Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 11:14 PM GMT

PDB ID	:	1WUE
Title	:	Crystal structure of protein GI:29375081, unknown member of enolase superfamily from enterococcus faecalis V583
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-05
Resolution	:	2.10 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 (i) symbol.

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

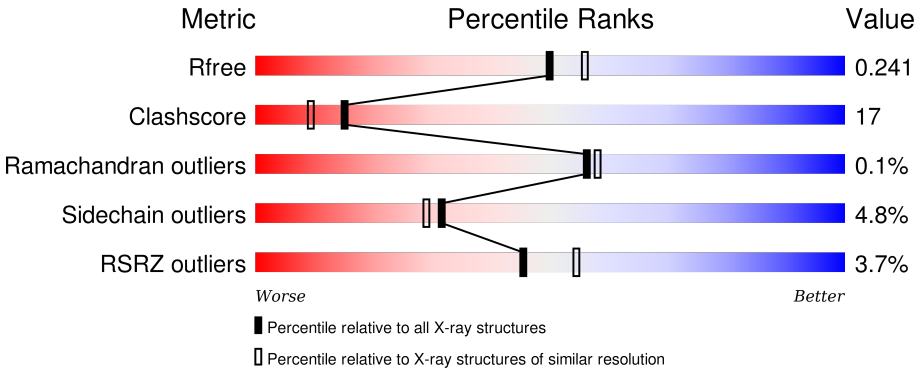
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	386	6% 66% 27%
1	B	386	% 65% 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6319 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 mandelate racemase/muconate lactonizing enzyme family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2959	1900	497	551	11			
1	B	369	Total	C	N	O	S	0	0	0
			2955	1898	496	550	11			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	GLY	-	EXPRESSION TAG	UNP Q838J7
A	983	HIS	-	EXPRESSION TAG	UNP Q838J7
A	984	HIS	-	EXPRESSION TAG	UNP Q838J7
A	985	HIS	-	EXPRESSION TAG	UNP Q838J7
A	986	HIS	-	EXPRESSION TAG	UNP Q838J7
A	987	HIS	-	EXPRESSION TAG	UNP Q838J7
A	988	HIS	-	EXPRESSION TAG	UNP Q838J7
A	989	HIS	-	EXPRESSION TAG	UNP Q838J7
A	990	HIS	-	EXPRESSION TAG	UNP Q838J7
A	991	HIS	-	EXPRESSION TAG	UNP Q838J7
A	992	HIS	-	EXPRESSION TAG	UNP Q838J7
A	993	GLY	-	EXPRESSION TAG	UNP Q838J7
A	994	LEU	-	EXPRESSION TAG	UNP Q838J7
A	995	VAL	-	EXPRESSION TAG	UNP Q838J7
A	996	PRO	-	EXPRESSION TAG	UNP Q838J7
A	997	ARG	-	EXPRESSION TAG	UNP Q838J7
A	998	GLY	-	EXPRESSION TAG	UNP Q838J7
A	999	SER	-	EXPRESSION TAG	UNP Q838J7
A	1000	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1982	GLY	-	EXPRESSION TAG	UNP Q838J7
B	1983	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1984	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1985	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1986	HIS	-	EXPRESSION TAG	UNP Q838J7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1987	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1988	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1989	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1990	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1991	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1992	HIS	-	EXPRESSION TAG	UNP Q838J7
B	1993	GLY	-	EXPRESSION TAG	UNP Q838J7
B	1994	LEU	-	EXPRESSION TAG	UNP Q838J7
B	1995	VAL	-	EXPRESSION TAG	UNP Q838J7
B	1996	PRO	-	EXPRESSION TAG	UNP Q838J7
B	1997	ARG	-	EXPRESSION TAG	UNP Q838J7
B	1998	GLY	-	EXPRESSION TAG	UNP Q838J7
B	1999	SER	-	EXPRESSION TAG	UNP Q838J7
B	2000	HIS	-	EXPRESSION TAG	UNP Q838J7

- Molecule 2 is water.

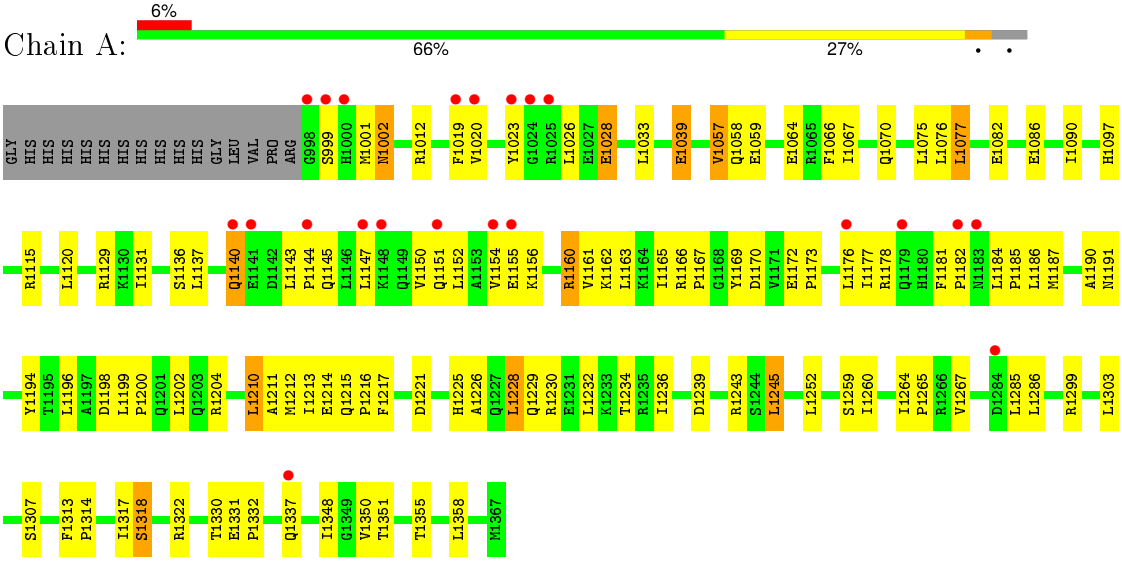
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	220	Total O 220 220	0	0
2	B	185	Total O 185 185	0	0

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.

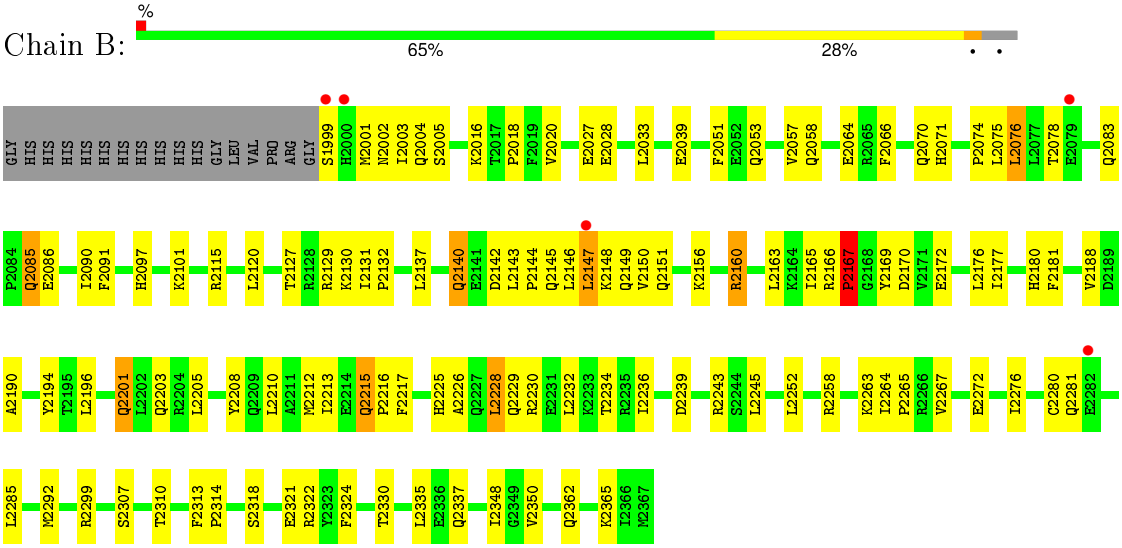
- Molecule 1: mandelate racemase/muconate lactonizing enzyme family protein

Chain A:



- Molecule 1: mandelate racemase/muconate lactonizing enzyme family protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	136.81Å 136.81Å 112.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.10 28.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.10) 98.6 (28.65-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.32 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.242 0.206 , 0.241	Depositor DCC
R_{free} test set	2260 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.1	EDS
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 45927 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6319	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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	0.34	0/3021	0.72	3/4093 (0.1%)
1	B	0.32	0/3017	0.65	4/4088 (0.1%)
All	All	0.33	0/6038	0.68	7/8181 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1196	LEU	CB-CG-CD2	-19.36	78.08	111.00
1	A	1351	THR	CA-CB-OG1	9.95	129.90	109.00
1	B	2172	GLU	CA-CB-CG	-9.88	91.67	113.40
1	B	2201	GLN	CA-CB-CG	6.83	128.43	113.40
1	A	1318	SER	CA-CB-OG	5.85	126.99	111.20
1	B	2330	THR	CA-CB-CG2	-5.57	104.61	112.40
1	B	2330	THR	CA-CB-OG1	5.44	120.43	109.00

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	2959	0	2973	103	0
1	B	2955	0	2970	109	0
2	A	220	0	0	7	0
2	B	185	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6319	0	5943	207	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 17.

All (207) 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:B:2163:LEU:HD11	1:B:2177:ILE:HD12	1.39	1.03
1:A:1165:ILE:HD12	1:A:1170:ASP:HA	1.52	0.89
1:B:2071:HIS:O	1:B:2075:LEU:HD13	1.74	0.87
1:A:1163:LEU:HD11	1:A:1177:ILE:HD12	1.56	0.87
1:B:2165:ILE:HD12	1:B:2170:ASP:HA	1.58	0.85
1:B:2213:ILE:HD13	1:B:2234:THR:HG21	1.59	0.84
1:B:2267:VAL:HG21	1:B:2276:ILE:HD12	1.61	0.82
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.81	0.81
1:A:1215:GLN:HE22	1:A:1239:ASP:H	1.29	0.80
1:A:1330:THR:HG23	1:A:1331:GLU:HG2	1.65	0.78
1:A:1210:LEU:HD23	1:A:1213:ILE:HD11	1.64	0.78
1:A:1152:LEU:HD11	1:A:1156:LYS:HE2	1.64	0.78
1:A:1213:ILE:HD13	1:A:1234:THR:HG21	1.67	0.77
1:B:2001:MET:HG3	1:B:2115:ARG:HE	1.50	0.77
1:A:1002:ASN:HB3	1:A:1039:GLU:CG	2.17	0.74
1:B:2215:GLN:HE22	1:B:2239:ASP:H	1.36	0.74
1:A:1066:PHE:CZ	1:A:1070:GLN:HG3	2.22	0.74
1:B:2281:GLN:NE2	1:B:2310:THR:HG23	2.01	0.74
1:B:2229:GLN:HE22	1:B:2236:ILE:H	1.37	0.72
1:B:2057:VAL:CG2	1:B:2243:ARG:NH2	2.53	0.72
1:A:1002:ASN:HB3	1:A:1039:GLU:HG3	1.72	0.71
1:B:2001:MET:HG3	1:B:2115:ARG:NE	2.05	0.71
1:B:2066:PHE:CZ	1:B:2070:GLN:HG3	2.26	0.71
1:B:2143:LEU:H	1:B:2143:LEU:HD12	1.56	0.70
1:B:2086:GLU:O	1:B:2090:ILE:HG12	1.92	0.70
1:A:1214:GLU:OE1	2:A:3054:HOH:O	2.10	0.68
1:B:2083:GLN:HB3	1:B:2085:GLN:NE2	2.09	0.68
1:B:2001:MET:HA	1:B:2115:ARG:NH2	2.09	0.68
1:A:1086:GLU:O	1:A:1090:ILE:HG12	1.93	0.67
1:A:1229:GLN:HE22	1:A:1236:ILE:H	1.40	0.67
1:B:2215:GLN:NE2	1:B:2239:ASP:H	1.91	0.67
1:B:2085:GLN:NE2	1:B:2085:GLN:H	1.92	0.67
1:A:1215:GLN:NE2	1:A:1239:ASP:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2230:ARG:NH2	2:B:3243:HOH:O	2.24	0.67
1:A:1165:ILE:CG2	1:A:1170:ASP:HB3	2.25	0.66
1:B:2057:VAL:HG21	1:B:2243:ARG:NH2	2.10	0.66
1:B:2165:ILE:CG2	1:B:2170:ASP:HB3	2.25	0.65
1:B:2267:VAL:HG22	1:B:2272:GLU:HB3	1.78	0.65
1:A:1358:LEU:HD23	1:A:1358:LEU:O	1.96	0.65
1:B:2066:PHE:CE2	1:B:2070:GLN:HG3	2.33	0.63
1:B:1999:SER:HB2	2:B:3061:HOH:O	1.98	0.63
1:B:2142:ASP:OD2	1:B:2144:PRO:HD2	1.99	0.62
1:B:2057:VAL:HG22	1:B:2243:ARG:NH2	2.14	0.62
1:B:2085:GLN:HE21	1:B:2085:GLN:H	1.48	0.62
1:B:2147:LEU:HD23	1:B:2176:LEU:HG	1.82	0.60
1:A:1012:ARG:HB3	1:A:1028:GLU:HG3	1.84	0.59
1:A:1140:GLN:NE2	1:A:1145:GLN:HB3	2.17	0.59
1:A:1228:LEU:HD13	1:A:1236:ILE:HD11	1.84	0.59
1:B:2076:LEU:HD13	1:B:2076:LEU:O	2.03	0.59
1:B:2001:MET:HA	1:B:2115:ARG:HH21	1.65	0.59
1:B:2064:GLU:OE1	1:B:2097:HIS:HD2	1.86	0.58
1:B:2196:LEU:HD13	1:B:2196:LEU:O	2.03	0.58
1:A:1097:HIS:HE1	1:B:2058:GLN:O	1.86	0.58
1:A:1213:ILE:CD1	1:A:1234:THR:HG21	2.33	0.57
1:A:1064:GLU:OE1	1:A:1097:HIS:HD2	1.87	0.57
1:B:2190:ALA:HB3	1:B:2216:PRO:HA	1.87	0.57
1:A:1199:LEU:HB3	1:A:1200:PRO:HD3	1.85	0.57
1:A:1129:ARG:HG3	1:A:1129:ARG:HH21	1.70	0.57
1:B:2267:VAL:HG22	1:B:2267:VAL:O	2.04	0.57
1:A:1020:VAL:O	1:A:1020:VAL:HG13	2.04	0.57
1:A:1165:ILE:HG22	1:A:1194:TYR:OH	2.05	0.56
1:B:2165:ILE:HG23	1:B:2170:ASP:HB3	1.87	0.56
1:B:2163:LEU:HD11	1:B:2177:ILE:CD1	2.26	0.56
1:A:1212:MET:C	1:A:1213:ILE:HD12	2.26	0.56
2:A:4004:HOH:O	1:B:2058:GLN:HG3	2.04	0.56
1:A:1001:MET:HG2	1:A:1115:ARG:CD	2.36	0.56
1:B:2213:ILE:CD1	1:B:2234:THR:HG21	2.33	0.55
1:B:2074:PRO:O	1:B:2078:THR:HG23	2.06	0.55
1:B:2020:VAL:HG13	1:B:2020:VAL:O	2.06	0.55
1:A:1057:VAL:HG22	1:A:1243:ARG:NH2	2.22	0.55
1:B:2205:LEU:HD12	1:B:2205:LEU:N	2.22	0.55
1:A:1067:ILE:HG13	1:A:1097:HIS:CD2	2.41	0.55
1:A:1190:ALA:CB	1:A:1216:PRO:HA	2.37	0.55
1:A:1165:ILE:HG23	1:A:1170:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:VAL:CG2	1:A:1243:ARG:NH2	2.71	0.54
1:B:2217:PHE:H	1:B:2225:HIS:CE1	2.25	0.54
1:A:999:SER:O	1:A:1082:GLU:HG2	2.07	0.54
1:B:2165:ILE:HG23	1:B:2169:TYR:O	2.07	0.54
1:B:2131:ILE:HG21	1:B:2307:SER:HA	1.88	0.54
1:A:1057:VAL:HG13	1:A:1059:GLU:OE1	2.07	0.54
1:B:2348:ILE:HG13	1:B:2350:VAL:HG22	1.88	0.54
1:A:1204:ARG:HH11	1:A:1204:ARG:HG3	1.73	0.54
1:A:1217:PHE:H	1:A:1225:HIS:CE1	2.26	0.53
1:B:2208:TYR:HB2	1:B:2210:LEU:HD21	1.90	0.53
1:B:2203:GLN:HA	1:B:2232:LEU:HD21	1.88	0.53
1:B:2213:ILE:HD13	1:B:2234:THR:CG2	2.35	0.53
1:B:2143:LEU:H	1:B:2143:LEU:CD1	2.22	0.53
1:A:1058:GLN:O	1:B:2097:HIS:HE1	1.92	0.53
1:B:2130:LYS:HB2	1:B:2130:LYS:NZ	2.24	0.53
1:B:2143:LEU:N	1:B:2143:LEU:HD12	2.23	0.53
1:A:1143:LEU:HB2	1:A:1144:PRO:HD3	1.91	0.53
1:A:1131:ILE:HG21	1:A:1307:SER:HA	1.90	0.53
1:A:1190:ALA:HB3	1:A:1216:PRO:HA	1.92	0.52
1:A:1140:GLN:HE22	1:A:1145:GLN:HB3	1.75	0.52
1:B:2156:LYS:O	1:B:2337:GLN:HA	2.10	0.52
1:A:1252:LEU:O	1:A:1252:LEU:HD13	2.10	0.51
1:B:2151:GLN:HG3	1:B:2181:PHE:HZ	1.75	0.51
1:A:1260:ILE:CD1	1:A:1285:LEU:HD13	2.40	0.51
1:A:1245:LEU:HD22	1:A:1245:LEU:O	2.11	0.51
1:A:1286:LEU:HD23	1:A:1286:LEU:C	2.30	0.51
1:B:2264:ILE:HB	1:B:2265:PRO:HD3	1.92	0.51
1:B:2226:ALA:O	1:B:2230:ARG:HG3	2.11	0.51
1:B:2051:PHE:HB3	1:B:2053:GLN:NE2	2.25	0.51
1:A:1162:LYS:HE3	1:A:1187:MET:HE3	1.93	0.50
1:B:2281:GLN:CD	1:B:2310:THR:HG23	2.31	0.50
1:A:1165:ILE:HG21	1:A:1170:ASP:HB3	1.92	0.50
1:B:2137:LEU:HD13	1:B:2149:GLN:HE21	1.76	0.50
1:A:1152:LEU:CD1	1:A:1156:LYS:HE2	2.36	0.50
1:B:2229:GLN:NE2	1:B:2236:ILE:H	2.07	0.50
1:B:2210:LEU:HD22	1:B:2210:LEU:N	2.26	0.50
1:B:2212:MET:C	1:B:2213:ILE:HD12	2.32	0.50
1:A:1129:ARG:NH2	1:A:1129:ARG:HG3	2.27	0.50
1:A:1160:ARG:NH1	1:A:1314:PRO:O	2.44	0.49
1:A:1213:ILE:HD13	1:A:1234:THR:CG2	2.41	0.49
1:A:1178:ARG:HD3	1:A:1182:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:HB3	1:A:1176:LEU:CD2	2.43	0.49
1:A:1165:ILE:HG23	1:A:1169:TYR:O	2.13	0.49
1:A:1163:LEU:HD11	1:A:1177:ILE:CD1	2.34	0.49
1:A:1299:ARG:HD3	1:A:1318:SER:O	2.13	0.49
1:B:2165:ILE:HG21	1:B:2170:ASP:HB3	1.93	0.48
1:A:1229:GLN:NE2	1:A:1236:ILE:H	2.10	0.48
1:A:1147:LEU:O	1:A:1151:GLN:HG3	2.13	0.48
1:A:1160:ARG:HD2	1:A:1161:VAL:N	2.29	0.48
1:A:1172:GLU:HB3	1:A:1173:PRO:CD	2.43	0.48
1:A:1162:LYS:HB2	1:A:1187:MET:HE3	1.96	0.48
1:A:1163:LEU:CD1	1:A:1177:ILE:HD12	2.38	0.47
1:B:2145:GLN:O	1:B:2148:LYS:HB3	2.15	0.47
1:B:2039:GLU:OE1	1:B:2115:ARG:NH2	2.47	0.47
1:B:2299:ARG:HD3	1:B:2318:SER:O	2.14	0.47
1:A:1198:ASP:O	1:A:1202:LEU:HD23	2.15	0.47
1:B:2016:LYS:HE3	1:B:2324:PHE:O	2.15	0.47
1:B:2140:GLN:HB3	1:B:2146:LEU:HB2	1.97	0.46
1:A:1058:GLN:HG3	2:A:4004:HOH:O	2.14	0.46
1:B:2127:THR:HB	1:B:2307:SER:OG	2.16	0.46
1:B:2140:GLN:OE1	1:B:2142:ASP:N	2.49	0.46
1:B:2143:LEU:HB2	1:B:2144:PRO:HD3	1.97	0.46
1:B:2005:SER:HB2	1:B:2365:LYS:NZ	2.31	0.45
1:A:1229:GLN:HB2	1:A:1236:ILE:HD12	1.97	0.45
1:A:1226:ALA:O	1:A:1230:ARG:HG3	2.16	0.45
1:B:2003:ILE:CD1	1:B:2076:LEU:HD12	2.46	0.45
1:B:2243:ARG:O	1:B:2267:VAL:HG23	2.16	0.45
1:B:2003:ILE:HD12	1:B:2076:LEU:HD12	1.99	0.45
1:A:1204:ARG:NH1	2:A:3225:HOH:O	2.50	0.45
1:A:1019:PHE:HB2	1:A:1026:LEU:HB2	1.99	0.45
1:B:2165:ILE:CG1	1:B:2188:VAL:HG13	2.47	0.45
1:A:1002:ASN:HB3	1:A:1039:GLU:HG2	1.94	0.45
1:B:2083:GLN:HB3	1:B:2085:GLN:HE22	1.80	0.45
1:A:1166:ARG:HG2	2:A:3090:HOH:O	2.17	0.45
1:B:2190:ALA:CB	1:B:2216:PRO:HA	2.47	0.44
1:A:1259:SER:C	1:A:1260:ILE:HD12	2.38	0.44
1:B:2335:LEU:HD23	1:B:2335:LEU:C	2.37	0.44
1:A:1267:VAL:CG1	1:A:1267:VAL:O	2.65	0.44
1:A:1228:LEU:HD13	1:A:1236:ILE:CD1	2.46	0.44
1:B:2321:GLU:CD	1:B:2321:GLU:H	2.20	0.44
1:B:2057:VAL:HG22	1:B:2058:GLN:OE1	2.18	0.44
1:B:2018:PRO:HB3	1:B:2027:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2129:ARG:HH21	1:B:2129:ARG:HG3	1.82	0.44
1:A:1217:PHE:H	1:A:1225:HIS:HE1	1.66	0.43
1:A:1260:ILE:HD11	1:A:1285:LEU:HD13	1.99	0.43
1:B:2165:ILE:CG2	1:B:2166:ARG:N	2.80	0.43
1:A:1154:VAL:HG21	1:A:1181:PHE:CE2	2.53	0.43
1:A:1058:GLN:O	1:B:2097:HIS:CE1	2.71	0.43
1:A:1215:GLN:NE2	1:A:1239:ASP:N	2.64	0.43
1:B:2166:ARG:HH11	1:B:2166:ARG:HG3	1.84	0.43
1:B:2160:ARG:HG2	1:B:2314:PRO:HB2	2.00	0.43
1:B:2280:CYS:HB3	1:B:2285:LEU:O	2.19	0.43
1:B:2147:LEU:HD21	1:B:2180:HIS:CD2	2.53	0.43
1:B:2150:VAL:HG21	1:B:2177:ILE:HD13	2.00	0.43
1:B:2362:GLN:NE2	1:B:2362:GLN:HA	2.34	0.43
1:A:1150:VAL:HG21	1:A:1177:ILE:CD1	2.49	0.43
1:A:1332:PRO:HA	2:A:4059:HOH:O	2.18	0.43
1:B:2131:ILE:HA	1:B:2132:PRO:HD3	1.93	0.42
1:A:1303:LEU:CD2	1:A:1317:ILE:HG21	2.49	0.42
1:B:2165:ILE:HG22	1:B:2194:TYR:OH	2.20	0.42
1:A:1143:LEU:H	1:A:1143:LEU:HD22	1.83	0.42
1:A:1160:ARG:HD3	1:A:1313:PHE:CZ	2.55	0.42
1:A:1023:TYR:CE1	1:B:2075:LEU:HD11	2.54	0.42
1:A:1023:TYR:HE1	1:B:2075:LEU:HD11	1.83	0.42
1:B:2166:ARG:HB2	1:B:2167:PRO:HD2	2.00	0.42
1:A:1057:VAL:HG22	1:A:1243:ARG:HH21	1.83	0.42
1:B:2091:PHE:HB3	1:B:2101:LYS:HE2	2.02	0.42
1:A:1156:LYS:O	1:A:1337:GLN:HA	2.20	0.42
1:B:2004:GLN:CG	1:B:2039:GLU:HA	2.50	0.42
1:A:1184:LEU:HD12	1:A:1185:PRO:HD2	2.00	0.42
1:A:1077:LEU:CD1	1:A:1077:LEU:N	2.83	0.42
1:B:2160:ARG:HD3	1:B:2313:PHE:CZ	2.54	0.42
1:A:1355:THR:HG23	2:A:3276:HOH:O	2.20	0.42
1:A:1136:SER:O	1:A:1137:LEU:HD23	2.19	0.41
1:A:1264:ILE:HB	1:A:1265:PRO:HD3	2.02	0.41
1:A:1166:ARG:CG	1:A:1167:PRO:HD2	2.50	0.41
1:A:1228:LEU:HD22	1:A:1232:LEU:HG	2.01	0.41
1:A:1211:ALA:O	1:A:1212:MET:HB3	2.20	0.41
1:B:2205:LEU:O	1:B:2210:LEU:HD23	2.21	0.41
1:A:1348:ILE:HG13	1:A:1350:VAL:HG22	2.02	0.41
1:B:2267:VAL:HG21	1:B:2276:ILE:CD1	2.41	0.41
1:B:2245:LEU:HD23	1:B:2245:LEU:O	2.21	0.41
1:B:2215:GLN:NE2	1:B:2239:ASP:N	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ASP:O	1:A:1225:HIS:HD2	2.04	0.41
1:B:2228:LEU:HD22	1:B:2232:LEU:HG	2.02	0.41
1:A:1163:LEU:HG	1:A:1186:LEU:HD11	2.02	0.41
1:B:2143:LEU:HB3	1:B:2176:LEU:HD22	2.03	0.41
1:A:1162:LYS:CE	1:A:1187:MET:HE3	2.50	0.41
1:A:1166:ARG:HG3	1:A:1166:ARG:HH11	1.86	0.41
1:B:2263:LYS:HD3	1:B:2292:MET:CG	2.51	0.40
1:A:1150:VAL:HG21	1:A:1177:ILE:HD13	2.03	0.40
1:B:2064:GLU:OE1	1:B:2097:HIS:CD2	2.70	0.40
1:B:2229:GLN:NE2	1:B:2258:ARG:HG3	2.35	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	368/386 (95%)	355 (96%)	13 (4%)	0	100	100
1	B	367/386 (95%)	356 (97%)	10 (3%)	1 (0%)	46	45
All	All	735/772 (95%)	711 (97%)	23 (3%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2167	PRO

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	322/336 (96%)	306 (95%)	16 (5%)	30	27
1	B	322/336 (96%)	307 (95%)	15 (5%)	32	30
All	All	644/672 (96%)	613 (95%)	31 (5%)	31	29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	ASN
1	A	1028	GLU
1	A	1033	LEU
1	A	1039	GLU
1	A	1057	VAL
1	A	1075	LEU
1	A	1076	LEU
1	A	1077	LEU
1	A	1120	LEU
1	A	1140	GLN
1	A	1160	ARG
1	A	1191	ASN
1	A	1210	LEU
1	A	1228	LEU
1	A	1245	LEU
1	A	1322	ARG
1	B	2002	ASN
1	B	2028	GLU
1	B	2033	LEU
1	B	2076	LEU
1	B	2085	GLN
1	B	2120	LEU
1	B	2140	GLN
1	B	2147	LEU
1	B	2160	ARG
1	B	2167	PRO
1	B	2201	GLN
1	B	2215	GLN
1	B	2228	LEU
1	B	2252	LEU
1	B	2322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1002	ASN
1	A	1004	GLN
1	A	1010	GLN
1	A	1069	GLN
1	A	1085	GLN
1	A	1097	HIS
1	A	1117	GLN
1	A	1140	GLN
1	A	1145	GLN
1	A	1149	GLN
1	A	1180	HIS
1	A	1215	GLN
1	A	1225	HIS
1	A	1229	GLN
1	A	1249	GLN
1	A	1283	ASN
1	A	1304	GLN
1	A	1354	GLN
1	A	1362	GLN
1	A	1364	GLN
1	B	2002	ASN
1	B	2010	GLN
1	B	2042	ASN
1	B	2053	GLN
1	B	2085	GLN
1	B	2097	HIS
1	B	2149	GLN
1	B	2151	GLN
1	B	2159	GLN
1	B	2180	HIS
1	B	2215	GLN
1	B	2225	HIS
1	B	2229	GLN
1	B	2249	GLN
1	B	2281	GLN
1	B	2304	GLN
1	B	2354	GLN
1	B	2362	GLN
1	B	2364	GLN

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	370/386 (95%)	0.26	22 (5%) 26 34	9, 21, 45, 55	0
1	B	369/386 (95%)	0.14	5 (1%) 78 82	11, 24, 42, 51	0
All	All	739/772 (95%)	0.20	27 (3%) 45 54	9, 23, 43, 55	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1024	GLY	4.6
1	A	998	GLY	4.6
1	A	1023	TYR	4.4
1	A	1155	GLU	3.7
1	A	1141	GLU	3.6
1	B	2000	HIS	3.6
1	A	1020	VAL	3.2
1	A	1179	GLN	3.2
1	B	1999	SER	3.1
1	A	1147	LEU	3.0
1	A	1025	ARG	2.9
1	A	1183	ASN	2.9
1	B	2079	GLU	2.7
1	B	2147	LEU	2.7
1	B	2282	GLU	2.7
1	A	1182	PRO	2.6
1	A	1337	GLN	2.5
1	A	1148	LYS	2.5
1	A	1144	PRO	2.4
1	A	999	SER	2.3
1	A	1140	GLN	2.3
1	A	1284	ASP	2.3
1	A	1000	HIS	2.2
1	A	1151	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1019	PHE	2.1
1	A	1176	LEU	2.1
1	A	1154	VAL	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.