Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:06 pm BST

PDB ID	:	5DEC
Title	:	Crystal structure of the small alarmone synthetase 1 from Bacillus subtilis
Authors	:	Steinchen, W.; Altegoer, A.; Schuhmacher, J.S.; Bange, G.
Deposited on	:	2015-08-25
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

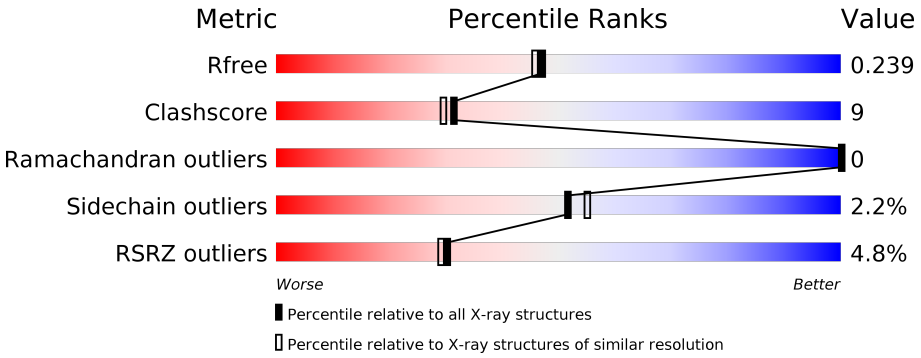
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	218	2% 72% 14% 14%
1	B	218	4% 72% 14% • 12%
1	C	218	4% 67% 16% • 16%
1	D	218	7% 68% 17% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6542 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 GTP pyrophosphokinase YjbM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1546	985	270	285	6			
1	B	191	Total	C	N	O	S	0	0	0
			1572	1001	276	289	6			
1	C	183	Total	C	N	O	S	0	0	0
			1507	960	262	279	6			
1	D	189	Total	C	N	O	S	0	0	0
			1552	988	271	287	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP O31611
A	-5	GLY	-	expression tag	UNP O31611
A	-4	HIS	-	expression tag	UNP O31611
A	-3	HIS	-	expression tag	UNP O31611
A	-2	HIS	-	expression tag	UNP O31611
A	-1	HIS	-	expression tag	UNP O31611
A	0	HIS	-	expression tag	UNP O31611
A	1	HIS	-	expression tag	UNP O31611
A	4	ASP	LYS	conflict	UNP O31611
A	5	LYS	GLN	conflict	UNP O31611
B	-6	MET	-	expression tag	UNP O31611
B	-5	GLY	-	expression tag	UNP O31611
B	-4	HIS	-	expression tag	UNP O31611
B	-3	HIS	-	expression tag	UNP O31611
B	-2	HIS	-	expression tag	UNP O31611
B	-1	HIS	-	expression tag	UNP O31611
B	0	HIS	-	expression tag	UNP O31611
B	1	HIS	-	expression tag	UNP O31611
B	4	ASP	LYS	conflict	UNP O31611
B	5	LYS	GLN	conflict	UNP O31611
C	-6	MET	-	expression tag	UNP O31611

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP O31611
C	-4	HIS	-	expression tag	UNP O31611
C	-3	HIS	-	expression tag	UNP O31611
C	-2	HIS	-	expression tag	UNP O31611
C	-1	HIS	-	expression tag	UNP O31611
C	0	HIS	-	expression tag	UNP O31611
C	1	HIS	-	expression tag	UNP O31611
C	4	ASP	LYS	conflict	UNP O31611
C	5	LYS	GLN	conflict	UNP O31611
D	-6	MET	-	expression tag	UNP O31611
D	-5	GLY	-	expression tag	UNP O31611
D	-4	HIS	-	expression tag	UNP O31611
D	-3	HIS	-	expression tag	UNP O31611
D	-2	HIS	-	expression tag	UNP O31611
D	-1	HIS	-	expression tag	UNP O31611
D	0	HIS	-	expression tag	UNP O31611
D	1	HIS	-	expression tag	UNP O31611
D	4	ASP	LYS	conflict	UNP O31611
D	5	LYS	GLN	conflict	UNP O31611

- Molecule 2 is water.

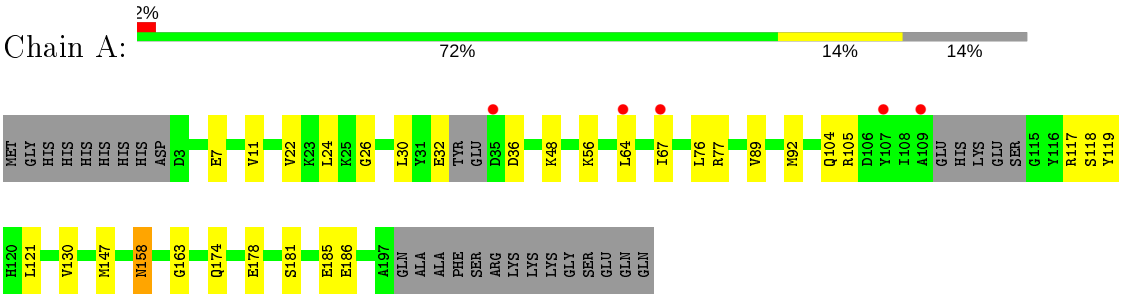
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	90	Total O 90 90	0	0
2	B	96	Total O 96 96	0	0
2	C	92	Total O 92 92	0	0
2	D	87	Total O 87 87	0	0

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 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.

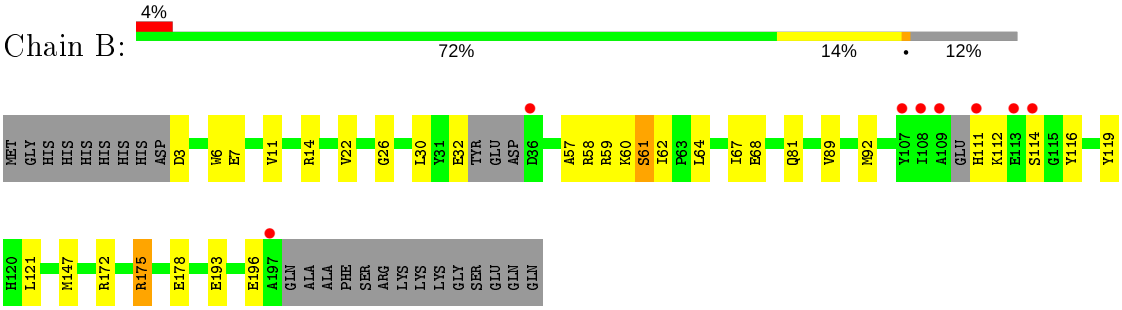
- Molecule 1: GTP pyrophosphokinase YjbM

Chain A:



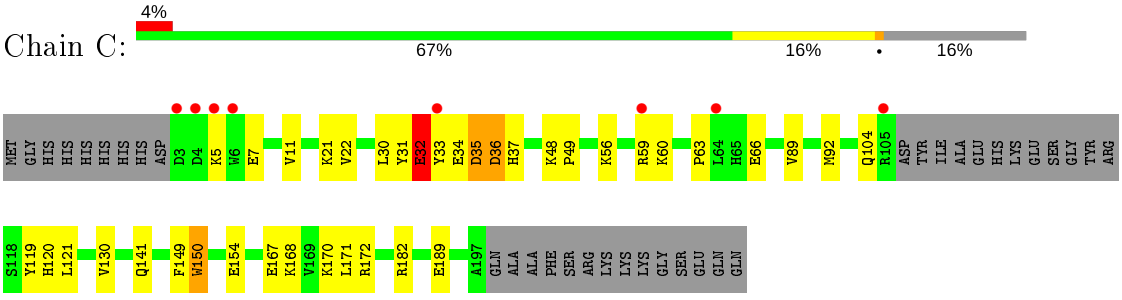
- Molecule 1: GTP pyrophosphokinase YjbM

Chain B:



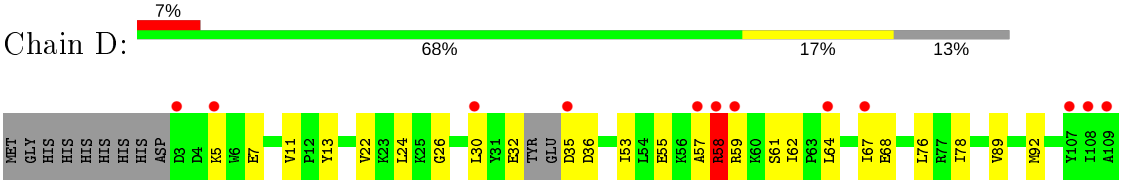
- Molecule 1: GTP pyrophosphokinase YjbM

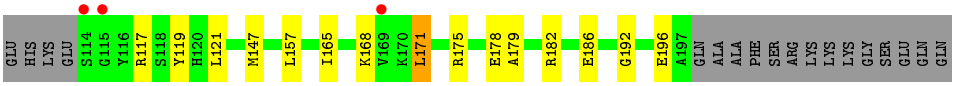
Chain C:



- Molecule 1: GTP pyrophosphokinase YjbM

Chain D:




GLU
HIS
LYS
GLU
S114
G115
Y116
R117
S118
Y119
H120
L121
M147
L157
I165
K168
V169
K170
L171
R175
E178
A179
R182
E186
G192
E196
A197
GLN
ALA
ALA
PHE
SER
ARG
LYS
LYS
LYS
GLY
SER
GLU
GLN
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.13Å 77.69Å 81.61Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	56.63 – 2.00 56.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (56.63-2.00) 96.4 (56.63-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1685	Depositor
R, R_{free}	0.194 , 0.238 0.197 , 0.239	Depositor DCC
R_{free} test set	2025 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.017 for -h,-l,-k 0.001 for -h,l,k 0.023 for k,h,-l 0.034 for -k,-h,-l 0.002 for l,h,k 0.002 for k,l,h 0.001 for -l,-h,k 0.001 for -k,-l,h 0.026 for h,-k,-l 0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6542	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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, 0.333 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	0.45	0/1572	0.62	0/2116
1	B	0.42	0/1599	0.61	1/2151 (0.0%)
1	C	0.55	1/1533 (0.1%)	0.62	0/2065
1	D	0.49	0/1578	0.68	2/2124 (0.1%)
All	All	0.48	1/6282 (0.0%)	0.64	3/8456 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	TRP	CB-CG	-5.59	1.40	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	58	ARG	CA-CB-CG	5.92	126.42	113.40
1	D	171	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	175	ARG	NE-CZ-NH2	-5.73	117.44	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	32	GLU	Peptide
1	D	58	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1546	0	1567	24	0
1	B	1572	0	1594	28	1
1	C	1507	0	1529	39	0
1	D	1552	0	1572	31	1
2	A	90	0	0	2	0
2	B	96	0	0	4	0
2	C	92	0	0	6	0
2	D	87	0	0	9	0
All	All	6542	0	6262	112	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 9.

All (112) 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:33:TYR:C	1:C:35:ASP:OD1	1.79	1.21
1:D:32:GLU:C	1:D:35:ASP:OD2	1.80	1.19
1:D:32:GLU:O	1:D:35:ASP:CG	1.84	1.14
1:C:32:GLU:C	1:C:35:ASP:OD1	1.93	1.06
1:C:32:GLU:O	1:C:35:ASP:OD2	1.85	0.94
1:A:22:VAL:HG21	1:C:22:VAL:HG21	1.48	0.94
1:A:158:ASN:ND2	1:A:163:GLY:HA2	1.82	0.93
1:C:36:ASP:OD1	1:C:37:HIS:N	2.03	0.91
1:D:147:MET:SD	2:D:352:HOH:O	2.30	0.89
1:C:167:GLU:O	2:C:301:HOH:O	1.90	0.88
1:B:22:VAL:HG21	1:D:22:VAL:HG21	1.55	0.88
1:C:33:TYR:CA	1:C:35:ASP:OD1	2.24	0.84
1:D:192:GLY:O	2:D:301:HOH:O	1.94	0.84
1:C:34:GLU:N	1:C:35:ASP:OD1	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:MET:SD	2:B:383:HOH:O	2.38	0.81
1:C:5:LYS:NZ	2:C:302:HOH:O	2.14	0.81
1:C:32:GLU:O	1:C:35:ASP:CG	2.18	0.81
1:A:158:ASN:HD21	1:A:163:GLY:HA2	1.46	0.80
1:D:196:GLU:N	2:D:301:HOH:O	2.14	0.79
1:D:168:LYS:O	2:D:302:HOH:O	2.02	0.77
1:C:32:GLU:O	1:C:35:ASP:OD1	2.03	0.76
1:B:196:GLU:OE2	1:C:168:LYS:NZ	2.18	0.76
1:C:31:TYR:O	1:C:34:GLU:HB2	1.88	0.73
1:B:61:SER:O	1:B:61:SER:OG	2.05	0.72
1:D:55:GLU:O	1:D:59:ARG:HG2	1.90	0.72
1:B:193:GLU:OE2	1:C:172:ARG:NH1	2.24	0.71
1:C:33:TYR:N	1:C:35:ASP:OD1	2.23	0.71
1:B:32:GLU:O	2:B:301:HOH:O	2.10	0.70
1:A:130:VAL:HG23	1:C:30:LEU:HD23	1.72	0.70
1:A:119:TYR:HE2	1:A:121:LEU:HD23	1.58	0.69
1:B:3:ASP:N	2:B:303:HOH:O	2.27	0.68
1:B:178:GLU:OE1	2:B:302:HOH:O	2.11	0.67
1:C:32:GLU:C	1:C:35:ASP:CG	2.52	0.67
1:B:7:GLU:OE2	1:B:14:ARG:NH2	2.28	0.66
1:A:186:GLU:HG3	2:D:303:HOH:O	1.96	0.65
1:B:119:TYR:HE2	1:B:121:LEU:HD23	1.62	0.64
1:B:193:GLU:O	1:B:196:GLU:HG2	1.98	0.63
1:C:56:LYS:NZ	1:C:60:LYS:HD2	2.14	0.61
1:B:112:LYS:HE2	1:B:114:SER:OG	2.00	0.61
1:D:58:ARG:HB2	1:D:62:ILE:H	1.65	0.60
1:D:182:ARG:NH1	2:D:306:HOH:O	2.25	0.59
1:C:120:HIS:ND1	1:C:141:GLN:HG2	2.18	0.59
1:D:119:TYR:HE2	1:D:121:LEU:HD23	1.66	0.58
1:D:13:TYR:OH	1:D:68:GLU:HG3	2.04	0.58
1:D:32:GLU:O	1:D:35:ASP:OD2	0.63	0.58
1:C:170:LYS:N	2:C:301:HOH:O	2.37	0.57
1:C:171:LEU:N	2:C:301:HOH:O	1.95	0.56
1:A:105:ARG:HG3	1:A:105:ARG:HH11	1.70	0.56
1:D:58:ARG:HD2	1:D:61:SER:HA	1.88	0.55
1:D:7:GLU:O	1:D:11:VAL:HG23	2.07	0.54
1:D:175:ARG:O	2:D:303:HOH:O	2.18	0.53
1:B:81:GLN:HG3	1:C:149:PHE:HE1	1.74	0.53
1:B:64:LEU:H	1:B:64:LEU:HD12	1.74	0.52
1:D:64:LEU:HA	1:D:67:ILE:HG23	1.91	0.52
1:A:7:GLU:O	1:A:11:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLU:HB3	1:D:59:ARG:HE	1.74	0.51
1:C:56:LYS:HZ3	1:C:60:LYS:HD2	1.77	0.50
1:C:7:GLU:O	1:C:11:VAL:HG23	2.12	0.50
1:D:165:ILE:HG12	2:D:325:HOH:O	2.11	0.50
1:D:157:LEU:HB3	1:D:165:ILE:HD12	1.94	0.49
1:C:63:PRO:HD2	1:C:66:GLU:OE1	2.11	0.49
1:B:26:GLY:O	1:B:30:LEU:HD13	2.13	0.49
1:A:174:GLN:NE2	1:A:178:GLU:OE2	2.32	0.49
1:B:111:HIS:HB2	1:B:116:TYR:O	2.14	0.48
1:C:150:TRP:CH2	1:C:154:GLU:OE1	2.66	0.48
1:A:48:LYS:HZ2	1:A:56:LYS:HD3	1.79	0.48
1:C:104:GLN:OE1	1:C:119:TYR:OH	2.19	0.48
1:B:3:ASP:O	1:B:6:TRP:HB2	2.14	0.47
1:A:30:LEU:HD23	1:C:130:VAL:HG22	1.96	0.47
1:A:77:ARG:NH1	2:A:301:HOH:O	2.20	0.47
1:C:119:TYR:HE2	1:C:121:LEU:HD23	1.79	0.47
1:A:89:VAL:HA	1:A:92:MET:CE	2.45	0.47
1:B:81:GLN:HG3	1:C:149:PHE:CE1	2.49	0.47
1:B:59:ARG:CZ	1:B:60:LYS:HE2	2.45	0.46
1:B:57:ALA:HB1	1:B:62:ILE:HB	1.96	0.46
1:B:7:GLU:O	1:B:11:VAL:HG23	2.15	0.46
1:A:89:VAL:HA	1:A:92:MET:HE2	1.97	0.46
1:D:58:ARG:HB2	1:D:62:ILE:N	2.30	0.46
1:D:58:ARG:HB2	1:D:61:SER:CA	2.46	0.45
1:A:26:GLY:O	1:A:30:LEU:HD13	2.17	0.45
1:C:120:HIS:ND1	1:C:141:GLN:CG	2.79	0.45
1:D:117:ARG:C	1:D:147:MET:HE3	2.37	0.45
1:A:118:SER:HA	1:A:147:MET:CE	2.47	0.45
1:B:89:VAL:HA	1:B:92:MET:CE	2.47	0.45
1:C:89:VAL:HA	1:C:92:MET:CE	2.48	0.44
1:D:24:LEU:HD13	1:D:78:ILE:HD11	1.99	0.44
1:C:21:LYS:NZ	2:C:304:HOH:O	2.29	0.44
1:C:182:ARG:HD3	1:C:182:ARG:HA	1.80	0.44
1:D:58:ARG:HB2	1:D:61:SER:HA	1.99	0.44
1:C:168:LYS:C	2:C:301:HOH:O	2.55	0.44
1:D:179:ALA:HB2	2:D:303:HOH:O	2.17	0.43
1:B:172:ARG:HE	1:C:189:GLU:HG2	1.82	0.43
1:A:105:ARG:NH1	1:A:105:ARG:HG3	2.32	0.43
1:A:104:GLN:HA	1:A:121:LEU:HA	2.00	0.43
1:A:181:SER:O	1:A:185:GLU:HG2	2.19	0.43
1:C:48:LYS:HA	1:C:49:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:GLU:O	1:B:196:GLU:HG3	2.19	0.42
1:D:57:ALA:O	1:D:62:ILE:HB	2.19	0.42
1:B:64:LEU:HA	1:B:67:ILE:HG23	2.02	0.42
1:C:104:GLN:HA	1:C:121:LEU:HA	2.01	0.42
1:D:178:GLU:HB3	1:D:182:ARG:NH2	2.34	0.42
1:D:53:ILE:O	1:D:57:ALA:N	2.52	0.42
1:A:24:LEU:HD12	1:A:76:LEU:HD22	2.01	0.42
1:D:26:GLY:O	1:D:30:LEU:HG	2.19	0.42
1:A:130:VAL:HG23	1:C:30:LEU:CD2	2.47	0.42
1:D:89:VAL:HA	1:D:92:MET:CE	2.49	0.41
1:A:117:ARG:HD3	2:A:308:HOH:O	2.21	0.41
1:A:117:ARG:HB2	1:A:147:MET:HG2	2.03	0.41
1:B:64:LEU:N	1:B:64:LEU:HD12	2.36	0.41
1:B:89:VAL:HA	1:B:92:MET:HE2	2.02	0.41
1:B:64:LEU:CD1	1:B:64:LEU:H	2.35	0.40
1:A:64:LEU:HA	1:A:67:ILE:HG23	2.04	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:B:175:ARG:NH2	1:D:186:GLU:OE1[1_556]	2.13	0.07

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	182/218 (84%)	180 (99%)	2 (1%)	0	100	100
1	B	185/218 (85%)	181 (98%)	4 (2%)	0	100	100
1	C	179/218 (82%)	178 (99%)	1 (1%)	0	100	100
1	D	183/218 (84%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	729/872 (84%)	718 (98%)	11 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/195 (87%)	166 (98%)	3 (2%)	59 63
1	B	172/195 (88%)	169 (98%)	3 (2%)	60 65
1	C	166/195 (85%)	162 (98%)	4 (2%)	49 51
1	D	170/195 (87%)	165 (97%)	5 (3%)	42 43
All	All	677/780 (87%)	662 (98%)	15 (2%)	52 55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	36	ASP
1	A	158	ASN
1	B	58	ARG
1	B	61	SER
1	B	68	GLU
1	C	32	GLU
1	C	35	ASP
1	C	36	ASP
1	C	59	ARG
1	D	5	LYS
1	D	36	ASP
1	D	58	ARG
1	D	76	LEU
1	D	171	LEU

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	158	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	188/218 (86%)	0.21	5 (2%)	54	53	21, 37, 88, 108	0
1	B	191/218 (87%)	0.27	8 (4%)	36	35	22, 39, 105, 121	0
1	C	183/218 (83%)	0.23	8 (4%)	34	33	19, 42, 96, 122	0
1	D	189/218 (86%)	0.41	15 (7%)	12	11	23, 43, 101, 125	0
All	All	751/872 (86%)	0.28	36 (4%)	30	29	19, 40, 99, 125	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	TYR	9.7
1	D	108	ILE	5.0
1	B	114	SER	4.9
1	A	35	ASP	4.3
1	D	58	ARG	4.1
1	B	113	GLU	4.0
1	C	59	ARG	3.8
1	D	107	TYR	3.6
1	B	109	ALA	3.5
1	B	111	HIS	3.4
1	A	109	ALA	3.3
1	D	169	VAL	3.2
1	D	115	GLY	3.1
1	D	67	ILE	3.1
1	C	64	LEU	3.0
1	B	36	ASP	3.0
1	B	197	ALA	2.9
1	B	107	TYR	2.9
1	C	4	ASP	2.7
1	A	107	TYR	2.7
1	D	109	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	57	ALA	2.6
1	D	5	LYS	2.5
1	C	105	ARG	2.4
1	C	3	ASP	2.4
1	D	64	LEU	2.3
1	B	108	ILE	2.2
1	D	114	SER	2.2
1	D	59	ARG	2.2
1	D	3	ASP	2.1
1	A	67	ILE	2.1
1	C	6	TRP	2.1
1	D	30	LEU	2.1
1	C	5	LYS	2.1
1	A	64	LEU	2.0
1	D	35	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.