Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 PM GMT

PDB ID	:	3VW5
Title	:	Crystal structure of sugar epimerase from ruminal bacterium
Authors	:	Fujiwara, T.; Saburi, W.; Tanaka, I.; Yao, M.
Deposited on	:	2012-08-02
Resolution	:	2.60 Å(reported)

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

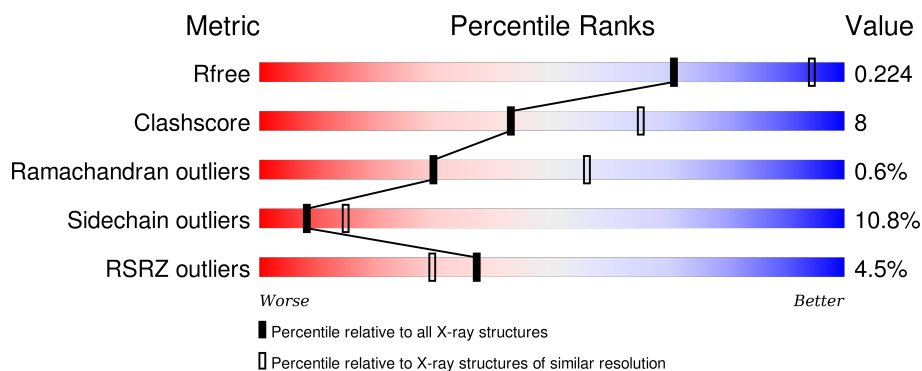|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		8
Ramachandran outliers		0.6%
Sidechain outliers		10.8%
RSRZ outliers		4.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	389	3% / 78% / 17% / 5%
1	B	389	3% / 78% / 19% / •
1	C	389	7% / 74% / 21% / 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9744 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 Cellobiose 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total 3196	C 2039	N 527	O 614	S 16	0	0	0
1	B	389	Total 3196	C 2039	N 527	O 614	S 16	0	0	0
1	C	389	Total 3196	C 2039	N 527	O 614	S 16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLU	GLY	ENGINEERED MUTATION	UNP A8CF79
A	138	LEU	PRO	ENGINEERED MUTATION	UNP A8CF79
B	38	GLU	GLY	ENGINEERED MUTATION	UNP A8CF79
B	138	LEU	PRO	ENGINEERED MUTATION	UNP A8CF79
C	38	GLU	GLY	ENGINEERED MUTATION	UNP A8CF79
C	138	LEU	PRO	ENGINEERED MUTATION	UNP A8CF79

- Molecule 2 is water.

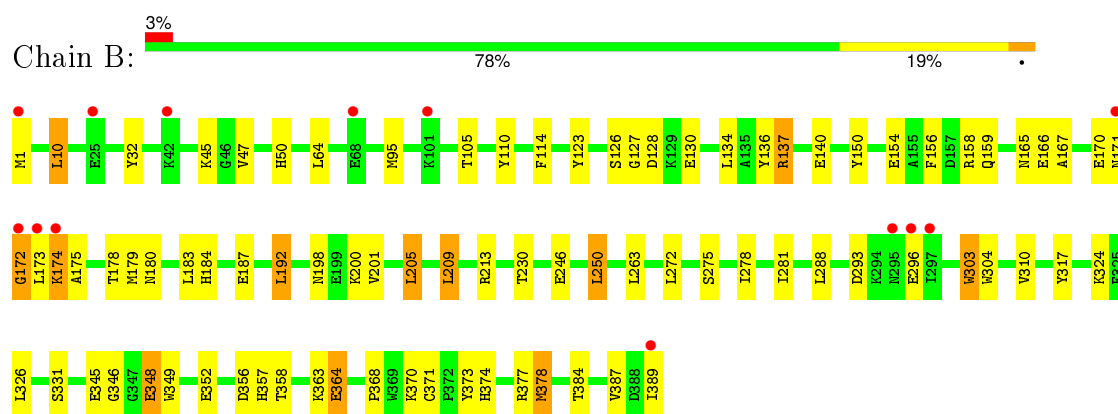| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total 57	O 57	0	0
2	B	59	Total 59	O 59	0	0
2	C	40	Total 40	O 40	0	0

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.
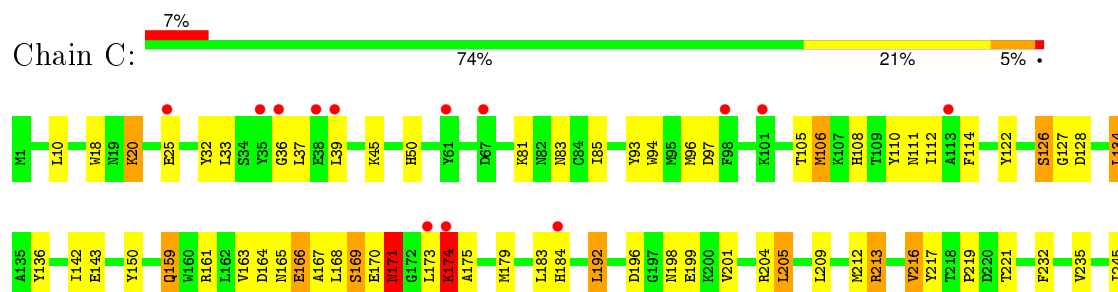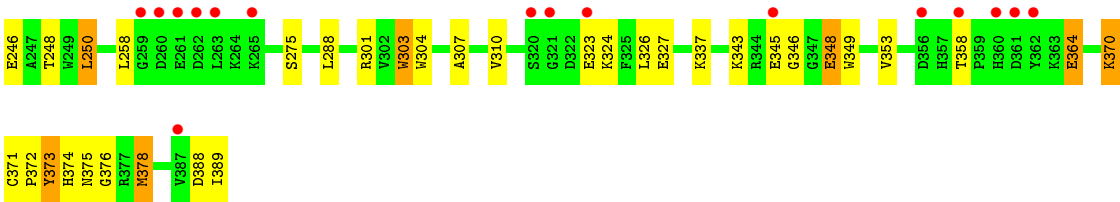
- Molecule 1: Cellobiose 2-epimerase

- Molecule 1: Cellobiose 2-epimerase

- Molecule 1: Cellobiose 2-epimerase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.93Å 100.88Å 186.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.60 43.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.13-2.60) 98.5 (43.68-2.60)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.26 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.173 , 0.222 0.170 , 0.224	Depositor DCC
R_{free} test set	2893 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 46.8	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.47$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 57195 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9744	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.46	0/3275	0.57	1/4427 (0.0%)
1	B	0.47	1/3275 (0.0%)	0.56	0/4427
1	C	0.47	0/3275	0.55	0/4427
All	All	0.47	1/9825 (0.0%)	0.56	1/13281 (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	A	0	1
1	B	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	B	371	CYS	CB-SG	6.21	1.92	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	GLY	N-CA-C	-5.65	98.98	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	SER	Peptide
1	B	126	SER	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	3196	0	3032	46	0
1	B	3196	0	3032	43	0
1	C	3196	0	3032	67	0
2	A	57	0	0	1	0
2	B	59	0	0	2	0
2	C	40	0	0	0	0
All	All	9744	0	9096	154	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 8.

All (154) 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:126:SER:HB3	1:C:128:ASP:H	1.26	0.99
1:A:166:GLU:HG3	1:A:174:LYS:HD3	1.53	0.91
1:C:173:LEU:O	1:C:175:ALA:N	2.10	0.84
1:A:169:SER:HB2	1:A:174:LYS:H	1.42	0.84
1:C:212:MET:HA	1:C:216:VAL:HG13	1.62	0.82
1:C:163:VAL:HG12	1:C:164:ASP:H	1.50	0.75
1:C:126:SER:CB	1:C:128:ASP:H	1.99	0.75
1:A:32:TYR:CE1	1:A:364:GLU:HG2	2.22	0.74
1:C:45:LYS:HB3	1:C:50:HIS:CE1	2.24	0.72
1:A:163:VAL:HG12	1:A:164:ASP:H	1.55	0.72
1:A:166:GLU:O	1:A:167:ALA:HB3	1.90	0.71
1:C:45:LYS:HB3	1:C:50:HIS:HE1	1.55	0.71
1:C:110:TYR:HE1	1:C:184:HIS:CD2	2.10	0.70
1:A:32:TYR:HE1	1:A:364:GLU:HG2	1.54	0.70
1:A:212:MET:HA	1:A:216:VAL:HG13	1.73	0.70
1:C:166:GLU:O	1:C:168:LEU:N	2.25	0.69
1:B:32:TYR:CE1	1:B:364:GLU:HG2	2.26	0.69
1:B:32:TYR:HE1	1:B:364:GLU:HG2	1.60	0.67
1:C:348:GLU:HG3	1:C:349:TRP:H	1.59	0.67
1:C:310:VAL:HG21	1:C:378:MET:HE1	1.78	0.66
1:B:10:LEU:HD13	1:B:64:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:LEU:C	1:C:175:ALA:H	2.00	0.65
1:C:170:GLU:HG2	1:C:171:ASN:OD1	1.97	0.64
1:A:246:GLU:HG2	1:A:250:LEU:HD22	1.79	0.64
1:C:348:GLU:CG	1:C:349:TRP:H	2.11	0.64
1:C:205:LEU:HD12	1:C:258:LEU:HD21	1.78	0.64
1:C:169:SER:OG	1:C:173:LEU:HA	1.98	0.63
1:C:192:LEU:HD13	1:C:201:VAL:HG21	1.81	0.63
1:C:126:SER:HB3	1:C:128:ASP:N	2.06	0.62
1:A:166:GLU:HG3	1:A:174:LYS:CD	2.29	0.62
1:A:175:ALA:HB1	1:A:228:PHE:O	2.00	0.61
1:B:110:TYR:HE1	1:B:184:HIS:CD2	2.18	0.61
1:B:348:GLU:HG3	1:B:349:TRP:H	1.66	0.61
1:C:32:TYR:CE1	1:C:364:GLU:HG2	2.35	0.61
1:A:180:ASN:HB2	2:A:447:HOH:O	2.01	0.59
1:A:183:LEU:HD11	1:A:250:LEU:HD23	1.84	0.59
1:B:192:LEU:HD13	1:B:201:VAL:HG21	1.83	0.59
1:A:52:ARG:HD3	1:A:371:CYS:SG	2.42	0.59
1:A:166:GLU:O	1:A:167:ALA:CB	2.51	0.59
1:C:32:TYR:HE1	1:C:364:GLU:HG2	1.65	0.59
1:B:246:GLU:HG2	1:B:250:LEU:HD22	1.86	0.57
1:A:10:LEU:HD13	1:A:64:LEU:HD11	1.87	0.57
1:B:205:LEU:HD22	1:B:209:LEU:HD22	1.86	0.56
1:A:45:LYS:HB3	1:A:50:HIS:HE1	1.72	0.55
1:C:307:ALA:HA	1:C:378:MET:CE	2.36	0.54
1:B:317:TYR:CG	1:B:326:LEU:HD13	2.43	0.54
1:C:173:LEU:C	1:C:175:ALA:N	2.58	0.54
1:B:165:ASN:HB3	1:B:175:ALA:O	2.07	0.54
1:C:348:GLU:HG3	1:C:349:TRP:N	2.23	0.54
1:C:205:LEU:HD13	1:C:258:LEU:HD11	1.91	0.53
1:A:45:LYS:HB3	1:A:50:HIS:CE1	2.44	0.53
1:B:154:GLU:HB2	1:B:165:ASN:ND2	2.24	0.53
1:B:45:LYS:HB3	1:B:50:HIS:HE1	1.74	0.53
1:C:122:TYR:CZ	1:C:126:SER:OG	2.60	0.53
1:C:171:ASN:N	1:C:171:ASN:OD1	2.41	0.53
1:B:326:LEU:HD11	1:B:387:VAL:HG21	1.90	0.53
1:B:310:VAL:HB	1:B:378:MET:HE2	1.89	0.53
1:B:171:ASN:ND2	1:B:293:ASP:OD2	2.42	0.52
1:B:304:TRP:HB2	1:B:374:HIS:CG	2.45	0.52
1:A:154:GLU:HB2	1:A:165:ASN:ND2	2.25	0.52
1:A:153:ARG:NH2	1:B:140:GLU:OE1	2.40	0.52
1:C:246:GLU:HG2	1:C:250:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:HG2	1:C:213:ARG:HH11	1.76	0.51
1:A:169:SER:HB2	1:A:174:LYS:N	2.18	0.51
1:C:304:TRP:HB2	1:C:374:HIS:CG	2.44	0.51
1:B:180:ASN:HB2	2:B:448:HOH:O	2.10	0.51
1:B:352:GLU:OE2	1:B:363:LYS:HE2	2.11	0.51
1:C:212:MET:HA	1:C:216:VAL:CG1	2.39	0.50
1:C:307:ALA:HA	1:C:378:MET:HE3	1.93	0.50
1:A:47:VAL:HG22	1:A:111:ASN:HD21	1.76	0.50
1:A:10:LEU:CD1	1:A:64:LEU:HD11	2.42	0.50
1:C:143:GLU:OE1	1:C:204:ARG:NE	2.46	0.49
1:B:187:GLU:OE1	1:B:377:ARG:NH1	2.42	0.49
1:B:45:LYS:HB3	1:B:50:HIS:CE1	2.47	0.49
1:B:105:THR:HB	1:B:158:ARG:HB2	1.94	0.48
1:C:20:LYS:HB3	1:C:20:LYS:NZ	2.28	0.48
1:B:348:GLU:CG	1:B:349:TRP:H	2.27	0.48
1:C:110:TYR:CE1	1:C:184:HIS:CD2	2.98	0.48
1:A:304:TRP:HB2	1:A:374:HIS:CG	2.49	0.48
1:C:304:TRP:HB2	1:C:374:HIS:CD2	2.49	0.48
1:C:159:GLN:HG2	1:C:159:GLN:H	1.46	0.48
1:B:95:MET:HE1	1:B:368:PRO:HG3	1.95	0.47
1:B:178:THR:HB	2:B:448:HOH:O	2.15	0.47
1:A:163:VAL:HG12	1:A:164:ASP:N	2.25	0.47
1:C:245:ILE:O	1:C:248:THR:OG1	2.33	0.47
1:C:371:CYS:SG	1:C:373:TYR:HB3	2.55	0.47
1:A:119:LEU:HD13	1:A:134:LEU:HB3	1.97	0.47
1:A:205:LEU:HD13	1:A:258:LEU:HD11	1.97	0.47
1:B:1:MET:HB3	1:B:389:ILE:O	2.15	0.46
1:C:159:GLN:HG3	1:C:161:ARG:HH21	1.80	0.46
1:A:348:GLU:CG	1:A:349:TRP:H	2.27	0.46
1:A:303:TRP:CZ2	1:A:370:LYS:HG3	2.51	0.46
1:B:356:ASP:O	1:B:357:HIS:HB2	2.16	0.46
1:B:272:LEU:HA	1:B:275:SER:HB2	1.98	0.45
1:C:348:GLU:CG	1:C:349:TRP:N	2.79	0.45
1:B:128:ASP:OD2	1:B:130:GLU:N	2.49	0.45
1:A:6:ILE:CG2	1:A:379:CYS:HA	2.47	0.45
1:C:165:ASN:HB3	1:C:175:ALA:O	2.17	0.45
1:C:375:ASN:OD1	1:C:376:GLY:N	2.49	0.45
1:A:192:LEU:HD13	1:A:201:VAL:HG21	1.99	0.45
1:C:97:ASP:OD1	1:C:97:ASP:C	2.55	0.45
1:C:81:LYS:HG3	1:C:134:LEU:HD21	1.98	0.45
1:B:303:TRP:CG	1:B:304:TRP:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:TRP:CG	1:C:304:TRP:N	2.86	0.44
1:A:159:GLN:OE1	1:A:161:ARG:NH2	2.50	0.44
1:A:250:LEU:HA	1:A:250:LEU:HD12	1.76	0.44
1:B:110:TYR:CE1	1:B:184:HIS:CD2	3.02	0.44
1:C:33:LEU:HD13	1:C:39:LEU:HD13	1.99	0.44
1:C:388:ASP:O	1:C:389:ILE:HB	2.18	0.44
1:C:301:ARG:HB2	1:C:353:VAL:O	2.18	0.44
1:C:20:LYS:HB3	1:C:20:LYS:HZ1	1.83	0.43
1:C:217:TYR:O	1:C:219:PRO:HD3	2.17	0.43
1:C:36:GLY:O	1:C:37:LEU:HB2	2.19	0.43
1:C:126:SER:CB	1:C:127:GLY:HA2	2.49	0.43
1:B:123:TYR:O	1:B:127:GLY:HA2	2.19	0.43
1:A:358:THR:HA	1:A:359:PRO:HD3	1.75	0.43
1:C:174:LYS:HB2	1:C:235:VAL:HG11	2.00	0.43
1:C:93:TYR:CD1	1:C:105:THR:HG22	2.54	0.43
1:C:112:ILE:HG22	1:C:142:ILE:HD11	2.01	0.42
1:C:85:ILE:CD1	1:C:134:LEU:HG	2.49	0.42
1:B:156:PHE:N	1:B:156:PHE:CD2	2.87	0.42
1:C:337:LYS:O	1:C:343:LYS:NZ	2.53	0.42
1:A:110:TYR:HE1	1:A:184:HIS:CD2	2.37	0.42
1:A:221:THR:HG22	1:A:223:ALA:H	1.84	0.42
1:B:172:GLY:HA3	1:B:173:LEU:HA	1.90	0.42
1:A:123:TYR:O	1:A:127:GLY:HA2	2.19	0.42
1:A:110:TYR:CE1	1:A:184:HIS:CD2	3.08	0.42
1:B:263:LEU:HA	1:B:263:LEU:HD23	1.94	0.42
1:B:250:LEU:HA	1:B:250:LEU:HD12	1.89	0.42
1:C:106:MET:SD	1:C:108:HIS:HB2	2.60	0.42
1:B:278:ILE:HA	1:B:278:ILE:HD13	1.82	0.42
1:A:371:CYS:HB2	1:A:372:PRO:HD2	2.01	0.41
1:A:213:ARG:HG2	1:A:214:ASP:OD1	2.20	0.41
1:A:303:TRP:CG	1:A:304:TRP:N	2.87	0.41
1:C:94:TRP:HZ3	1:C:111:ASN:HB2	1.85	0.41
1:A:345:GLU:HA	1:A:346:GLY:HA2	1.78	0.41
1:A:348:GLU:OE1	1:A:349:TRP:HB2	2.20	0.41
1:C:136:TYR:OH	1:C:198:ASN:HB2	2.20	0.41
1:C:83:ASN:HB3	1:C:96:MET:HE2	2.03	0.41
1:A:179:MET:HE2	1:A:179:MET:HB2	1.80	0.41
1:B:166:GLU:O	1:B:167:ALA:HB3	2.20	0.41
1:A:162:LEU:CD2	1:B:137:ARG:HH21	2.33	0.41
1:B:345:GLU:HA	1:B:346:GLY:HA2	1.89	0.41
1:B:174:LYS:HG2	1:B:174:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:TRP:CH2	1:C:372:PRO:HD3	2.56	0.41
1:C:303:TRP:CZ2	1:C:370:LYS:HD3	2.56	0.40
1:B:136:TYR:OH	1:B:198:ASN:HB2	2.20	0.40
1:A:48:ILE:HG13	1:A:111:ASN:OD1	2.21	0.40
1:A:123:TYR:O	1:A:127:GLY:CA	2.70	0.40
1:C:18:TRP:CD1	1:C:372:PRO:HB3	2.56	0.40
1:C:18:TRP:NE1	1:C:372:PRO:HB3	2.36	0.40
1:C:345:GLU:HA	1:C:346:GLY:HA2	1.74	0.40
1:B:310:VAL:HG21	1:B:378:MET:HE1	2.04	0.40
1:C:349:TRP:CD1	1:C:349:TRP:N	2.88	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	387/389 (100%)	371 (96%)	15 (4%)	1 (0%)	46	72
1	B	387/389 (100%)	369 (95%)	17 (4%)	1 (0%)	46	72
1	C	387/389 (100%)	365 (94%)	17 (4%)	5 (1%)	15	30
All	All	1161/1167 (100%)	1105 (95%)	49 (4%)	7 (1%)	30	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	LYS
1	B	172	GLY
1	A	167	ALA
1	C	166	GLU
1	C	171	ASN
1	C	196	ASP
1	C	167	ALA

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	333/333 (100%)	292 (88%)	41 (12%)	6	11
1	B	333/333 (100%)	302 (91%)	31 (9%)	11	21
1	C	333/333 (100%)	297 (89%)	36 (11%)	8	15
All	All	999/999 (100%)	891 (89%)	108 (11%)	8	15

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	ARG
1	A	8	GLN
1	A	10	LEU
1	A	25	GLU
1	A	38	GLU
1	A	42	LYS
1	A	48	ILE
1	A	114	PHE
1	A	134	LEU
1	A	137	ARG
1	A	150	TYR
1	A	159	GLN
1	A	162	LEU
1	A	169	SER
1	A	170	GLU
1	A	173	LEU
1	A	179	MET
1	A	180	ASN
1	A	192	LEU
1	A	194	LYS
1	A	199	GLU
1	A	200	LYS
1	A	205	LEU
1	A	209	LEU
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	265	LYS
1	A	281	ILE
1	A	288	LEU
1	A	303	TRP
1	A	324	LYS
1	A	326	LEU
1	A	327	GLU
1	A	348	GLU
1	A	358	THR
1	A	364	GLU
1	A	371	CYS
1	A	373	TYR
1	A	384	THR
1	A	387	VAL
1	B	10	LEU
1	B	47	VAL
1	B	114	PHE
1	B	134	LEU
1	B	137	ARG
1	B	150	TYR
1	B	159	GLN
1	B	170	GLU
1	B	174	LYS
1	B	179	MET
1	B	183	LEU
1	B	192	LEU
1	B	200	LYS
1	B	205	LEU
1	B	209	LEU
1	B	213	ARG
1	B	230	THR
1	B	250	LEU
1	B	281	ILE
1	B	288	LEU
1	B	296	GLU
1	B	303	TRP
1	B	324	LYS
1	B	331	SER
1	B	348	GLU
1	B	358	THR
1	B	364	GLU

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Mol	Chain	Res	Type
1	B	370	LYS
1	B	373	TYR
1	B	378	MET
1	B	384	THR
1	C	10	LEU
1	C	20	LYS
1	C	25	GLU
1	C	106	MET
1	C	114	PHE
1	C	126	SER
1	C	134	LEU
1	C	150	TYR
1	C	159	GLN
1	C	169	SER
1	C	171	ASN
1	C	174	LYS
1	C	179	MET
1	C	183	LEU
1	C	192	LEU
1	C	199	GLU
1	C	205	LEU
1	C	209	LEU
1	C	213	ARG
1	C	216	VAL
1	C	221	THR
1	C	232	PHE
1	C	250	LEU
1	C	275	SER
1	C	288	LEU
1	C	303	TRP
1	C	323	GLU
1	C	324	LYS
1	C	326	LEU
1	C	327	GLU
1	C	348	GLU
1	C	358	THR
1	C	364	GLU
1	C	370	LYS
1	C	373	TYR
1	C	378	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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(Å²)	Q<0.9
1	A	389/389 (100%)	-0.09	10 (2%)	59	53	31, 43, 63, 85	0
1	B	389/389 (100%)	-0.02	13 (3%)	50	43	33, 44, 64, 89	0
1	C	389/389 (100%)	0.30	29 (7%)	17	12	35, 50, 67, 82	0
All	All	1167/1167 (100%)	0.06	52 (4%)	37	29	31, 46, 65, 89	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	GLY	6.4
1	C	259	GLY	3.7
1	A	261	GLU	3.7
1	B	1	MET	3.4
1	B	295	ASN	3.4
1	B	101	LYS	3.3
1	B	297	ILE	3.2
1	C	36	GLY	3.1
1	C	35	TYR	3.1
1	C	261	GLU	3.1
1	A	262	ASP	3.1
1	B	173	LEU	2.9
1	C	356	ASP	2.9
1	C	38	GLU	2.9
1	C	174	LYS	2.9
1	A	70	LEU	2.8
1	B	174	LYS	2.7
1	B	389	ILE	2.7
1	A	174	LYS	2.7
1	B	25	GLU	2.6
1	C	39	LEU	2.6
1	B	171	ASN	2.6
1	C	263	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	2.5
1	C	345	GLU	2.5
1	A	67	ASP	2.5
1	C	265	LYS	2.4
1	A	263	LEU	2.4
1	C	260	ASP	2.4
1	C	358	THR	2.3
1	C	323	GLU	2.3
1	C	173	LEU	2.3
1	A	101	LYS	2.3
1	C	61	TYR	2.3
1	B	68	GLU	2.3
1	C	362	TYR	2.3
1	C	67	ASP	2.3
1	C	360	HIS	2.2
1	A	265	LYS	2.2
1	C	101	LYS	2.2
1	C	184	HIS	2.2
1	B	296	GLU	2.2
1	C	387	VAL	2.1
1	B	42	LYS	2.1
1	C	320	SER	2.1
1	C	113	ALA	2.1
1	C	361	ASP	2.1
1	C	25	GLU	2.1
1	C	98	PHE	2.0
1	C	321	GLY	2.0
1	A	266	GLN	2.0
1	C	262	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.