0.41
1:A:172:SER:HB2	1:A:173:PRO:CD	2.50	0.41
1:A:260:GLU:O	1:A:261:TYR:HD2	2.02	0.41
1:A:22:GLU:O	1:A:22:GLU:HG3	2.17	0.41
1:A:245:ARG:NH1	1:A:283:LEU:HD12	2.36	0.41
1:A:231:GLN:O	1:A:232:LYS:C	2.60	0.40
1:A:191:GLU:CG	1:A:192:TRP:CD1	2.70	0.40
1:A:259:VAL:CG1	1:A:271:VAL:CG1	2.97	0.40
1:A:223:ASN:C	1:A:224:ILE:HD13	2.42	0.40
1:A:87:SER:HB3	2:A:313:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:CD2	1:A:260:GLU:OE1[2_555]	1.79	0.41

## 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	279/292 (96%)	249 (89%)	18 (6%)	12 (4%)	<b>3</b> <b>6</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	162	ILE
1	A	266	GLU
1	A	285	ASP
1	A	64	GLN
1	A	259	VAL
1	A	5	ILE
1	A	160	GLU
1	A	204	ASP
1	A	232	LYS
1	A	272	PRO
1	A	284	ASP

### 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	248/255 (97%)	187 (75%)	61 (25%)	<b>1</b> <b>2</b>

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	9	ILE
1	A	17	ARG
1	A	18	THR
1	A	20	LEU
1	A	28	SER
1	A	33	MET
1	A	35	ARG
1	A	44	ILE
1	A	50	ASP
1	A	53	THR
1	A	55	SER
1	A	56	ILE
1	A	57	THR
1	A	59	SER

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Mol	Chain	Res	Type
1	A	64	GLN
1	A	65	ASP
1	A	87	SER
1	A	91	THR
1	A	93	VAL
1	A	95	GLU
1	A	97	LYS
1	A	102	VAL
1	A	109	SER
1	A	122	GLU
1	A	129	ARG
1	A	130	LYS
1	A	141	LEU
1	A	149	LYS
1	A	150	GLU
1	A	152	THR
1	A	153	ILE
1	A	157	SER
1	A	160	GLU
1	A	162	ILE
1	A	163	LYS
1	A	168	LYS
1	A	174	VAL
1	A	186	LYS
1	A	194	SER
1	A	200	THR
1	A	204	ASP
1	A	208	ASP
1	A	243	THR
1	A	245	ARG
1	A	250	VAL
1	A	260	GLU
1	A	263	ASN
1	A	266	GLU
1	A	268	LYS
1	A	269	ILE
1	A	273	ASN
1	A	274	LYS
1	A	275	GLU
1	A	277	LYS
1	A	278	LYS
1	A	279	LYS

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	284	ASP
1	A	285	ASP
1	A	291	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	45	ASN
1	A	64	GLN
1	A	82	HIS
1	A	106	HIS
1	A	136	HIS
1	A	138	ASN
1	A	182	GLN
1	A	256	HIS
1	A	263	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	283/292 (96%)	0.69	38 (13%) 4 3	21, 36, 66, 79	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ILE	13.3
1	A	280	ASP	7.9
1	A	261	TYR	6.5
1	A	268	LYS	6.2
1	A	260	GLU	5.7
1	A	276	ALA	5.6
1	A	272	PRO	5.3
1	A	278	LYS	4.6
1	A	271	VAL	4.2
1	A	275	GLU	3.8
1	A	263	ASN	3.7
1	A	266	GLU	3.7
1	A	248	LEU	3.7
1	A	270	GLU	3.5
1	A	267	LYS	3.4
1	A	186	LYS	3.3
1	A	279	LYS	3.2
1	A	259	VAL	3.2
1	A	164	ALA	2.9
1	A	4	PRO	2.9
1	A	192	TRP	2.8
1	A	274	LYS	2.6
1	A	5	ILE	2.6
1	A	18	THR	2.6
1	A	282	VAL	2.4
1	A	246	VAL	2.4
1	A	273	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	286	ILE	2.3
1	A	245	ARG	2.3
1	A	281	ILE	2.2
1	A	258	GLY	2.2
1	A	184	VAL	2.2
1	A	193	ASP	2.2
1	A	44	ILE	2.1
1	A	290	LEU	2.1
1	A	160	GLU	2.1
1	A	244	PRO	2.1
1	A	277	LYS	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.