Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID	:	3U49
Title	:	Crystal structure of YwfH, NADPH dependent reductase involved in Bacilysin biosynthesis
Authors	:	Rajavel, M.; Gopal, B.
Deposited on	:	2011-10-07
Resolution	:	1.75 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

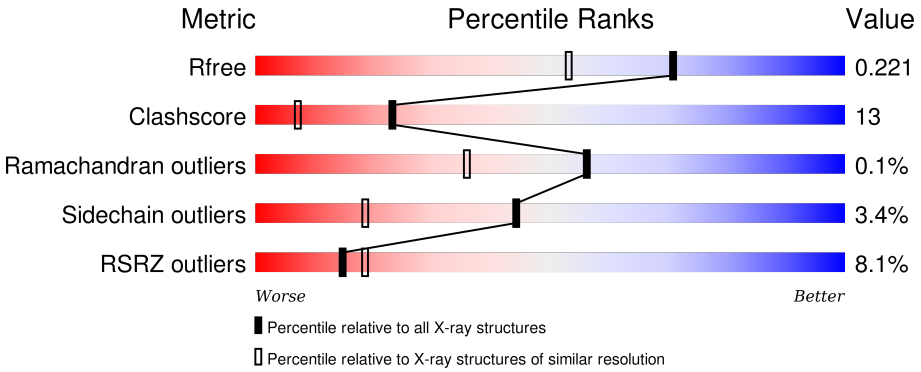
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 >=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 <=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	281	6% 75% 11% • 11%
1	B	281	7% 72% 15% • 11%
1	C	281	9% 70% 17% • 10%
1	D	281	6% 74% 11% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8008 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 Bacilysin biosynthesis oxidoreductase ywfH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1881	1174	330	364	13			
1	B	251	Total	C	N	O	S	0	4	0
			1941	1209	342	377	13			
1	C	252	Total	C	N	O	S	0	1	0
			1907	1186	338	370	13			
1	D	242	Total	C	N	O	S	0	4	0
			1869	1160	332	364	13			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P39644
A	-18	GLY	-	EXPRESSION TAG	UNP P39644
A	-17	SER	-	EXPRESSION TAG	UNP P39644
A	-16	SER	-	EXPRESSION TAG	UNP P39644
A	-15	HIS	-	EXPRESSION TAG	UNP P39644
A	-14	HIS	-	EXPRESSION TAG	UNP P39644
A	-13	HIS	-	EXPRESSION TAG	UNP P39644
A	-12	HIS	-	EXPRESSION TAG	UNP P39644
A	-11	HIS	-	EXPRESSION TAG	UNP P39644
A	-10	HIS	-	EXPRESSION TAG	UNP P39644
A	-9	SER	-	EXPRESSION TAG	UNP P39644
A	-8	SER	-	EXPRESSION TAG	UNP P39644
A	-7	GLY	-	EXPRESSION TAG	UNP P39644
A	-6	LEU	-	EXPRESSION TAG	UNP P39644
A	-5	VAL	-	EXPRESSION TAG	UNP P39644
A	-4	PRO	-	EXPRESSION TAG	UNP P39644
A	-3	ARG	-	EXPRESSION TAG	UNP P39644
A	-2	GLY	-	EXPRESSION TAG	UNP P39644
A	-1	SER	-	EXPRESSION TAG	UNP P39644
A	0	HIS	-	EXPRESSION TAG	UNP P39644
A	260	LEU	-	CLONING ARTIFACT	UNP P39644

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Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLU	-	CLONING ARTIFACT	UNP P39644
B	-19	MET	-	EXPRESSION TAG	UNP P39644
B	-18	GLY	-	EXPRESSION TAG	UNP P39644
B	-17	SER	-	EXPRESSION TAG	UNP P39644
B	-16	SER	-	EXPRESSION TAG	UNP P39644
B	-15	HIS	-	EXPRESSION TAG	UNP P39644
B	-14	HIS	-	EXPRESSION TAG	UNP P39644
B	-13	HIS	-	EXPRESSION TAG	UNP P39644
B	-12	HIS	-	EXPRESSION TAG	UNP P39644
B	-11	HIS	-	EXPRESSION TAG	UNP P39644
B	-10	HIS	-	EXPRESSION TAG	UNP P39644
B	-9	SER	-	EXPRESSION TAG	UNP P39644
B	-8	SER	-	EXPRESSION TAG	UNP P39644
B	-7	GLY	-	EXPRESSION TAG	UNP P39644
B	-6	LEU	-	EXPRESSION TAG	UNP P39644
B	-5	VAL	-	EXPRESSION TAG	UNP P39644
B	-4	PRO	-	EXPRESSION TAG	UNP P39644
B	-3	ARG	-	EXPRESSION TAG	UNP P39644
B	-2	GLY	-	EXPRESSION TAG	UNP P39644
B	-1	SER	-	EXPRESSION TAG	UNP P39644
B	0	HIS	-	EXPRESSION TAG	UNP P39644
B	260	LEU	-	CLONING ARTIFACT	UNP P39644
B	261	GLU	-	CLONING ARTIFACT	UNP P39644
C	-19	MET	-	EXPRESSION TAG	UNP P39644
C	-18	GLY	-	EXPRESSION TAG	UNP P39644
C	-17	SER	-	EXPRESSION TAG	UNP P39644
C	-16	SER	-	EXPRESSION TAG	UNP P39644
C	-15	HIS	-	EXPRESSION TAG	UNP P39644
C	-14	HIS	-	EXPRESSION TAG	UNP P39644
C	-13	HIS	-	EXPRESSION TAG	UNP P39644
C	-12	HIS	-	EXPRESSION TAG	UNP P39644
C	-11	HIS	-	EXPRESSION TAG	UNP P39644
C	-10	HIS	-	EXPRESSION TAG	UNP P39644
C	-9	SER	-	EXPRESSION TAG	UNP P39644
C	-8	SER	-	EXPRESSION TAG	UNP P39644
C	-7	GLY	-	EXPRESSION TAG	UNP P39644
C	-6	LEU	-	EXPRESSION TAG	UNP P39644
C	-5	VAL	-	EXPRESSION TAG	UNP P39644
C	-4	PRO	-	EXPRESSION TAG	UNP P39644
C	-3	ARG	-	EXPRESSION TAG	UNP P39644
C	-2	GLY	-	EXPRESSION TAG	UNP P39644
C	-1	SER	-	EXPRESSION TAG	UNP P39644

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	EXPRESSION TAG	UNP P39644
C	260	LEU	-	CLONING ARTIFACT	UNP P39644
C	261	GLU	-	CLONING ARTIFACT	UNP P39644
D	-19	MET	-	EXPRESSION TAG	UNP P39644
D	-18	GLY	-	EXPRESSION TAG	UNP P39644
D	-17	SER	-	EXPRESSION TAG	UNP P39644
D	-16	SER	-	EXPRESSION TAG	UNP P39644
D	-15	HIS	-	EXPRESSION TAG	UNP P39644
D	-14	HIS	-	EXPRESSION TAG	UNP P39644
D	-13	HIS	-	EXPRESSION TAG	UNP P39644
D	-12	HIS	-	EXPRESSION TAG	UNP P39644
D	-11	HIS	-	EXPRESSION TAG	UNP P39644
D	-10	HIS	-	EXPRESSION TAG	UNP P39644
D	-9	SER	-	EXPRESSION TAG	UNP P39644
D	-8	SER	-	EXPRESSION TAG	UNP P39644
D	-7	GLY	-	EXPRESSION TAG	UNP P39644
D	-6	LEU	-	EXPRESSION TAG	UNP P39644
D	-5	VAL	-	EXPRESSION TAG	UNP P39644
D	-4	PRO	-	EXPRESSION TAG	UNP P39644
D	-3	ARG	-	EXPRESSION TAG	UNP P39644
D	-2	GLY	-	EXPRESSION TAG	UNP P39644
D	-1	SER	-	EXPRESSION TAG	UNP P39644
D	0	HIS	-	EXPRESSION TAG	UNP P39644
D	260	LEU	-	CLONING ARTIFACT	UNP P39644
D	261	GLU	-	CLONING ARTIFACT	UNP P39644

- Molecule 2 is water.

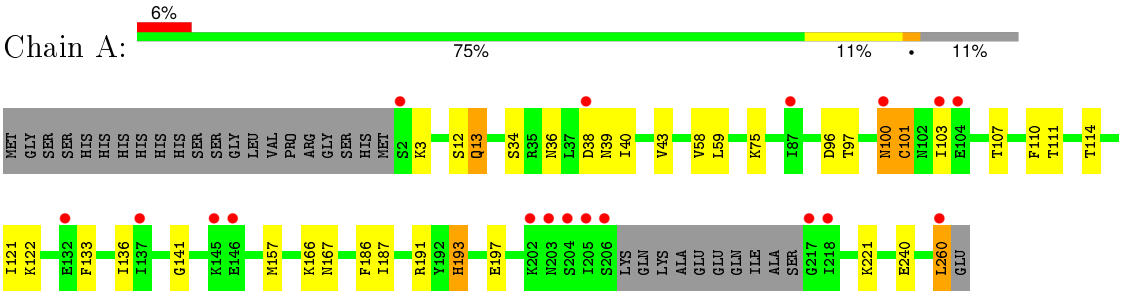
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	122	Total O 122 122	0	0
2	B	77	Total O 77 77	0	0
2	C	90	Total O 90 90	0	0
2	D	121	Total O 121 121	0	0

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 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.

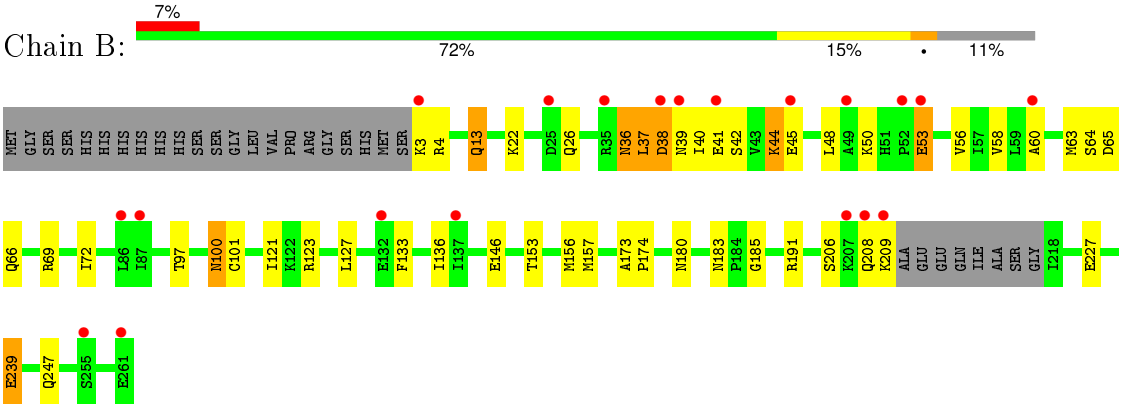
- Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain A:



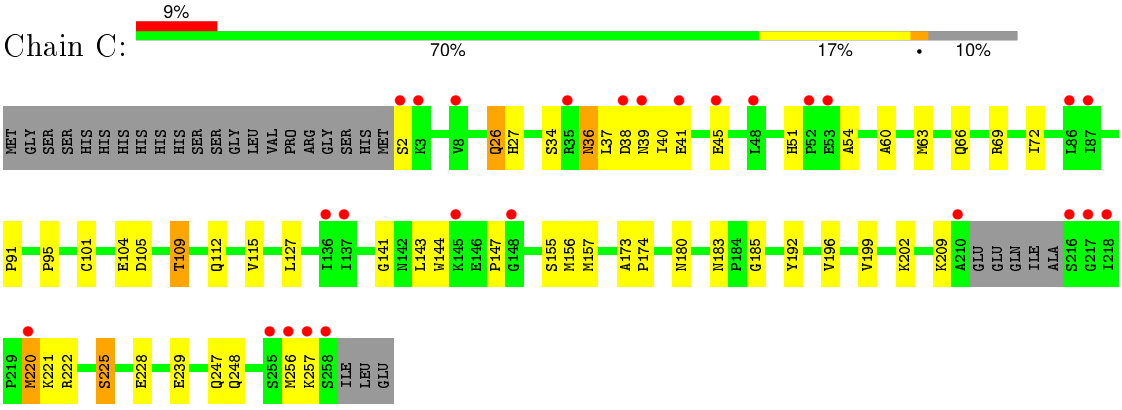
- Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain B:



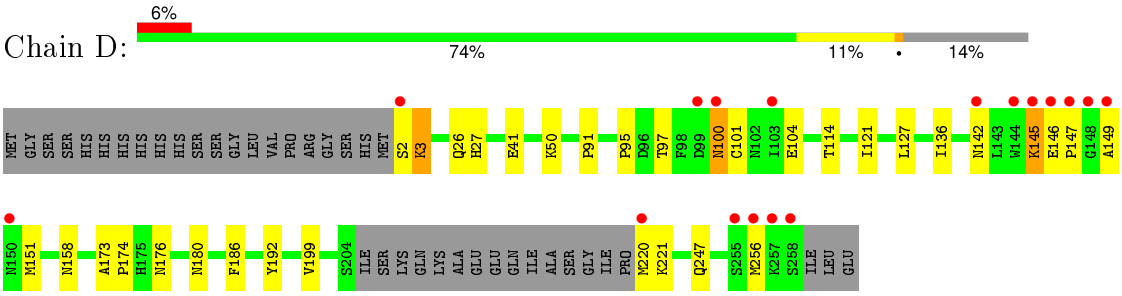
- Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain C:



- Molecule 1: Bacilysin biosynthesis oxidoreductase ywfH

Chain D:


6%
74%
11%
14%
MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET S2 K3 Q26 H27 E41 K50 P91 P95 D96 T97 F98 D99 N100 C101 N102 I103 E104 T114 I121 L127 I136 N142 L143 W144 K145 E146 P147 G148 A149
N150 M151 N158 A173 P174 H175 N176 N180 F186 Y192 V199 S204 ILE SER LYS GLN LYS ALA GLU GLU GLN ILE ALA SER GLY ILE PRO M220 K221 Q247 S255 M256 K257 S258 ILE LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.85Å 136.99Å 66.70Å 90.00° 117.99° 90.00°	Depositor
Resolution (Å)	68.50 – 1.75 31.55 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (68.50-1.75) 99.0 (31.55-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.222 0.188 , 0.221	Depositor DCC
R_{free} test set	5116 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.5	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.014 for h,-k,-h-l 0.015 for -h-l,-k,l 0.015 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 102213 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.54	0/1906	0.52	0/2570
1	B	0.46	1/1966 (0.1%)	0.54	0/2649
1	C	0.54	0/1932	0.56	0/2603
1	D	0.48	0/1893	0.53	0/2550
All	All	0.51	1/7697 (0.0%)	0.54	0/10372

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	SER	CB-OG	-5.88	1.34	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1881	0	1891	39	0
1	B	1941	0	1945	56	0
1	C	1907	0	1906	68	0
1	D	1869	0	1861	49	0
2	A	122	0	0	4	0
2	B	77	0	0	3	0
2	C	90	0	0	5	0
2	D	121	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8008	0	7603	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (204) 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:C:95:PRO:HG2	1:C:199:VAL:HG21	1.21	1.16
1:C:63:MET:HE1	1:C:72:ILE:HG13	1.26	1.08
1:D:100:ASN:C	1:D:100:ASN:HD22	1.65	1.00
1:A:100:ASN:C	1:A:100:ASN:HD22	1.67	0.96
1:C:63:MET:CE	1:C:72:ILE:HG13	1.96	0.96
1:A:187:ILE:H	1:A:193:HIS:HD2	1.03	0.96
1:D:95:PRO:HG2	1:D:199:VAL:CG2	1.99	0.93
1:C:248:GLN:HG3	2:C:316:HOH:O	1.68	0.92
1:B:38:ASP:CG	1:B:39:ASN:H	1.74	0.91
1:D:145:LYS:HD2	1:D:220:MET:HB2	1.53	0.89
1:C:36:ASN:HD22	1:C:38:ASP:H	1.21	0.88
1:D:41:GLU:HG3	2:D:340:HOH:O	1.73	0.87
1:B:50:LYS:HD3	2:B:370:HOH:O	1.74	0.86
1:C:202:LYS:HB2	1:C:202:LYS:NZ	1.90	0.85
1:B:42:SER:O	1:B:45:GLU:HB3	1.77	0.85
1:D:95:PRO:HG2	1:D:199:VAL:HG23	1.58	0.84
1:A:187:ILE:H	1:A:193:HIS:CD2	1.93	0.83
1:B:157:MET:HG3	2:B:286:HOH:O	1.79	0.81
1:C:37:LEU:CD1	1:C:60:ALA:HB2	2.11	0.81
1:B:63:MET:CE	1:B:72:ILE:HD12	2.11	0.81
1:C:95:PRO:HG2	1:C:199:VAL:CG2	2.09	0.80
1:D:147:PRO:O	1:D:151:MET:HB2	1.82	0.80
1:C:156:MET:HG3	1:C:157:MET:HE2	1.65	0.79
1:C:202:LYS:HZ2	1:C:202:LYS:HB2	1.46	0.79
1:C:63:MET:HE1	1:C:72:ILE:CG1	2.13	0.78
1:B:63:MET:HA	1:B:63:MET:HE2	1.66	0.77
1:C:220:MET:HG2	1:C:256:MET:SD	2.24	0.76
1:C:36:ASN:HD21	1:C:38:ASP:HB2	1.52	0.75
1:D:145:LYS:CD	1:D:220:MET:HB2	2.16	0.74
1:B:44:LYS:HD2	1:B:56:VAL:CG1	2.16	0.74
1:C:105:ASP:O	1:C:109:THR:HG23	1.87	0.73
1:D:100:ASN:C	1:D:100:ASN:ND2	2.40	0.73
1:D:95:PRO:HG2	1:D:199:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:MET:HA	1:B:63:MET:CE	2.18	0.73
1:B:13:GLN:HE22	1:B:191:ARG:H	1.36	0.73
1:B:63:MET:HE1	1:B:72:ILE:HD12	1.71	0.72
1:B:44:LYS:HD2	1:B:56:VAL:HG13	1.72	0.72
1:D:146:GLU:OE2	1:D:146:GLU:HA	1.90	0.71
1:A:103:ILE:HG23	1:C:115:VAL:CG1	2.21	0.71
1:D:97:THR:HG22	1:D:149:ALA:O	1.91	0.71
1:C:221:LYS:O	1:C:256:MET:HB2	1.91	0.70
1:A:100:ASN:C	1:A:100:ASN:ND2	2.40	0.70
1:A:240:GLU:HG3	2:A:278:HOH:O	1.92	0.69
1:A:187:ILE:N	1:A:193:HIS:HD2	1.86	0.69
1:C:196:VAL:O	1:C:199:VAL:HG22	1.93	0.69
1:A:97:THR:O	1:A:101:CYS:HB3	1.94	0.68
1:B:100:ASN:HD22	1:B:100:ASN:C	1.96	0.68
1:C:63:MET:HA	1:C:63:MET:HE2	1.76	0.68
1:B:38:ASP:CG	1:B:39:ASN:N	2.45	0.68
1:A:34:SER:HB3	1:A:40:ILE:HB	1.77	0.67
1:C:248:GLN:CG	2:C:316:HOH:O	2.31	0.66
1:C:37:LEU:HD12	1:C:60:ALA:HB2	1.77	0.66
1:A:100:ASN:HD22	1:A:101:CYS:N	1.92	0.66
1:A:103:ILE:HG23	1:C:115:VAL:HG13	1.79	0.65
1:B:37:LEU:CD2	1:B:60:ALA:HB2	2.26	0.65
1:A:166:LYS:HE3	2:A:409:HOH:O	1.97	0.65
1:C:202:LYS:CB	1:C:202:LYS:NZ	2.59	0.64
1:B:156:MET:HG3	1:B:157:MET:HE3	1.80	0.64
1:A:13:GLN:NE2	1:A:191:ARG:H	1.96	0.64
1:D:145:LYS:NZ	1:D:220:MET:HB2	2.14	0.63
1:D:97:THR:O	1:D:101:CYS:HB2	1.99	0.63
1:B:157:MET:CE	1:B:157:MET:HA	2.29	0.63
1:D:145:LYS:HD2	1:D:220:MET:CB	2.27	0.63
1:B:13:GLN:NE2	1:B:191:ARG:H	1.96	0.63
1:D:186:PHE:CG	1:D:221:LYS:HD2	2.34	0.62
1:D:186:PHE:CD2	1:D:221:LYS:HD2	2.34	0.62
1:B:37:LEU:HD12	1:B:41:GLU:OE1	2.00	0.61
1:C:221:LYS:O	1:C:256:MET:CB	2.49	0.60
1:A:103:ILE:CG2	1:C:115:VAL:HG11	2.31	0.60
1:D:95:PRO:CG	1:D:199:VAL:HG21	2.30	0.60
1:B:97:THR:H	1:B:100:ASN:ND2	2.00	0.60
1:A:107:THR:O	1:A:111:THR:HG23	2.00	0.60
1:D:145:LYS:H	1:D:145:LYS:HD3	1.67	0.60
1:A:197:GLU:OE2	1:A:221:LYS:NZ	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PRO:CD	1:D:199:VAL:HG21	2.31	0.59
1:C:2:SER:N	1:C:27:HIS:O	2.36	0.59
1:C:248:GLN:CD	2:C:316:HOH:O	2.41	0.59
1:C:41:GLU:O	1:C:41:GLU:HG2	1.95	0.59
1:D:142:ASN:HB3	1:D:147:PRO:CB	2.33	0.58
1:B:63:MET:HE3	1:B:72:ILE:HD12	1.87	0.57
1:C:180:ASN:HD22	1:C:247:GLN:H	1.53	0.56
1:C:109:THR:HG21	2:C:341:HOH:O	2.05	0.56
1:C:36:ASN:ND2	1:C:38:ASP:HB2	2.19	0.56
1:D:146:GLU:OE2	1:D:146:GLU:CA	2.54	0.56
1:B:40:ILE:HD13	1:B:58:VAL:HG13	1.88	0.56
1:A:260:LEU:C	1:A:260:LEU:HD12	2.26	0.56
1:B:53:GLU:OE2	1:B:53:GLU:N	2.39	0.55
1:D:104:GLU:O	1:D:104:GLU:HG2	2.05	0.55
1:C:220:MET:HA	1:C:220:MET:HE2	1.88	0.55
1:C:63:MET:HA	1:C:63:MET:CE	2.36	0.55
1:A:103:ILE:CG2	1:C:115:VAL:CG1	2.85	0.55
1:C:36:ASN:ND2	1:C:38:ASP:H	1.99	0.54
1:B:37:LEU:HD23	1:B:60:ALA:HB2	1.89	0.54
1:B:44:LYS:HD2	1:B:56:VAL:HG11	1.86	0.54
1:A:36:ASN:ND2	1:A:39:ASN:H	2.05	0.54
1:A:36:ASN:HD22	1:A:39:ASN:H	1.55	0.54
1:A:103:ILE:HG23	1:C:115:VAL:HG11	1.88	0.54
1:D:180:ASN:HD22	1:D:247:GLN:H	1.55	0.53
1:B:50:LYS:CD	2:B:370:HOH:O	2.46	0.53
1:B:97:THR:H	1:B:100:ASN:HD21	1.54	0.53
1:B:157:MET:N	1:B:157:MET:HE3	2.24	0.53
1:B:239[B]:GLU:CD	1:B:239[B]:GLU:H	2.12	0.53
1:B:180:ASN:HD22	1:B:247:GLN:H	1.57	0.52
1:D:145:LYS:CE	1:D:220:MET:HB2	2.40	0.52
1:D:142:ASN:HB3	1:D:147:PRO:HB3	1.91	0.52
1:C:222:ARG:HD2	1:C:256:MET:CE	2.40	0.51
1:A:260:LEU:C	1:A:260:LEU:CD1	2.79	0.51
1:A:166:LYS:HD3	1:A:166:LYS:O	2.10	0.51
1:C:225:SER:OG	1:C:228:GLU:HG2	2.11	0.51
1:B:22:LYS:HE3	1:B:26:GLN:HE21	1.75	0.51
1:B:66[A]:GLN:HE22	1:B:123:ARG:HH21	1.57	0.51
1:A:12:SER:HA	1:A:43:VAL:HG21	1.92	0.51
1:D:2:SER:N	1:D:27:HIS:O	2.44	0.50
1:D:26:GLN:OE1	2:D:297:HOH:O	2.20	0.50
1:B:206:SER:O	1:B:208:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ASP:OD2	1:B:39:ASN:N	2.40	0.50
1:C:112:GLN:HB3	2:C:313:HOH:O	2.12	0.49
1:B:180:ASN:ND2	1:B:247:GLN:H	2.11	0.49
1:D:91:PRO:HB3	1:D:192:TYR:CG	2.48	0.49
1:C:220:MET:CE	1:C:220:MET:HA	2.43	0.49
1:A:3:LYS:HE3	2:A:349:HOH:O	2.12	0.49
1:D:146:GLU:N	1:D:147:PRO:HD3	2.28	0.49
1:C:109:THR:HA	1:C:112:GLN:HG2	1.94	0.49
1:A:40:ILE:HG23	1:A:58:VAL:HG11	1.96	0.48
1:B:123:ARG:O	1:B:127:LEU:HD13	2.13	0.48
1:D:145:LYS:HZ2	1:D:220:MET:HB2	1.76	0.48
1:C:63:MET:CE	1:C:69:ARG:HA	2.43	0.48
1:B:183:ASN:ND2	1:B:185:GLY:H	2.11	0.48
1:C:41:GLU:O	1:C:45:GLU:HG3	2.13	0.48
1:B:146:GLU:HA	1:B:146:GLU:OE2	2.14	0.48
1:B:208:GLN:O	1:B:209:LYS:HG3	2.14	0.48
1:D:145:LYS:CD	1:D:220:MET:O	2.62	0.47
1:C:144:TRP:CZ3	1:C:221:LYS:HG2	2.48	0.47
1:D:121:ILE:HG23	1:D:136:ILE:HD13	1.94	0.47
1:A:122:LYS:NZ	1:C:101:CYS:O	2.47	0.47
1:C:147:PRO:HB2	1:C:155:SER:OG	2.14	0.47
1:D:145:LYS:HD3	1:D:220:MET:O	2.14	0.47
1:C:36:ASN:ND2	1:C:38:ASP:CB	2.77	0.47
1:A:141:GLY:HA3	2:A:369:HOH:O	2.14	0.47
1:C:26:GLN:HA	1:C:26:GLN:HE21	1.80	0.47
1:C:157:MET:CE	1:C:157:MET:HA	2.46	0.46
1:C:34:SER:HB2	1:C:40:ILE:HD13	1.96	0.46
1:C:202:LYS:CB	1:C:202:LYS:HZ3	2.29	0.46
1:B:153:THR:O	1:B:157:MET:HG2	2.16	0.46
1:B:3:LYS:HG2	1:B:4:ARG:N	2.31	0.46
1:C:104:GLU:H	1:C:104:GLU:CD	2.19	0.46
1:B:36:ASN:HD22	1:B:38:ASP:H	1.63	0.46
1:C:183:ASN:ND2	1:C:185:GLY:H	2.14	0.46
1:D:3:LYS:HG2	1:D:3:LYS:O	2.15	0.46
1:A:121:ILE:HG23	1:A:136:ILE:HD13	1.97	0.46
1:D:95:PRO:HD2	1:D:199:VAL:HG21	1.98	0.45
1:B:157:MET:CE	1:B:157:MET:CA	2.95	0.45
1:C:180:ASN:ND2	1:C:247:GLN:H	2.13	0.45
1:B:239[B]:GLU:N	1:B:239[B]:GLU:CD	2.69	0.45
1:C:51:HIS:HB2	1:C:54:ALA:HB2	1.99	0.45
1:A:133:PHE:CD2	1:A:133:PHE:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ASN:HD21	1:C:38:ASP:CB	2.25	0.45
1:B:100:ASN:C	1:B:100:ASN:ND2	2.67	0.45
1:D:97:THR:H	1:D:100:ASN:ND2	2.15	0.45
1:A:114:THR:CG2	1:C:156:MET:HE1	2.47	0.45
1:B:156:MET:HG3	1:B:157:MET:CE	2.46	0.45
1:C:173:ALA:N	1:C:174:PRO:CD	2.80	0.44
1:C:37:LEU:CD1	1:C:60:ALA:CB	2.91	0.44
1:A:186:PHE:CD2	1:A:221:LYS:HD3	2.53	0.44
1:B:157:MET:HE3	1:B:157:MET:CA	2.47	0.44
1:D:220:MET:HB3	1:D:256:MET:CE	2.48	0.44
1:D:173:ALA:N	1:D:174:PRO:CD	2.81	0.44
1:A:96:ASP:HB2	1:A:100:ASN:HD21	1.82	0.44
1:A:13:GLN:HE22	1:A:191:ARG:H	1.67	0.43
1:D:145:LYS:O	1:D:146:GLU:HB2	2.19	0.43
1:B:156:MET:HE1	1:D:114:THR:CG2	2.49	0.43
1:C:222:ARG:HH11	1:C:256:MET:CE	2.31	0.43
1:A:59:LEU:HD22	1:A:75:LYS:HD2	1.99	0.43
1:B:173:ALA:N	1:B:174:PRO:CD	2.81	0.43
1:C:156:MET:HG3	1:C:157:MET:CE	2.42	0.43
1:D:50:LYS:HB3	1:D:50:LYS:HE2	1.76	0.43
1:D:100:ASN:HD22	1:D:101:CYS:N	2.12	0.42
1:C:143:LEU:N	1:C:143:LEU:HD23	2.34	0.42
1:C:222:ARG:HD2	1:C:256:MET:HE1	2.01	0.42
1:B:63:MET:CE	1:B:69:ARG:HA	2.49	0.42
1:C:95:PRO:CG	1:C:199:VAL:HG21	2.15	0.42
1:D:180:ASN:ND2	1:D:247:GLN:H	2.17	0.42
1:B:133:PHE:C	1:B:133:PHE:CD2	2.93	0.42
1:B:100:ASN:HD22	1:B:101:CYS:N	2.17	0.42
1:B:208:GLN:C	1:B:209:LYS:HG3	2.40	0.42
1:D:176[A]:ASN:O	1:D:176[A]:ASN:CG	2.59	0.42
1:C:105:ASP:O	1:C:109:THR:CG2	2.64	0.42
1:B:37:LEU:HD23	1:B:60:ALA:CB	2.50	0.42
1:D:3:LYS:HE3	2:D:296:HOH:O	2.20	0.41
1:D:146:GLU:N	1:D:147:PRO:CD	2.83	0.41
1:B:157:MET:HE3	1:B:157:MET:HA	2.03	0.41
1:C:38:ASP:O	1:C:39:ASN:HB2	2.19	0.41
1:A:40:ILE:HG23	1:A:58:VAL:CG1	2.49	0.41
1:C:222:ARG:HD2	1:C:256:MET:HE2	2.02	0.41
1:D:142:ASN:ND2	1:D:158:ASN:HD22	2.17	0.41
1:B:48:LEU:C	1:B:50:LYS:H	2.23	0.41
1:C:141:GLY:HA3	1:C:183:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PRO:HB3	1:C:192:TYR:CG	2.55	0.41
1:D:220:MET:HB3	1:D:256:MET:HE2	2.02	0.41
1:D:91:PRO:HB3	1:D:192:TYR:CD1	2.56	0.40
1:B:121:ILE:HG23	1:B:136:ILE:HD13	2.02	0.40
1:A:167:ASN:HA	1:A:167:ASN:HD22	1.73	0.40
1:A:110:PHE:HB2	1:A:157:MET:HE3	2.02	0.40
1:A:36:ASN:HD21	1:A:38:ASP:HB2	1.86	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	245/281 (87%)	241 (98%)	4 (2%)	0	100 100
1	B	251/281 (89%)	242 (96%)	8 (3%)	1 (0%)	39 19
1	C	249/281 (89%)	243 (98%)	6 (2%)	0	100 100
1	D	242/281 (86%)	236 (98%)	6 (2%)	0	100 100
All	All	987/1124 (88%)	962 (98%)	24 (2%)	1 (0%)	56 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	38	ASP

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	204/231 (88%)	199 (98%)	5 (2%)	55 30
1	B	211/231 (91%)	201 (95%)	10 (5%)	32 10
1	C	205/231 (89%)	195 (95%)	10 (5%)	31 9
1	D	202/231 (87%)	198 (98%)	4 (2%)	63 39
All	All	822/924 (89%)	793 (96%)	29 (4%)	44 17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	100	ASN
1	A	101	CYS
1	A	193	HIS
1	A	260	LEU
1	B	13	GLN
1	B	36	ASN
1	B	37	LEU
1	B	44	LYS
1	B	53	GLU
1	B	65	ASP
1	B	100	ASN
1	B	227	GLU
1	B	239[A]	GLU
1	B	239[B]	GLU
1	C	26	GLN
1	C	36	ASN
1	C	66	GLN
1	C	109	THR
1	C	127	LEU
1	C	209	LYS
1	C	220	MET
1	C	225	SER
1	C	239	GLU
1	C	257	LYS
1	D	3	LYS
1	D	100	ASN
1	D	127	LEU
1	D	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	36	ASN
1	A	39	ASN
1	A	100	ASN
1	A	102	ASN
1	A	167	ASN
1	A	193	HIS
1	A	194	GLN
1	A	198	ASN
1	A	203	ASN
1	B	13	GLN
1	B	36	ASN
1	B	67	HIS
1	B	79	GLN
1	B	100	ASN
1	B	167	ASN
1	B	180	ASN
1	B	183	ASN
1	B	194	GLN
1	B	198	ASN
1	B	208	GLN
1	C	26	GLN
1	C	36	ASN
1	C	66	GLN
1	C	112	GLN
1	C	158	ASN
1	C	163	ASN
1	C	167	ASN
1	C	171	GLN
1	C	180	ASN
1	C	183	ASN
1	C	198	ASN
1	D	66	GLN
1	D	100	ASN
1	D	142	ASN
1	D	167	ASN
1	D	180	ASN
1	D	203	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^{th} 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^2)	Q<0.9
1	A	249/281 (88%)	0.33	18 (7%)	18	24	13, 23, 47, 69	0
1	B	251/281 (89%)	0.53	20 (7%)	15	19	13, 29, 63, 73	0
1	C	252/281 (89%)	0.55	26 (10%)	9	11	14, 25, 55, 83	0
1	D	242/281 (86%)	0.43	17 (7%)	19	24	12, 21, 50, 74	0
All	All	994/1124 (88%)	0.46	81 (8%)	15	18	12, 24, 55, 83	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	SER	9.5
1	D	256	MET	8.5
1	C	216	SER	8.0
1	C	217	GLY	7.9
1	A	2	SER	7.0
1	C	2	SER	6.9
1	D	2	SER	6.8
1	A	205	ILE	6.5
1	D	257	LYS	5.9
1	B	209	LYS	5.4
1	C	256	MET	5.2
1	D	146	GLU	5.1
1	A	204	SER	5.1
1	A	218	ILE	4.9
1	C	255	SER	4.8
1	C	218	ILE	4.8
1	D	149	ALA	4.7
1	B	49	ALA	4.6
1	D	145	LYS	4.5
1	D	103	ILE	4.4
1	B	39	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	210	ALA	4.2
1	A	103	ILE	4.2
1	A	260	LEU	4.2
1	D	144	TRP	4.1
1	D	220	MET	3.8
1	B	208	GLN	3.8
1	A	217	GLY	3.7
1	D	255	SER	3.6
1	C	257	LYS	3.4
1	C	53	GLU	3.3
1	B	207	LYS	3.3
1	B	38	ASP	3.2
1	C	220	MET	3.2
1	C	258	SER	3.1
1	B	35	ARG	3.1
1	C	52	PRO	3.1
1	D	148	GLY	3.1
1	C	136	ILE	3.0
1	B	41	GLU	2.9
1	B	261	GLU	2.9
1	C	48	LEU	2.9
1	A	38	ASP	2.8
1	C	87	ILE	2.8
1	D	147	PRO	2.8
1	C	148	GLY	2.8
1	B	137	ILE	2.7
1	B	52	PRO	2.7
1	C	38	ASP	2.7
1	C	86	LEU	2.6
1	B	53	GLU	2.6
1	C	35	ARG	2.6
1	A	104	GLU	2.6
1	C	41	GLU	2.6
1	C	3	LYS	2.6
1	B	3	LYS	2.6
1	B	87	ILE	2.5
1	A	132	GLU	2.5
1	A	206	SER	2.5
1	D	100	ASN	2.4
1	A	87	ILE	2.4
1	C	39	ASN	2.4
1	D	99	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	132	GLU	2.3
1	C	8	VAL	2.3
1	C	145	LYS	2.3
1	D	150	ASN	2.3
1	A	145	LYS	2.3
1	B	45	GLU	2.3
1	D	142	ASN	2.3
1	B	86	LEU	2.2
1	C	45	GLU	2.2
1	A	202	LYS	2.2
1	C	137	ILE	2.1
1	B	60	ALA	2.1
1	B	25	ASP	2.1
1	A	203	ASN	2.1
1	A	137	ILE	2.1
1	A	100	ASN	2.0
1	A	146	GLU	2.0
1	B	255	SER	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.