



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 1TZZ / pdb_00001tzz
Title : Crystal structure of the protein L1841, unknown member of enolase superfamily from Bradyrhizobium japonicum
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 : 2004-07-12
Resolution : 1.86 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

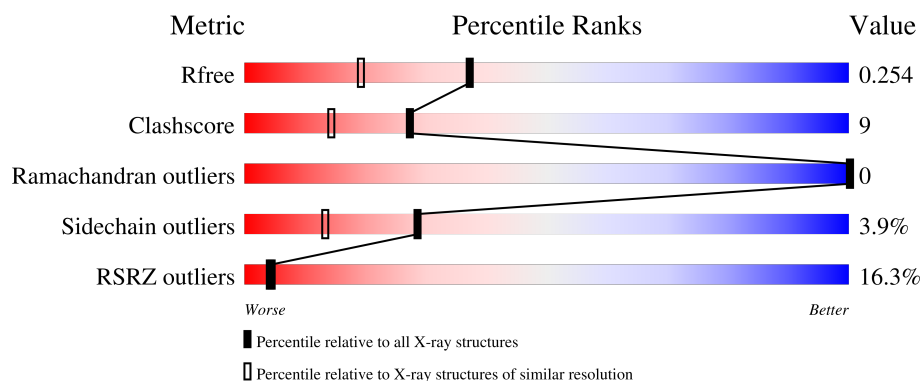
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 of 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 $\leq 5\%$. 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	392	20% 73% 20% 5%
1	B	392	12% 76% 18% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6155 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 Hypothetical protein L1841.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2906	1840	511	538	17			
1	B	379	Total	C	N	O	S	0	0	0
			2944	1865	517	545	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1001	GLY	-	cloning artifact	UNP Q89FH0
A	1002	SER	-	cloning artifact	UNP Q89FH0
A	1003	HIS	-	cloning artifact	UNP Q89FH0
B	2001	GLY	-	cloning artifact	UNP Q89FH0
B	2002	SER	-	cloning artifact	UNP Q89FH0
B	2003	HIS	-	cloning artifact	UNP Q89FH0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

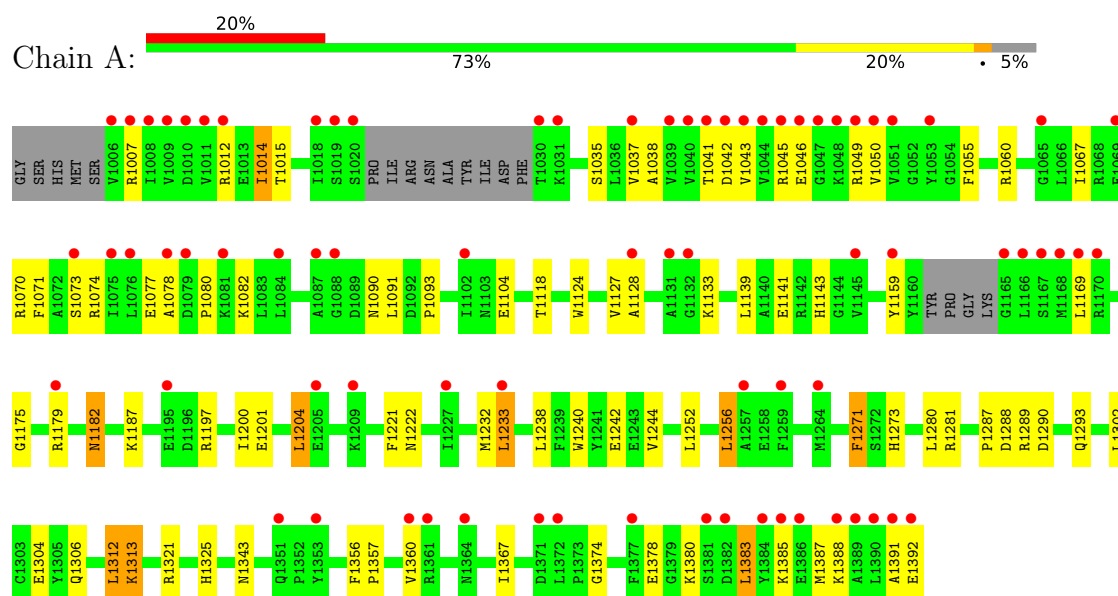
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	181	Total	O	0	0
			181	181		

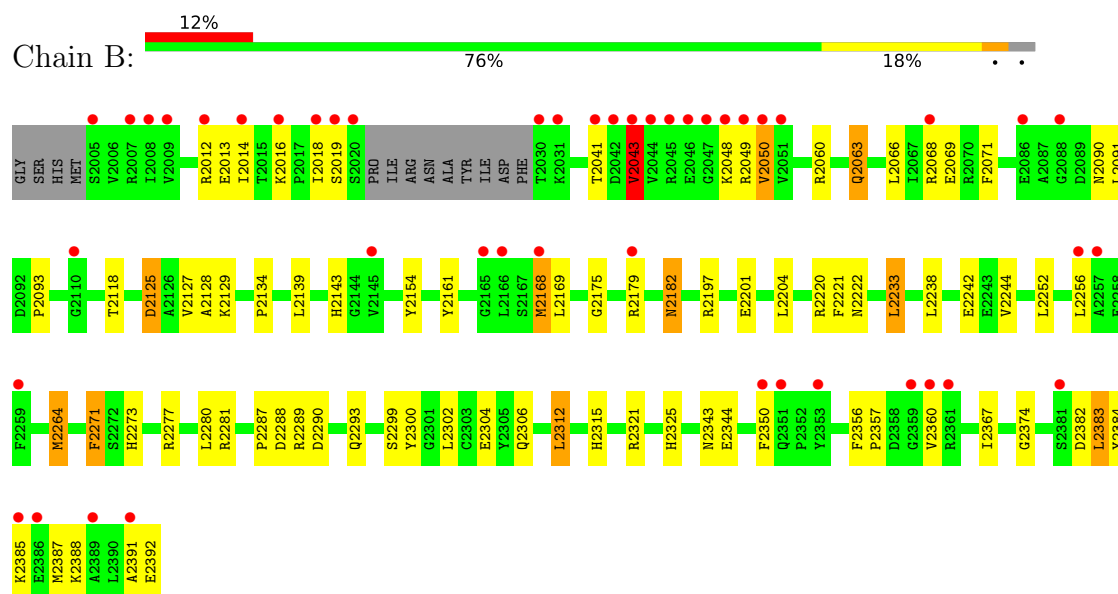
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Hypothetical protein L1841



• Molecule 1: Hypothetical protein L1841



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.97Å 178.00Å 110.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.86 30.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.86) 99.3 (30.00-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 1.87Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.254 0.235 , 0.254	Depositor DCC
R_{free} test set	3989 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6155	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/2969	0.89	7/4006 (0.2%)
1	B	0.38	1/3010 (0.0%)	0.90	13/4063 (0.3%)
All	All	0.37	1/5979 (0.0%)	0.89	20/8069 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2264	MET	SD-CE	-5.29	1.66	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1221	PHE	N-CA-C	8.55	123.71	110.20
1	B	2221	PHE	N-CA-C	7.63	122.45	110.32
1	A	1271	PHE	N-CA-C	7.22	121.40	112.59
1	A	1071	PHE	N-CA-C	6.87	119.78	111.40
1	B	2271	PHE	N-CA-C	6.77	120.85	112.59
1	A	1242	GLU	N-CA-C	6.59	120.58	109.76
1	B	2242	GLU	N-CA-C	6.52	120.46	109.76
1	B	2071	PHE	N-CA-C	6.26	119.39	111.69
1	B	2069	GLU	N-CA-C	6.21	118.12	111.36
1	B	2220	ARG	N-CA-C	6.14	118.94	111.82
1	A	1293	GLN	N-CA-C	6.12	119.49	112.57
1	B	2222	ASN	N-CA-C	-6.00	101.06	110.36
1	B	2325	HIS	N-CA-C	-5.92	102.15	110.50
1	B	2293	GLN	N-CA-C	5.85	119.72	112.59
1	A	1222	ASN	N-CA-C	-5.67	101.57	110.36
1	B	2043	VAL	N-CA-C	5.59	116.79	109.58
1	B	2134	PRO	N-CA-C	-5.14	103.12	111.19
1	B	2233	LEU	N-CA-C	5.09	116.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1325	HIS	N-CA-C	-5.08	103.34	110.50
1	B	2125	ASP	N-CA-C	-5.06	105.66	111.07

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	2906	0	2861	53	0
1	B	2944	0	2899	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	122	0	0	2	0
3	B	181	0	0	1	0
All	All	6155	0	5760	106	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 9.

All (106) 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:2244:VAL:HG11	1:B:2256:LEU:HD21	1.60	0.84
1:B:2256:LEU:HD23	1:B:2264:MET:HE1	1.63	0.81
1:B:2041:THR:OG1	1:B:2050:VAL:HG13	1.83	0.79
1:B:2357:PRO:O	1:B:2360:VAL:HG22	1.81	0.79
1:B:2161:TYR:CD2	1:B:2168:MET:HG2	2.20	0.77
1:B:2357:PRO:HD2	1:B:2360:VAL:HG21	1.71	0.73
1:A:1093:PRO:HG3	1:A:1127:VAL:HG21	1.68	0.73
1:A:1012:ARG:HD2	1:A:1391:ALA:HB2	1.70	0.72
1:A:1014:ILE:HD13	1:A:1015:THR:N	2.06	0.71
1:B:2288:ASP:OD1	1:B:2289:ARG:HD3	1.90	0.70
1:A:1357:PRO:O	1:A:1360:VAL:HG22	1.92	0.69
1:A:1385:LYS:HA	1:A:1388:LYS:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1357:PRO:HD2	1:A:1360:VAL:HG21	1.74	0.68
1:A:1288:ASP:OD1	1:A:1289:ARG:HD3	1.94	0.66
1:B:2244:VAL:HG21	1:B:2256:LEU:HD23	1.78	0.66
1:A:1244:VAL:HG11	1:A:1256:LEU:HD21	1.77	0.65
1:B:2384:TYR:CE2	1:B:2388:LYS:HD2	2.32	0.63
1:A:1041:THR:OG1	1:A:1050:VAL:HG13	1.98	0.63
1:B:2290:ASP:O	1:B:2321:ARG:HD3	1.98	0.62
1:B:2175:GLY:O	1:B:2179:ARG:HG2	1.99	0.62
1:B:2273:HIS:HD2	1:B:2304:GLU:OE2	1.85	0.60
1:A:1043:VAL:O	1:A:1050:VAL:HG12	2.03	0.59
1:A:1290:ASP:O	1:A:1321:ARG:HD3	2.03	0.59
1:B:2049:ARG:HH21	1:B:2392:GLU:C	2.11	0.58
1:B:2383:LEU:HD22	1:B:2387:MET:HE3	1.85	0.58
1:B:2281:ARG:HG2	1:B:2315:HIS:CE1	2.37	0.58
1:B:2043:VAL:O	1:B:2050:VAL:HG12	2.04	0.57
1:B:2383:LEU:CD2	1:B:2387:MET:HE3	2.34	0.57
1:A:1175:GLY:O	1:A:1179:ARG:HG2	2.04	0.57
1:A:1273:HIS:HD2	1:A:1304:GLU:OE2	1.87	0.56
1:A:1244:VAL:HG21	1:A:1256:LEU:HD23	1.87	0.56
1:B:2280:LEU:HD11	1:B:2312:LEU:HD22	1.88	0.56
1:A:1280:LEU:HD11	1:A:1312:LEU:HD22	1.89	0.55
1:A:1128:ALA:HB3	1:A:1374:GLY:HA2	1.90	0.54
1:B:2277:ARG:O	1:B:2281:ARG:HG3	2.08	0.54
1:B:2118:THR:HG21	3:B:3025:HOH:O	2.07	0.54
1:A:1139:LEU:HD21	1:A:1302:LEU:HD21	1.91	0.53
1:B:2182:ASN:HD22	1:B:2182:ASN:C	2.17	0.53
1:B:2252:LEU:O	1:B:2256:LEU:HD13	2.09	0.53
1:B:2043:VAL:HG13	1:B:2050:VAL:CG1	2.39	0.52
1:B:2244:VAL:HG21	1:B:2256:LEU:CD2	2.38	0.52
1:B:2154:TYR:CE2	1:B:2344:GLU:HB3	2.45	0.52
1:A:1197:ARG:O	1:A:1201:GLU:HG3	2.09	0.52
1:B:2128:ALA:HB3	1:B:2374:GLY:HA2	1.91	0.51
1:B:2244:VAL:HG21	1:B:2264:MET:HE1	1.93	0.51
1:A:1014:ILE:HD13	1:A:1014:ILE:C	2.36	0.51
1:A:1133:LYS:HE2	1:A:1141:GLU:OE2	2.11	0.51
1:A:1143:HIS:HE1	1:A:1306:GLN:NE2	2.08	0.51
1:A:1367:ILE:C	1:A:1367:ILE:HD12	2.36	0.51
1:A:1090:ASN:OD1	1:A:1091:LEU:N	2.43	0.51
1:B:2382:ASP:O	1:B:2385:LYS:HG2	2.11	0.51
1:B:2018:ILE:HG13	1:B:2019:SER:N	2.26	0.50
1:B:2197:ARG:O	1:B:2201:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LYS:HB2	1:A:1313:LYS:NZ	2.27	0.49
1:A:1070:ARG:HD3	1:A:1104:GLU:OE2	2.12	0.49
1:B:2093:PRO:HG3	1:B:2127:VAL:HG21	1.95	0.49
1:B:2143:HIS:HE1	1:B:2306:GLN:NE2	2.11	0.49
1:B:2018:ILE:HG13	1:B:2019:SER:H	1.78	0.48
1:A:1182:ASN:HD22	1:A:1182:ASN:C	2.21	0.47
1:A:1200:ILE:HD12	1:A:1232:MET:HE1	1.97	0.47
1:A:1232:MET:SD	1:A:1233:LEU:HD12	2.54	0.47
1:B:2384:TYR:CD2	1:B:2388:LYS:HD2	2.50	0.46
1:B:2012:ARG:HD2	1:B:2391:ALA:HB2	1.97	0.46
1:B:2125:ASP:OD1	1:B:2129:LYS:HE3	2.16	0.46
1:A:1118:THR:HG21	3:A:3263:HOH:O	2.15	0.46
1:A:1060:ARG:HD2	1:A:1271:PHE:CZ	2.52	0.45
1:A:1078:ALA:O	1:A:1080:PRO:HD3	2.17	0.45
1:A:1380:LYS:HD3	1:A:1383:LEU:HD12	1.98	0.45
1:A:1378:GLU:H	1:A:1378:GLU:CD	2.25	0.44
1:A:1240:TRP:CD1	1:A:1240:TRP:C	2.96	0.44
1:B:2013:GLU:OE1	1:B:2068:ARG:NE	2.51	0.44
1:A:1055:PHE:C	1:A:1118:THR:HG22	2.43	0.44
1:A:1356:PHE:HB2	1:A:1360:VAL:HG23	2.00	0.44
1:A:1037:VAL:HG21	1:A:1067:ILE:HD13	2.00	0.44
1:A:1073:SER:O	1:A:1077:GLU:HG3	2.17	0.44
1:B:2367:ILE:C	1:B:2367:ILE:HD12	2.42	0.43
1:A:1037:VAL:HG12	1:A:1038:ALA:N	2.33	0.43
1:B:2244:VAL:HG21	1:B:2264:MET:CE	2.48	0.43
1:A:1252:LEU:C	1:A:1252:LEU:HD23	2.42	0.43
1:A:1046:GLU:HG3	1:A:1046:GLU:O	2.19	0.43
1:B:2060:ARG:HD2	1:B:2271:PHE:CZ	2.54	0.43
1:A:1049:ARG:HH21	1:A:1392:GLU:C	2.27	0.43
1:A:1070:ARG:HG2	1:A:1074:ARG:CZ	2.49	0.43
1:A:1287:PRO:HG2	1:B:2287:PRO:HG2	2.01	0.43
1:B:2356:PHE:HB2	1:B:2360:VAL:HG23	2.00	0.43
1:B:2356:PHE:HB3	1:B:2360:VAL:CG2	2.49	0.43
1:A:1080:PRO:C	1:A:1082:LYS:H	2.27	0.42
1:B:2018:ILE:HG12	1:B:2350:PHE:HD2	1.85	0.42
1:B:2014:ILE:HD13	1:B:2016:LYS:HE2	2.02	0.42
1:B:2090:ASN:OD1	1:B:2091:LEU:N	2.49	0.42
1:B:2360:VAL:HG23	1:B:2360:VAL:O	2.20	0.42
1:A:1124:TRP:CD2	1:A:1302:LEU:HD23	2.55	0.41
1:B:2356:PHE:CB	1:B:2360:VAL:HG23	2.50	0.41
1:B:2139:LEU:HD21	1:B:2302:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:LEU:HD12	1:A:1204:LEU:HA	1.92	0.41
1:B:2281:ARG:HG2	1:B:2315:HIS:HE1	1.85	0.41
1:A:1035:SER:HB2	3:A:3263:HOH:O	2.21	0.41
1:A:1281:ARG:HH11	1:A:1281:ARG:HG3	1.86	0.41
1:A:1159:TYR:CD1	1:A:1187:LYS:HE3	2.56	0.40
1:A:1007:ARG:HG2	1:A:1042:ASP:CG	2.45	0.40
1:A:1383:LEU:HD21	1:A:1387:MET:HE3	2.03	0.40
1:B:2063:GLN:HG3	1:B:2066:LEU:HD12	2.03	0.40
1:B:2299:SER:O	1:B:2300:TYR:HB2	2.20	0.40
1:B:2356:PHE:CB	1:B:2360:VAL:CG2	2.99	0.40
1:B:2048:LYS:HE3	1:B:2048:LYS:HB3	1.95	0.40
1:A:1045:ARG:O	1:A:1046:GLU:C	2.65	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	368/392 (94%)	355 (96%)	13 (4%)	0	100	100
1	B	375/392 (96%)	367 (98%)	8 (2%)	0	100	100
All	All	743/784 (95%)	722 (97%)	21 (3%)	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	296/311 (95%)	285 (96%)	11 (4%)	30	15
1	B	300/311 (96%)	288 (96%)	12 (4%)	28	13
All	All	596/622 (96%)	573 (96%)	23 (4%)	28	13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1014	ILE
1	A	1169	LEU
1	A	1182	ASN
1	A	1204	LEU
1	A	1233	LEU
1	A	1238	LEU
1	A	1256	LEU
1	A	1312	LEU
1	A	1313	LYS
1	A	1343	ASN
1	A	1383	LEU
1	B	2043	VAL
1	B	2050	VAL
1	B	2063	GLN
1	B	2168	MET
1	B	2169	LEU
1	B	2182	ASN
1	B	2204	LEU
1	B	2233	LEU
1	B	2238	LEU
1	B	2312	LEU
1	B	2343	ASN
1	B	2383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1143	HIS
1	A	1182	ASN
1	A	1253	GLN
1	A	1269	ASN
1	A	1273	HIS

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Mol	Chain	Res	Type
1	A	1306	GLN
1	A	1329	GLN
1	A	1351	GLN
1	B	2143	HIS
1	B	2182	ASN
1	B	2273	HIS
1	B	2306	GLN
1	B	2329	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	374/392 (95%)	1.08	77 (20%) 2 2	15, 30, 50, 62	0
1	B	379/392 (96%)	0.61	46 (12%) 8 8	14, 25, 49, 61	0
All	All	753/784 (96%)	0.85	123 (16%) 4 4	14, 27, 49, 62	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1009	VAL	5.1
1	B	2018	ILE	5.0
1	B	2042	ASP	4.9
1	B	2043	VAL	4.8
1	B	2020	SER	4.7
1	A	1019	SER	4.7
1	A	1165	GLY	4.7
1	A	1389	ALA	4.6
1	B	2044	VAL	4.6
1	A	1006	VAL	4.3
1	A	1030	THR	4.3
1	A	1041	THR	4.2
1	A	1051	VAL	4.2
1	A	1040	VAL	4.2
1	A	1018	ILE	4.2
1	A	1050	VAL	4.1
1	B	2030	THR	4.1
1	A	1020	SER	4.1
1	A	1047	GLY	4.1
1	B	2046	GLU	4.0
1	A	1081	LYS	4.0
1	A	1043	VAL	4.0
1	B	2048	LYS	3.9
1	A	1259	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1087	ALA	3.7
1	A	1179	ARG	3.7
1	A	1166	LEU	3.7
1	A	1168	MET	3.6
1	A	1031	LYS	3.6
1	A	1053	TYR	3.6
1	A	1385	LYS	3.6
1	B	2360	VAL	3.5
1	A	1007	ARG	3.5
1	A	1048	LYS	3.4
1	A	1076	LEU	3.4
1	B	2019	SER	3.4
1	B	2050	VAL	3.3
1	B	2385	LYS	3.3
1	B	2041	THR	3.2
1	A	1388	LYS	3.1
1	A	1012	ARG	3.1
1	A	1390	LEU	3.1
1	B	2386	GLU	3.1
1	B	2179	ARG	3.1
1	A	1361	ARG	3.1
1	A	1372	LEU	3.0
1	A	1044	VAL	3.0
1	B	2257	ALA	3.0
1	A	1159	TYR	3.0
1	A	1381	SER	3.0
1	A	1046	GLU	3.0
1	A	1132	GLY	2.9
1	B	2007	ARG	2.9
1	A	1010	ASP	2.9
1	A	1075	ILE	2.9
1	B	2086	GLU	2.9
1	A	1384	TYR	2.9
1	B	2012	ARG	2.9
1	A	1167	SER	2.9
1	B	2391	ALA	2.8
1	A	1169	LEU	2.8
1	B	2009	VAL	2.8
1	A	1392	GLU	2.8
1	A	1195	GLU	2.8
1	B	2381	SER	2.7
1	A	1078	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	2068	ARG	2.7
1	A	1257	ALA	2.7
1	B	2389	ALA	2.7
1	B	2165	GLY	2.7
1	B	2045	ARG	2.7
1	A	1008	ILE	2.7
1	A	1084	LEU	2.6
1	B	2031	LYS	2.6
1	A	1049	ARG	2.6
1	A	1011	VAL	2.6
1	B	2168	MET	2.5
1	A	1073	SER	2.5
1	B	2359	GLY	2.5
1	A	1391	ALA	2.5
1	A	1209	LYS	2.5
1	A	1128	ALA	2.5
1	A	1386	GLU	2.4
1	A	1353	TYR	2.4
1	B	2166	LEU	2.4
1	B	2353	TYR	2.4
1	B	2016	LYS	2.4
1	A	1102	ILE	2.4
1	A	1037	VAL	2.4
1	A	1264	MET	2.4
1	B	2008	ILE	2.4
1	B	2049	ARG	2.4
1	A	1351	GLN	2.4
1	B	2047	GLY	2.4
1	B	2088	GLY	2.3
1	B	2259	PHE	2.3
1	A	1065	GLY	2.3
1	B	2005	SER	2.3
1	A	1079	ASP	2.3
1	B	2350	PHE	2.3
1	A	1131	ALA	2.3
1	A	1088	GLY	2.3
1	A	1069	GLU	2.3
1	A	1039	VAL	2.2
1	A	1377	PHE	2.2
1	B	2361	ARG	2.2
1	A	1042	ASP	2.2
1	A	1382	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2351	GLN	2.1
1	B	2145	VAL	2.1
1	A	1233	LEU	2.1
1	A	1371	ASP	2.1
1	B	2051	VAL	2.1
1	A	1205	GLU	2.1
1	B	2014	ILE	2.1
1	A	1045	ARG	2.1
1	A	1360	VAL	2.1
1	A	1364	ASN	2.1
1	A	1227	ILE	2.0
1	B	2256	LEU	2.0
1	A	1170	ARG	2.0
1	B	2110	GLY	2.0
1	A	1145	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	3501	1/1	0.92	0.07	25,25,25,25	0
2	MG	B	3502	1/1	0.93	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.