Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:03 AM GMT

PDB ID	:	3H1B
Title	:	Crystal structure of EstE5, was soaked by isopropyl alcohol
Authors	:	Hwang, K.Y.; Nam, K.H.
Deposited on	:	2009-04-11
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) 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 2.10 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.
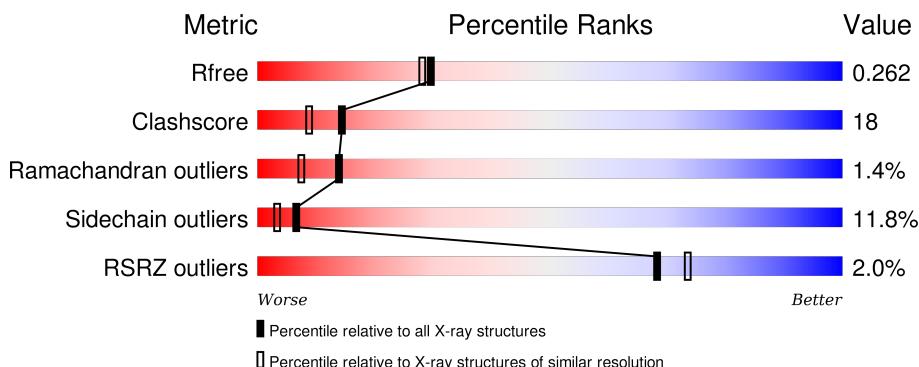
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	322	
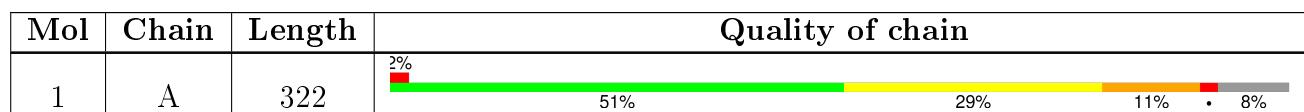
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2261 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 Esterase/lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2241	1426	393	407	15	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP Q0GMU2
A	-11	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	-10	SER	-	EXPRESSION TAG	UNP Q0GMU2
A	-9	MET	-	EXPRESSION TAG	UNP Q0GMU2
A	-8	THR	-	EXPRESSION TAG	UNP Q0GMU2
A	-7	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-6	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-5	GLN	-	EXPRESSION TAG	UNP Q0GMU2
A	-4	GLN	-	EXPRESSION TAG	UNP Q0GMU2
A	-3	MET	-	EXPRESSION TAG	UNP Q0GMU2
A	-2	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	-1	ARG	-	EXPRESSION TAG	UNP Q0GMU2
A	0	GLY	-	EXPRESSION TAG	UNP Q0GMU2
A	298	LEU	-	EXPRESSION TAG	UNP Q0GMU2
A	299	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	300	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	301	ALA	-	EXPRESSION TAG	UNP Q0GMU2
A	302	LEU	-	EXPRESSION TAG	UNP Q0GMU2
A	303	GLU	-	EXPRESSION TAG	UNP Q0GMU2
A	304	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	305	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	306	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	307	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	308	HIS	-	EXPRESSION TAG	UNP Q0GMU2
A	309	HIS	-	EXPRESSION TAG	UNP Q0GMU2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total 20	O 20	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: Esterase/lipase
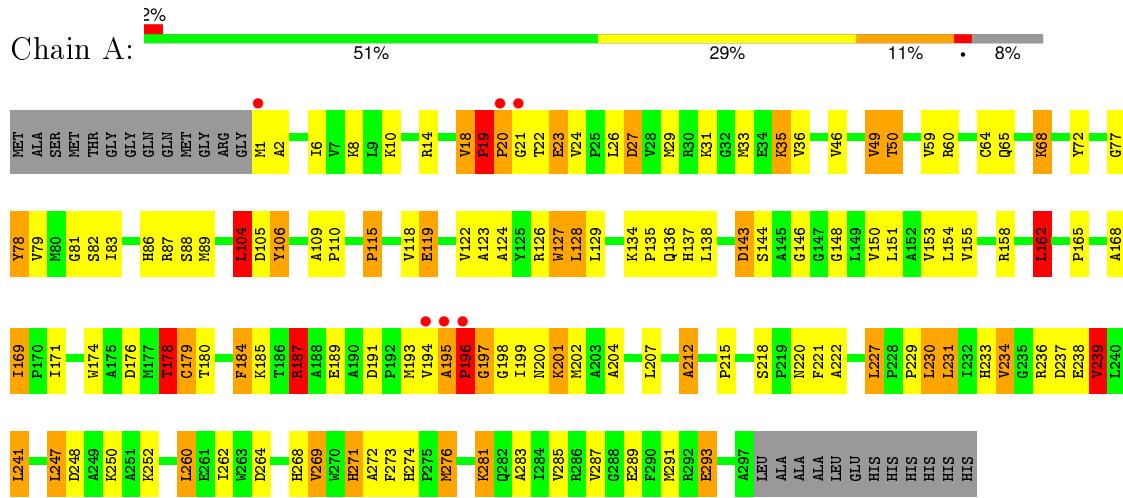
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	61.31Å 61.31Å 150.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.10 47.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.49-2.10) 90.7 (47.48-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.295 0.247 , 0.262	Depositor DCC
R_{free} test set	806 reflections (5.35%)	DCC
Wilson B-factor (Å²)	18.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 15894 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	2261	wwPDB-VP
Average B, all atoms (Å²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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	1.88	36/2295 (1.6%)	1.69	47/3116 (1.5%)

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	8

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	CYS	CB-SG	-10.19	1.65	1.82
1	A	88	SER	CB-OG	9.41	1.54	1.42
1	A	189	GLU	CG-CD	8.30	1.64	1.51
1	A	59	VAL	CB-CG2	-8.27	1.35	1.52
1	A	106	TYR	CE2-CZ	8.04	1.49	1.38
1	A	18	VAL	CB-CG1	-7.65	1.36	1.52
1	A	293	GLU	CD-OE1	7.16	1.33	1.25
1	A	144	SER	CB-OG	7.04	1.51	1.42
1	A	2	ALA	CA-CB	7.03	1.67	1.52
1	A	184	PHE	CE2-CZ	6.94	1.50	1.37
1	A	238	GLU	CD-OE1	6.84	1.33	1.25
1	A	272	ALA	CA-CB	-6.67	1.38	1.52
1	A	115	PRO	N-CA	-6.50	1.36	1.47
1	A	281	LYS	CE-NZ	6.50	1.65	1.49
1	A	36	VAL	CB-CG1	6.19	1.65	1.52
1	A	35	LYS	CD-CE	6.16	1.66	1.51
1	A	221	PHE	CD1-CE1	-6.14	1.26	1.39
1	A	273	PHE	CD1-CE1	-6.08	1.27	1.39
1	A	49	VAL	CB-CG2	-6.02	1.40	1.52
1	A	72	TYR	CZ-OH	-5.95	1.27	1.37

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLU	CD-OE2	5.93	1.32	1.25
1	A	283	ALA	CA-CB	-5.88	1.40	1.52
1	A	155	VAL	CB-CG1	-5.86	1.40	1.52
1	A	234	VAL	CB-CG1	5.79	1.65	1.52
1	A	126	ARG	CZ-NH1	5.60	1.40	1.33
1	A	78	TYR	CD2-CE2	-5.54	1.31	1.39
1	A	153	VAL	N-CA	5.45	1.57	1.46
1	A	123	ALA	CA-CB	-5.41	1.41	1.52
1	A	148	GLY	N-CA	-5.37	1.38	1.46
1	A	115	PRO	C-O	-5.35	1.12	1.23
1	A	64	CYS	CB-SG	5.27	1.91	1.82
1	A	230	LEU	CG-CD2	-5.09	1.33	1.51
1	A	174	TRP	CE3-CZ3	5.09	1.47	1.38
1	A	230	LEU	CG-CD1	5.06	1.70	1.51
1	A	106	TYR	CZ-OH	5.05	1.46	1.37
1	A	46	VAL	CA-CB	-5.02	1.44	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	MET	CG-SD-CE	13.27	121.44	100.20
1	A	60	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	176	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	A	178	THR	CB-CA-C	-9.99	84.62	111.60
1	A	89	MET	CG-SD-CE	-9.94	84.29	100.20
1	A	134	LYS	CD-CE-NZ	-9.08	90.81	111.70
1	A	19	PRO	CB-CA-C	-8.67	90.33	112.00
1	A	264	ASP	CB-CG-OD1	-8.34	110.79	118.30
1	A	187	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	104	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	14	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	260	LEU	CB-CG-CD1	-7.78	97.78	111.00
1	A	19	PRO	N-CA-C	7.53	131.67	112.10
1	A	252	LYS	CD-CE-NZ	-7.48	94.50	111.70
1	A	178	THR	C-N-CA	7.38	140.15	121.70
1	A	105	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	105	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	83	ILE	CG1-CB-CG2	-6.89	96.23	111.40
1	A	236	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	143	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	87	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	A	230	LEU	CB-CG-CD1	6.65	122.31	111.00

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LEU	CB-CG-CD2	6.61	122.24	111.00
1	A	191	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	126	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	230	LEU	CB-CG-CD2	-6.51	99.94	111.00
1	A	274	HIS	C-N-CD	6.44	141.93	128.40
1	A	87	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	23	GLU	N-CA-C	-6.40	93.72	111.00
1	A	68	LYS	CB-CA-C	6.33	123.06	110.40
1	A	60	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	50	THR	CB-CA-C	5.98	127.74	111.60
1	A	127	TRP	CB-CA-C	-5.95	98.49	110.40
1	A	227	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	A	126	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	128	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	A	162	LEU	CB-CG-CD2	5.75	120.78	111.00
1	A	46	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	A	250	LYS	CD-CE-NZ	-5.74	98.51	111.70
1	A	239	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	A	158	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	248	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	207	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	A	247	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	276	MET	CG-SD-CE	5.10	108.35	100.20
1	A	176	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	237	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	THR	Peptide
1	A	179	CYS	Peptide
1	A	19	PRO	Peptide
1	A	195	ALA	Peptide
1	A	196	PRO	Peptide
1	A	197	GLY	Peptide
1	A	20	PRO	Peptide
1	A	21	GLY	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	2241	0	2254	81	0
2	A	20	0	0	0	0
All	All	2261	0	2254	81	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 18.

All (81) 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:18:VAL:CG1	1:A:22:THR:HG21	1.77	1.12
1:A:18:VAL:CG1	1:A:22:THR:CG2	2.29	1.11
1:A:195:ALA:H	1:A:196:PRO:HG3	1.17	1.06
1:A:18:VAL:HG13	1:A:22:THR:HG21	1.32	1.05
1:A:195:ALA:N	1:A:196:PRO:HG3	1.84	0.91
1:A:178:THR:O	1:A:180:THR:HG23	1.74	0.86
1:A:18:VAL:HG12	1:A:22:THR:CG2	2.06	0.82
1:A:195:ALA:HB3	1:A:196:PRO:CB	2.11	0.81
1:A:169:ILE:HD12	1:A:169:ILE:N	1.95	0.81
1:A:196:PRO:HB2	1:A:198:GLY:N	1.97	0.78
1:A:195:ALA:HB3	1:A:196:PRO:HB3	1.67	0.76
1:A:168:ALA:HB3	1:A:230:LEU:HD12	1.71	0.73
1:A:233:HIS:HD2	1:A:271:HIS:NE2	1.90	0.69
1:A:104:LEU:HD13	1:A:106:TYR:HB3	1.74	0.67
1:A:195:ALA:N	1:A:196:PRO:CG	2.58	0.66
1:A:194:VAL:HG12	1:A:196:PRO:HD3	1.78	0.65
1:A:6:ILE:HG13	1:A:10:LYS:HD2	1.80	0.64
1:A:187:ARG:HD3	1:A:241:LEU:HD12	1.79	0.64
1:A:184:PHE:HA	1:A:239:VAL:HG22	1.80	0.63
1:A:18:VAL:HG12	1:A:22:THR:HG22	1.78	0.63
1:A:271:HIS:HD1	1:A:271:HIS:H	1.47	0.63
1:A:178:THR:O	1:A:180:THR:CG2	2.47	0.62
1:A:196:PRO:CB	1:A:198:GLY:H	2.13	0.61
1:A:18:VAL:HG11	1:A:22:THR:CG2	2.28	0.58
1:A:195:ALA:N	1:A:196:PRO:CD	2.66	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLY:O	1:A:78:TYR:HB2	2.04	0.57
1:A:195:ALA:HB3	1:A:196:PRO:CA	2.34	0.57
1:A:178:THR:C	1:A:180:THR:HG23	2.25	0.57
1:A:24:VAL:HG12	1:A:29:MET:HG3	1.88	0.54
1:A:169:ILE:HD13	1:A:291:MET:HE2	1.88	0.54
1:A:109:ALA:HB1	1:A:110:PRO:HA	1.90	0.54
1:A:195:ALA:CA	1:A:196:PRO:HG3	2.38	0.54
1:A:220:ASN:OD1	1:A:247:LEU:HB2	2.09	0.53
1:A:27:ASP:O	1:A:31:LYS:HG3	2.09	0.53
1:A:195:ALA:CB	1:A:196:PRO:CA	2.86	0.53
1:A:128:LEU:HD13	1:A:138:LEU:HD22	1.91	0.53
1:A:194:VAL:HG11	1:A:199:ILE:HD12	1.92	0.52
1:A:195:ALA:N	1:A:196:PRO:HD3	2.24	0.52
1:A:268:HIS:O	1:A:269:VAL:C	2.48	0.51
1:A:285:VAL:O	1:A:289:GLU:HG3	2.11	0.51
1:A:154:LEU:HD11	1:A:168:ALA:HB2	1.94	0.50
1:A:196:PRO:CB	1:A:198:GLY:N	2.68	0.50
1:A:195:ALA:HB3	1:A:196:PRO:CG	2.41	0.50
1:A:168:ALA:C	1:A:169:ILE:HD12	2.31	0.50
1:A:169:ILE:CD1	1:A:169:ILE:N	2.71	0.50
1:A:79:VAL:HA	1:A:109:ALA:O	2.11	0.50
1:A:196:PRO:HD2	1:A:199:ILE:HG22	1.94	0.49
1:A:233:HIS:CD2	1:A:271:HIS:NE2	2.75	0.49
1:A:289:GLU:O	1:A:293:GLU:HG3	2.13	0.48
1:A:195:ALA:CA	1:A:196:PRO:CG	2.92	0.48
1:A:194:VAL:HG12	1:A:196:PRO:CD	2.42	0.48
1:A:143:ASP:HB2	1:A:269:VAL:CG2	2.43	0.48
1:A:124:ALA:O	1:A:127:TRP:HB3	2.14	0.48
1:A:196:PRO:HB2	1:A:199:ILE:H	1.79	0.48
1:A:143:ASP:HA	1:A:171:ILE:O	2.15	0.47
1:A:169:ILE:HG21	1:A:287:VAL:HG13	1.97	0.47
1:A:195:ALA:CB	1:A:196:PRO:HA	2.45	0.46
1:A:169:ILE:HG13	1:A:231:LEU:HB3	1.97	0.46
1:A:146:GLY:O	1:A:150:VAL:HG23	2.16	0.46
1:A:195:ALA:HB3	1:A:196:PRO:HG3	1.98	0.46
1:A:86:HIS:HE2	1:A:143:ASP:CG	2.19	0.45
1:A:18:VAL:HG11	1:A:22:THR:HG23	1.97	0.45
1:A:195:ALA:H	1:A:196:PRO:CG	2.06	0.45
1:A:115:PRO:O	1:A:119:GLU:HG3	2.17	0.45
1:A:215:PRO:HB3	1:A:222:ALA:HA	1.99	0.44
1:A:118:VAL:O	1:A:122:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HA	1:A:19:PRO:HD3	1.97	0.44
1:A:162:LEU:HA	1:A:162:LEU:HD12	1.74	0.43
1:A:201:LYS:O	1:A:204:ALA:HB3	2.19	0.43
1:A:129:LEU:HD21	1:A:135:PRO:HG3	1.99	0.43
1:A:18:VAL:CG1	1:A:22:THR:HG23	2.36	0.43
1:A:197:GLY:CA	1:A:200:ASN:HB2	2.49	0.42
1:A:178:THR:HB	1:A:180:THR:HG23	2.01	0.42
1:A:154:LEU:HB3	1:A:227:LEU:HD13	2.02	0.42
1:A:287:VAL:O	1:A:291:MET:HG3	2.21	0.41
1:A:212:ALA:O	1:A:218:SER:OG	2.23	0.41
1:A:234:VAL:HG13	1:A:262:ILE:HG23	2.02	0.41
1:A:68:LYS:HG2	1:A:137:HIS:HB3	2.03	0.41
1:A:195:ALA:CB	1:A:196:PRO:HG3	2.51	0.40
1:A:81:GLY:O	1:A:82:SER:HB3	2.21	0.40
1:A:20:PRO:HA	1:A:22:THR:H	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	295/322 (92%)	263 (89%)	28 (10%)	4 (1%)	14 7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	PRO
1	A	212	ALA
1	A	271	HIS
1	A	269	VAL

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	229/246 (93%)	202 (88%)	27 (12%)	6 3

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	23	GLU
1	A	26	LEU
1	A	27	ASP
1	A	33	MET
1	A	35	LYS
1	A	49	VAL
1	A	50	THR
1	A	65	GLN
1	A	104	LEU
1	A	136	GLN
1	A	151	LEU
1	A	162	LEU
1	A	165	PRO
1	A	169	ILE
1	A	178	THR
1	A	185	LYS
1	A	187	ARG
1	A	193	MET
1	A	201	LYS
1	A	229	PRO
1	A	239	VAL
1	A	241	LEU
1	A	260	LEU
1	A	276	MET
1	A	281	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	131	GLN
1	A	181	ASN
1	A	208	ASN
1	A	223	ASN
1	A	233	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 95th 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	297/322 (92%)	-0.24	6 (2%)	68	73	6, 16, 33, 46	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PRO	3.7
1	A	195	ALA	3.6
1	A	194	VAL	3.5
1	A	196	PRO	3.0
1	A	21	GLY	2.6
1	A	1	MET	2.5

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.