



Full wwPDB X-ray Structure Validation Report

Jun 10, 2014 – 11:35 AM EDT

PDB ID : 1WUF
Title : Crystal structure of protein GI:16801725, member of Enolase superfamily from *Listeria innocua* Clip11262
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 : 2004-12-07
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

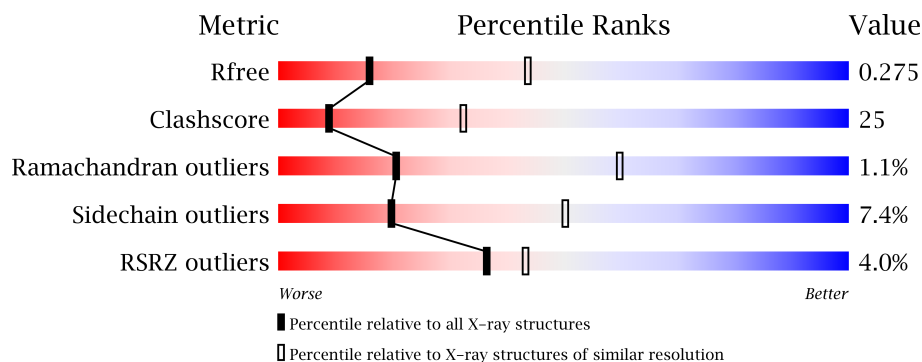
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	393	
1	B	393	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	5001	-	X
2	MG	B	5002	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5894 atoms, of which 0 are hydrogen and 0 are deuterium.

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 hypothetical protein lin2664.

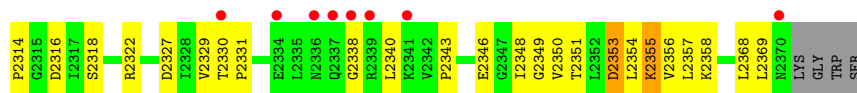
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2946	1891	495	548	12			
1	B	371	Total	C	N	O	S	0	0	0
			2946	1891	495	548	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1000	HIS	-	EXPRESSION TAG	UNP Q927X3
B	2000	HIS	-	EXPRESSION TAG	UNP Q927X3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.72Å 87.35Å 161.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 29.65 – 2.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.90) 95.1 (29.65-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.236 , 0.274 0.235 , 0.275	Depositor DCC
R_{free} test set	811 reflections (4.73%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17929 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5894	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.42	0/2998	0.68	1/4044 (0.0%)
1	B	0.43	0/2998	0.69	1/4044 (0.0%)
All	All	0.42	0/5996	0.69	2/8088 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1079	ARG	N-CA-C	6.15	127.60	111.00
1	B	2079	ARG	N-CA-C	6.08	127.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2946	0	3006	158	0
1	B	2946	0	3006	158	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	5894	0	6012	302	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (302) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2330:THR:OG1	1:B:2331:PRO:HD3	1.71	0.90
1:A:1241:ASN:H	1:A:1241:ASN:ND2	1.69	0.89
1:B:2241:ASN:H	1:B:2241:ASN:HD22	0.90	0.89
1:B:2241:ASN:HD22	1:B:2241:ASN:N	1.66	0.88
1:A:1241:ASN:HD22	1:A:1241:ASN:H	0.91	0.88
1:A:1241:ASN:HD22	1:A:1241:ASN:N	1.67	0.87
1:A:1330:THR:OG1	1:A:1331:PRO:HD3	1.76	0.86
1:A:1222:PHE:H	1:B:2250:GLN:NE2	1.74	0.86
1:A:1223:VAL:H	1:B:2250:GLN:HE21	1.23	0.83
1:B:2241:ASN:ND2	1:B:2241:ASN:H	1.69	0.83
1:A:1355:LYS:H	1:A:1355:LYS:HD3	1.45	0.82
1:B:2355:LYS:H	1:B:2355:LYS:HD3	1.42	0.82
1:A:1223:VAL:H	1:B:2250:GLN:NE2	1.77	0.81
1:B:2329:VAL:HG13	1:B:2350:VAL:HB	1.63	0.80
1:A:1222:PHE:H	1:B:2250:GLN:HE22	1.26	0.80
1:B:2215:GLN:HE22	1:B:2239:ASP:H	1.29	0.80
1:A:1250:GLN:NE2	1:B:2222:PHE:H	1.79	0.79
1:A:1329:VAL:HG13	1:A:1350:VAL:HB	1.65	0.78
1:B:2027:LYS:HD3	1:B:2027:LYS:N	1.99	0.78
1:B:2267:VAL:HG21	1:B:2276:ILE:HD12	1.67	0.77
1:A:1270:MET:HE2	1:A:1274:LEU:HG	1.66	0.77
1:B:2318:SER:HB2	1:B:2322:ARG:HD3	1.67	0.77
1:B:2270:MET:HE2	1:B:2274:LEU:HG	1.65	0.77
1:A:1318:SER:HB2	1:A:1322:ARG:HD3	1.67	0.76
1:A:1215:GLN:HE22	1:A:1239:ASP:H	1.33	0.76
1:A:1250:GLN:HE22	1:B:2222:PHE:H	1.30	0.75
1:A:1027:LYS:HD3	1:A:1027:LYS:N	2.02	0.75
1:A:1267:VAL:HG21	1:A:1276:ILE:HD12	1.67	0.74
1:B:2160:ARG:HG2	1:B:2314:PRO:HB2	1.70	0.74
1:A:1160:ARG:HG2	1:A:1314:PRO:HB2	1.72	0.72
1:A:1080:LYS:HD3	1:A:1080:LYS:N	2.05	0.71
1:B:2080:LYS:HD3	1:B:2080:LYS:N	2.06	0.71
1:A:1250:GLN:HE21	1:B:2223:VAL:H	1.39	0.70
1:A:1020:LYS:HD2	1:A:1020:LYS:H	1.56	0.69
1:B:2160:ARG:NH1	1:B:2314:PRO:O	2.25	0.69
1:A:1119:SER:HB2	1:A:1122:LYS:HG2	1.73	0.69
1:B:2020:LYS:HD2	1:B:2020:LYS:H	1.57	0.69
1:B:2119:SER:HB2	1:B:2122:LYS:HG2	1.73	0.69
1:A:1170:ASP:OD2	1:A:1171:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2035:GLU:OE1	1:B:2043:HIS:HD2	1.76	0.68
1:A:1222:PHE:N	1:B:2250:GLN:HE22	1.91	0.68
1:B:2170:ASP:OD2	1:B:2171:ILE:HG13	1.94	0.67
1:A:1132:LYS:HD3	1:A:1159:GLU:OE1	1.96	0.66
1:B:2171:ILE:HG12	1:B:2205:LEU:HD11	1.78	0.66
1:B:2203:LYS:HE2	1:B:2231:GLN:HB3	1.78	0.66
1:B:2132:LYS:HD3	1:B:2159:GLU:OE1	1.96	0.66
1:A:1203:LYS:HE2	1:A:1231:GLN:HB3	1.78	0.65
1:A:1035:GLU:OE1	1:A:1043:HIS:HD2	1.79	0.65
1:A:1142:ASN:HD22	1:A:1145:THR:HG21	1.61	0.65
1:B:2165:ILE:HD12	1:B:2170:ASP:HA	1.79	0.65
1:B:2215:GLN:NE2	1:B:2239:ASP:H	1.94	0.65
1:A:1250:GLN:HE22	1:B:2222:PHE:N	1.95	0.64
1:B:2171:ILE:HG12	1:B:2205:LEU:CD1	2.27	0.64
1:A:1165:ILE:HD12	1:A:1170:ASP:HA	1.80	0.64
1:A:1171:ILE:HG12	1:A:1205:LEU:HD11	1.80	0.64
1:B:2142:ASN:HD22	1:B:2145:THR:HG21	1.63	0.64
1:A:1250:GLN:NE2	1:B:2223:VAL:H	1.95	0.64
1:A:1160:ARG:NH1	1:A:1314:PRO:O	2.31	0.64
1:A:1215:GLN:NE2	1:A:1239:ASP:H	1.97	0.62
1:A:1075:LEU:HB3	1:A:1090:LEU:HD12	1.82	0.62
1:B:2027:LYS:HD3	1:B:2027:LYS:H	1.63	0.62
1:A:1078:GLN:HG2	1:A:1079:ARG:H	1.64	0.62
1:A:1171:ILE:HG12	1:A:1205:LEU:CD1	2.30	0.61
1:B:2142:ASN:HB2	1:B:2145:THR:HG23	1.82	0.60
1:B:2124:ILE:HD11	1:B:2304:ALA:O	2.02	0.59
1:B:2075:LEU:HB3	1:B:2090:LEU:HD12	1.83	0.59
1:A:1027:LYS:HD3	1:A:1027:LYS:H	1.66	0.59
1:B:2119:SER:HB2	1:B:2122:LYS:H	1.67	0.59
1:A:1002:TYR:CZ	1:A:1080:LYS:HB3	2.38	0.59
1:B:2019:PHE:HB3	1:B:2026:LEU:HB2	1.84	0.59
1:B:2165:ILE:HG23	1:B:2170:ASP:HB3	1.85	0.59
1:A:1142:ASN:HB2	1:A:1145:THR:HG23	1.85	0.59
1:A:1152:GLN:O	1:A:1156:GLN:HG3	2.03	0.59
1:A:1086:GLU:O	1:A:1090:LEU:HD23	2.02	0.58
1:A:1053:LEU:HD22	1:B:2071:GLN:HE22	1.66	0.58
1:A:1080:LYS:HD3	1:A:1080:LYS:H	1.68	0.58
1:B:2002:TYR:CZ	1:B:2080:LYS:HB3	2.38	0.58
1:B:2082:ARG:HH11	1:B:2082:ARG:HG3	1.68	0.58
1:A:1318:SER:CB	1:A:1322:ARG:HD3	2.33	0.58
1:B:2130:SER:HA	1:B:2340:LEU:O	2.04	0.57
1:B:2078:GLN:HG2	1:B:2079:ARG:H	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2170:ASP:O	1:B:2174:VAL:HG23	2.04	0.57
1:B:2318:SER:CB	1:B:2322:ARG:HD3	2.33	0.57
1:A:1165:ILE:HG23	1:A:1170:ASP:HB3	1.86	0.56
1:B:2152:GLN:O	1:B:2156:GLN:HG3	2.04	0.56
1:B:2267:VAL:HG21	1:B:2276:ILE:CD1	2.34	0.56
1:A:1119:SER:HB2	1:A:1122:LYS:H	1.69	0.56
1:A:1226:ALA:HA	1:A:1255:GLY:O	2.06	0.56
1:B:2020:LYS:HD2	1:B:2020:LYS:N	2.21	0.56
1:B:2013:LEU:O	1:B:2028:SER:HB2	2.06	0.56
1:A:1053:LEU:HD22	1:B:2071:GLN:NE2	2.21	0.56
1:A:1019:PHE:HB3	1:A:1026:LEU:HB2	1.87	0.56
1:B:2119:SER:CB	1:B:2122:LYS:HG2	2.35	0.56
1:A:1124:ILE:HD11	1:A:1304:ALA:O	2.05	0.56
1:A:1134:GLY:HA3	1:A:1160:ARG:HG3	1.87	0.56
1:A:1229:GLN:HE22	1:A:1236:ILE:H	1.53	0.56
1:B:2226:ALA:HA	1:B:2255:GLY:O	2.06	0.56
1:A:1023:TYR:O	1:A:1023:TYR:CD1	2.60	0.55
1:A:1245:VAL:HG21	1:A:1275:LYS:HB3	1.89	0.55
1:A:1020:LYS:N	1:A:1020:LYS:HD2	2.21	0.55
1:B:2229:GLN:HE22	1:B:2236:ILE:H	1.54	0.55
1:A:1130:SER:HA	1:A:1340:LEU:O	2.06	0.55
1:A:1146:LEU:HD22	1:A:1173:PHE:HD2	1.71	0.55
1:A:1242:ILE:HG13	1:A:1260:ILE:HD12	1.89	0.55
1:B:2086:GLU:O	1:B:2090:LEU:HD23	2.06	0.55
1:A:1280:CYS:HB3	1:A:1285:ILE:O	2.06	0.55
1:B:2080:LYS:HD3	1:B:2080:LYS:H	1.70	0.55
1:B:2353:ASP:HB2	1:B:2356:VAL:HB	1.88	0.55
1:B:2187:MET:HE1	1:B:2313:PHE:HE2	1.72	0.54
1:B:2280:CYS:HB3	1:B:2285:ILE:O	2.07	0.54
1:B:2146:LEU:O	1:B:2150:VAL:HG23	2.07	0.54
1:B:2146:LEU:HD22	1:B:2173:PHE:HD2	1.72	0.54
1:A:1119:SER:CB	1:A:1122:LYS:HG2	2.37	0.54
1:B:2242:ILE:HG13	1:B:2260:ILE:HD12	1.90	0.54
1:A:1146:LEU:O	1:A:1150:VAL:HG23	2.08	0.54
1:A:1353:ASP:HB2	1:A:1356:VAL:HB	1.90	0.53
1:A:1160:ARG:HD3	1:A:1313:PHE:CZ	2.44	0.53
1:B:2353:ASP:HA	1:B:2355:LYS:HZ3	1.74	0.53
1:B:2355:LYS:H	1:B:2355:LYS:CD	2.19	0.53
1:B:2153:TYR:HB3	1:B:2158:TYR:HD1	1.73	0.53
1:B:2007:ARG:HB3	1:B:2035:GLU:HB3	1.90	0.53
1:A:1007:ARG:HB3	1:A:1035:GLU:HB3	1.91	0.52
1:B:2287:VAL:HG22	1:B:2311:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2160:ARG:HD3	1:B:2313:PHE:CZ	2.44	0.52
1:B:2134:GLY:HA3	1:B:2160:ARG:HG3	1.92	0.52
1:A:1252:HIS:HE1	1:A:1283:ASN:HD22	1.58	0.52
1:A:1013:LEU:O	1:A:1028:SER:HB2	2.09	0.52
1:A:1082:ARG:HH11	1:A:1082:ARG:HG3	1.73	0.52
1:B:2023:TYR:O	1:B:2023:TYR:CD1	2.62	0.52
1:B:2216:PRO:HD2	1:B:2225:HIS:CE1	2.45	0.52
1:A:1038:ASN:HB3	1:A:1042:ILE:H	1.75	0.51
1:A:1175:GLU:HG2	1:A:1208:TYR:CZ	2.45	0.51
1:A:1153:TYR:HB3	1:A:1158:TYR:HD1	1.75	0.51
1:A:1355:LYS:N	1:A:1355:LYS:HD3	2.22	0.51
1:A:1216:PRO:HD2	1:A:1225:HIS:CE1	2.45	0.51
1:B:2245:VAL:HG21	1:B:2275:LYS:HB3	1.91	0.51
1:B:2079:ARG:HD2	1:B:2090:LEU:HD13	1.93	0.51
1:A:1170:ASP:O	1:A:1174:VAL:HG23	2.10	0.51
1:A:1210:LEU:O	1:A:1234:THR:HG23	2.12	0.51
1:A:1267:VAL:HG21	1:A:1276:ILE:CD1	2.37	0.50
1:A:1355:LYS:CD	1:A:1355:LYS:H	2.21	0.50
1:B:2175:GLU:HG2	1:B:2208:TYR:CZ	2.46	0.50
1:B:2264:LEU:HG	1:B:2305:LEU:HD22	1.93	0.50
1:A:1343:PRO:HB3	1:A:1349:GLY:HA3	1.93	0.50
1:A:1354:LEU:O	1:A:1358:LYS:HG3	2.12	0.50
1:B:2038:ASN:HB3	1:B:2042:ILE:H	1.76	0.50
1:B:2354:LEU:O	1:B:2358:LYS:HG3	2.12	0.49
1:A:1264:LEU:HG	1:A:1305:LEU:HD22	1.94	0.49
1:B:2252:HIS:HE1	1:B:2283:ASN:HD22	1.60	0.49
1:A:1252:HIS:CE1	1:A:1283:ASN:HB3	2.47	0.49
1:B:2329:VAL:CG1	1:B:2350:VAL:HB	2.40	0.49
1:A:1160:ARG:NH2	1:A:1316:ASP:OD1	2.46	0.49
1:A:1175:GLU:HG2	1:A:1208:TYR:OH	2.12	0.49
1:B:2175:GLU:HG2	1:B:2208:TYR:OH	2.12	0.49
1:A:1079:ARG:HD2	1:A:1090:LEU:HD13	1.94	0.49
1:A:1187:MET:HE1	1:A:1313:PHE:HE2	1.78	0.49
1:A:1142:ASN:HD22	1:A:1145:THR:CG2	2.25	0.48
1:B:2036:LEU:HD22	1:B:2107:ALA:HB3	1.95	0.48
1:A:1027:LYS:CD	1:A:1027:LYS:H	2.27	0.48
1:B:2160:ARG:NH2	1:B:2316:ASP:OD1	2.47	0.48
1:B:2355:LYS:N	1:B:2355:LYS:HD3	2.20	0.48
1:B:2006:ALA:HB2	1:B:2369:LEU:HD11	1.94	0.48
1:A:1029:LYS:HD3	1:A:1293:LEU:O	2.14	0.48
1:A:1029:LYS:HG3	1:A:1031:PHE:HD1	1.79	0.48
1:A:1353:ASP:HA	1:A:1355:LYS:NZ	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2215:GLN:NE2	1:B:2239:ASP:N	2.62	0.48
1:B:2211:GLU:HG2	1:B:2313:PHE:CE1	2.48	0.48
1:A:1211:GLU:HG2	1:A:1313:PHE:CE1	2.49	0.47
1:B:2082:ARG:NH1	1:B:2082:ARG:HG3	2.28	0.47
1:B:2210:LEU:O	1:B:2234:THR:HG23	2.15	0.47
1:B:2343:PRO:HB3	1:B:2349:GLY:HA3	1.95	0.47
1:B:2117:LYS:HA	1:B:2346:GLU:HG2	1.97	0.47
1:B:2353:ASP:HA	1:B:2355:LYS:NZ	2.29	0.47
1:A:1161:VAL:HB	1:A:1186:LEU:CD1	2.45	0.47
1:B:2047:GLU:OE2	1:B:2049:GLU:OE2	2.33	0.47
1:B:2165:ILE:CG2	1:B:2166:ALA:N	2.78	0.46
1:B:2241:ASN:ND2	1:B:2241:ASN:N	2.40	0.46
1:B:2252:HIS:CE1	1:B:2283:ASN:HB3	2.50	0.46
1:B:2287:VAL:HG22	1:B:2311:PHE:CE1	2.50	0.46
1:A:1132:LYS:HA	1:A:1338:GLY:O	2.16	0.46
1:B:2161:VAL:HB	1:B:2186:LEU:CD1	2.45	0.46
1:B:2210:LEU:HA	1:B:2210:LEU:HD12	1.81	0.46
1:A:1222:PHE:HB2	1:B:2250:GLN:HE22	1.81	0.46
1:B:2270:MET:HE3	1:B:2305:LEU:HD13	1.98	0.46
1:A:1027:LYS:CD	1:A:1027:LYS:N	2.73	0.46
1:B:2237:CYS:HA	1:B:2259:ALA:O	2.16	0.46
1:B:2161:VAL:O	1:B:2186:LEU:HD12	2.15	0.46
1:A:1036:LEU:HD22	1:A:1107:ALA:HB3	1.98	0.45
1:A:1117:LYS:HA	1:A:1346:GLU:HG2	1.98	0.45
1:B:2027:LYS:H	1:B:2027:LYS:CD	2.24	0.45
1:B:2142:ASN:CB	1:B:2145:THR:HG23	2.45	0.45
1:B:2215:GLN:HE21	1:B:2215:GLN:HB2	1.60	0.45
1:A:1161:VAL:O	1:A:1186:LEU:HD12	2.16	0.45
1:A:1327:ASP:O	1:A:1356:VAL:HG11	2.17	0.45
1:B:2142:ASN:HD22	1:B:2145:THR:CG2	2.26	0.45
1:B:2327:ASP:O	1:B:2356:VAL:HG11	2.17	0.45
1:A:1065:ILE:HD12	1:A:1068:ILE:HD12	1.99	0.45
1:A:1141:GLN:NE2	1:A:1169:LYS:HE2	2.31	0.45
1:A:1279:TYR:CD1	1:A:1279:TYR:C	2.91	0.45
1:B:2175:GLU:HG2	1:B:2208:TYR:CE2	2.52	0.45
1:A:1133:VAL:HG11	1:A:1340:LEU:HD12	1.99	0.44
1:A:1301:HIS:CE1	1:A:1348:ILE:HG21	2.51	0.44
1:A:1241:ASN:ND2	1:A:1241:ASN:N	2.40	0.44
1:A:1287:VAL:HG22	1:A:1311:PHE:HE1	1.82	0.44
1:A:1142:ASN:CB	1:A:1145:THR:HG23	2.47	0.44
1:A:1135:VAL:HG21	1:A:1153:TYR:CE2	2.52	0.44
1:B:2199:PHE:O	1:B:2203:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1228:LEU:HD22	1:A:1232:LEU:CD1	2.47	0.44
1:A:1239:ASP:HB3	1:A:1240:GLU:OE2	2.18	0.44
1:A:1045:TYR:O	1:A:1301:HIS:HE1	2.00	0.44
1:B:2206:ASP:CG	1:B:2233:LYS:H	2.20	0.44
1:A:1283:ASN:O	1:A:1285:ILE:HG13	2.18	0.44
1:B:2250:GLN:O	1:B:2254:ILE:HG13	2.17	0.44
1:B:2132:LYS:HA	1:B:2338:GLY:O	2.18	0.44
1:A:1175:GLU:HG2	1:A:1208:TYR:CE2	2.52	0.44
1:A:1187:MET:CE	1:A:1313:PHE:HE2	2.31	0.44
1:B:2116:GLU:OE1	1:B:2118:ARG:NH1	2.51	0.44
1:B:2239:ASP:HB3	1:B:2240:GLU:OE2	2.18	0.44
1:B:2045:TYR:O	1:B:2301:HIS:HE1	2.01	0.44
1:A:1165:ILE:CG2	1:A:1166:ALA:N	2.80	0.44
1:B:2187:MET:CE	1:B:2313:PHE:HE2	2.31	0.44
1:A:1270:MET:HE3	1:A:1305:LEU:HD13	2.00	0.44
1:B:2015:LEU:HG	1:B:2028:SER:HA	2.00	0.43
1:A:1082:ARG:NH1	1:A:1082:ARG:HG3	2.33	0.43
1:A:1215:GLN:NE2	1:A:1239:ASP:N	2.65	0.43
1:B:2141:GLN:NE2	1:B:2169:LYS:HE2	2.32	0.43
1:A:1229:GLN:NE2	1:A:1236:ILE:H	2.16	0.43
1:B:2029:LYS:HD3	1:B:2293:LEU:O	2.17	0.43
1:A:1003:PHE:O	1:A:1369:LEU:HB2	2.19	0.43
1:B:2201:LEU:O	1:B:2205:LEU:HD13	2.18	0.43
1:A:1004:GLN:HA	1:A:1370:ASN:OD1	2.19	0.43
1:A:1080:LYS:CD	1:A:1080:LYS:N	2.75	0.43
1:B:2135:VAL:HG21	1:B:2153:TYR:CE2	2.53	0.43
1:B:2142:ASN:HB2	1:B:2145:THR:CG2	2.48	0.43
1:A:1047:GLU:OE2	1:A:1049:GLU:OE2	2.37	0.43
1:A:1162:LYS:HD3	1:A:1187:MET:HE3	2.01	0.43
1:B:2135:VAL:HG21	1:B:2153:TYR:CD2	2.54	0.43
1:A:1116:GLU:OE1	1:A:1118:ARG:NH1	2.51	0.42
1:B:2172:GLN:HG3	1:B:2173:PHE:CD1	2.54	0.42
1:B:2299:ARG:HH11	1:B:2299:ARG:HG3	1.83	0.42
1:A:1090:LEU:H	1:A:1090:LEU:HD23	1.84	0.42
1:B:2019:PHE:O	1:B:2026:LEU:N	2.47	0.42
1:A:1172:GLN:HG3	1:A:1173:PHE:CD1	2.54	0.42
1:A:1299:ARG:HH11	1:A:1299:ARG:HG3	1.84	0.42
1:A:1353:ASP:C	1:A:1355:LYS:N	2.73	0.42
1:B:2029:LYS:HG3	1:B:2031:PHE:HD1	1.84	0.42
1:A:1135:VAL:HG21	1:A:1153:TYR:CD2	2.54	0.42
1:B:2038:ASN:HD22	1:B:2042:ILE:HD12	1.85	0.42
1:A:1270:MET:CE	1:A:1305:LEU:HD13	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1071:GLN:HE22	1:B:2053:LEU:HD22	1.85	0.42
1:A:1175:GLU:O	1:A:1176:ALA:C	2.58	0.42
1:A:1329:VAL:CG1	1:A:1350:VAL:HB	2.41	0.42
1:A:1015:LEU:HG	1:A:1028:SER:HA	2.00	0.41
1:B:2065:ILE:HD12	1:B:2068:ILE:HD12	2.01	0.41
1:B:2163:LEU:HD11	1:B:2186:LEU:HD21	2.03	0.41
1:B:2142:ASN:ND2	1:B:2145:THR:HG21	2.31	0.41
1:B:2153:TYR:HB3	1:B:2158:TYR:CD1	2.55	0.41
1:B:2353:ASP:C	1:B:2355:LYS:N	2.72	0.41
1:A:1163:LEU:HD11	1:A:1186:LEU:HD21	2.02	0.41
1:A:1237:CYS:HA	1:A:1259:ALA:O	2.21	0.41
1:A:1043:HIS:O	1:A:1114:LYS:HE2	2.20	0.41
1:B:2056:TYR:CD1	1:B:2057:THR:HG23	2.55	0.41
1:B:2175:GLU:O	1:B:2176:ALA:C	2.59	0.41
1:B:2270:MET:CE	1:B:2305:LEU:HD13	2.51	0.41
1:A:1147:LEU:O	1:A:1147:LEU:HD13	2.20	0.41
1:A:1206:ASP:CG	1:A:1233:LYS:H	2.24	0.41
1:A:1250:GLN:O	1:A:1254:ILE:HG13	2.20	0.41
1:A:1128:LYS:HD2	1:A:1307:ALA:O	2.21	0.41
1:A:1353:ASP:HB3	1:A:1355:LYS:HE2	2.03	0.41
1:B:2043:HIS:O	1:B:2114:LYS:HE2	2.20	0.41
1:B:2090:LEU:H	1:B:2090:LEU:HD23	1.86	0.41
1:A:1210:LEU:HD12	1:A:1210:LEU:HA	1.85	0.41
1:A:1287:VAL:HG22	1:A:1311:PHE:CE1	2.56	0.41
1:B:2133:VAL:HG11	1:B:2340:LEU:HD12	2.03	0.41
1:A:1201:LEU:O	1:A:1205:LEU:HD13	2.21	0.41
1:A:1353:ASP:HA	1:A:1355:LYS:HZ3	1.85	0.41
1:B:2001:MET:HB2	1:B:2038:ASN:OD1	2.21	0.41
1:B:2036:LEU:HA	1:B:2036:LEU:HD12	1.88	0.41
1:B:2301:HIS:CE1	1:B:2348:ILE:HG21	2.56	0.41
1:A:1072:LEU:HD13	1:A:1101:LYS:HA	2.03	0.40
1:A:1144:GLU:O	1:A:1148:GLN:HG3	2.21	0.40
1:B:2144:GLU:O	1:B:2148:GLN:HG3	2.21	0.40
1:B:2158:TYR:OH	1:B:2322:ARG:HD2	2.21	0.40
1:B:2283:ASN:O	1:B:2285:ILE:HG13	2.21	0.40
1:A:1080:LYS:CD	1:A:1080:LYS:H	2.33	0.40
1:A:1142:ASN:ND2	1:A:1145:THR:HG21	2.30	0.40
1:A:1175:GLU:O	1:A:1178:ARG:N	2.54	0.40
1:A:1286:LEU:HD23	1:A:1287:VAL:N	2.36	0.40
1:B:2162:LYS:HD3	1:B:2187:MET:HE3	2.02	0.40
1:A:1228:LEU:HD22	1:A:1232:LEU:HD11	2.03	0.40
1:A:1158:TYR:OH	1:A:1322:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2147:LEU:HD13	1:B:2147:LEU:O	2.21	0.40
1:B:2279:TYR:CD1	1:B:2279:TYR:C	2.94	0.40
1:A:1199:PHE:O	1:A:1203:LYS:HG3	2.20	0.40
1:B:2207:GLN:H	1:B:2207:GLN:HG3	1.66	0.40
1:B:2353:ASP:HB3	1:B:2355:LYS:HE2	2.03	0.40
1:A:1001:MET:HB2	1:A:1038:ASN:OD1	2.21	0.40
1:A:1056:TYR:CD1	1:A:1057:THR:HG23	2.57	0.40
1:B:2035:GLU:OE1	1:B:2043:HIS:CD2	2.66	0.40
1:B:2072:LEU:HD13	1:B:2101:LYS:HA	2.03	0.40
1:B:2167:PRO:HG3	1:B:2194:TYR:CE1	2.56	0.40
1:B:2171:ILE:HD13	1:B:2204:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

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	369/393 (94%)	337 (91%)	28 (8%)	4 (1%)	21	60
1	B	369/393 (94%)	336 (91%)	29 (8%)	4 (1%)	21	60
All	All	738/786 (94%)	673 (91%)	57 (8%)	8 (1%)	21	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	SER
1	B	2180	SER
1	A	1079	ARG
1	B	2079	ARG
1	A	1191	ASN
1	B	2191	ASN
1	B	2167	PRO
1	A	1167	PRO

5.3.2 Protein sidechains ⓘ

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	316/334 (95%)	293 (93%)	23 (7%)	20	51
1	B	316/334 (95%)	292 (92%)	24 (8%)	19	48
All	All	632/668 (95%)	585 (93%)	47 (7%)	20	50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	LYS
1	A	1020	LYS
1	A	1027	LYS
1	A	1036	LEU
1	A	1049	GLU
1	A	1058	GLU
1	A	1075	LEU
1	A	1078	GLN
1	A	1079	ARG
1	A	1080	LYS
1	A	1105	GLU
1	A	1127	THR
1	A	1147	LEU
1	A	1160	ARG
1	A	1207	GLN
1	A	1215	GLN
1	A	1228	LEU
1	A	1241	ASN
1	A	1351	THR
1	A	1353	ASP
1	A	1355	LYS
1	A	1357	LEU
1	A	1368	LEU
1	B	2005	LYS
1	B	2020	LYS
1	B	2027	LYS
1	B	2036	LEU
1	B	2049	GLU
1	B	2058	GLU

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Mol	Chain	Res	Type
1	B	2075	LEU
1	B	2078	GLN
1	B	2079	ARG
1	B	2080	LYS
1	B	2105	GLU
1	B	2127	THR
1	B	2147	LEU
1	B	2160	ARG
1	B	2167	PRO
1	B	2207	GLN
1	B	2215	GLN
1	B	2228	LEU
1	B	2241	ASN
1	B	2351	THR
1	B	2353	ASP
1	B	2355	LYS
1	B	2357	LEU
1	B	2368	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1004	GLN
1	A	1043	HIS
1	A	1071	GLN
1	A	1141	GLN
1	A	1142	ASN
1	A	1152	GLN
1	A	1156	GLN
1	A	1172	GLN
1	A	1191	ASN
1	A	1215	GLN
1	A	1225	HIS
1	A	1229	GLN
1	A	1231	GLN
1	A	1241	ASN
1	A	1250	GLN
1	A	1283	ASN
1	A	1301	HIS
1	B	2004	GLN
1	B	2043	HIS
1	B	2071	GLN

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Mol	Chain	Res	Type
1	B	2141	GLN
1	B	2142	ASN
1	B	2152	GLN
1	B	2156	GLN
1	B	2191	ASN
1	B	2215	GLN
1	B	2225	HIS
1	B	2229	GLN
1	B	2231	GLN
1	B	2241	ASN
1	B	2250	GLN
1	B	2283	ASN
1	B	2301	HIS
1	B	2370	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	371/393 (94%)	0.17	6 (1%) 68 78	14, 39, 70, 87	0
1	B	371/393 (94%)	0.39	24 (6%) 18 22	15, 40, 70, 87	0
All	All	742/786 (94%)	0.28	30 (4%) 36 43	14, 40, 70, 87	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2199	PHE	3.7
1	B	2155	ASP	3.6
1	B	2000	HIS	3.6
1	B	2337	GLN	3.5
1	B	2154	VAL	3.4
1	B	2330	THR	3.4
1	B	2334	GLU	3.4
1	A	1023	TYR	3.3
1	B	2023	TYR	3.3
1	B	2147	LEU	3.2
1	B	2179	LYS	2.9
1	B	2282	LEU	2.8
1	B	2141	GLN	2.8
1	B	2181	PHE	2.6
1	B	2338	GLY	2.6
1	A	1320	SER	2.5
1	B	2144	GLU	2.5
1	A	1143	VAL	2.5
1	A	1341	LYS	2.4
1	A	1337	GLN	2.4
1	B	2078	GLN	2.4
1	B	2200	LEU	2.2
1	B	2341	LYS	2.2
1	B	2370	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2182	PRO	2.1
1	B	2336	ASN	2.1
1	B	2284	GLU	2.1
1	B	2126	ALA	2.1
1	A	1179	LYS	2.1
1	B	2339	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	5002	1/1	0.61	12.34	60,60,60,60	0
2	MG	A	5001	1/1	0.69	11.57	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.