



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:16 PM UTC

PDB ID : 3SQN / pdb_00003sqn
Title : Putative Mga family transcriptional regulator from *Enterococcus faecalis*
Authors : Osipiuk, J.; Wu, R.; Jedrzejczak, R.; Moy, S.; Joachimiak, A.; Midwest Center
for Structural Genomics (MCSG)
Deposited on : 2011-07-05
Resolution : 2.31 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
Mogul : 2022.3.0, CSD as543be (2022)
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

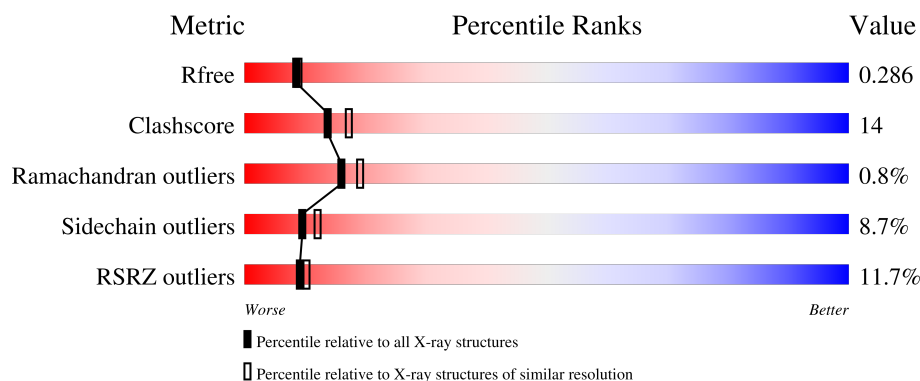
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	485	
1	B	485	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7103 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 Conserved domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	Se	0	1	0
			3883	2519	628	728	3	5			
1	B	381	Total	C	N	O	S	Se	0	3	0
			3181	2076	498	600	3	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q82ZN7
A	-1	ASN	-	expression tag	UNP Q82ZN7
A	0	ALA	-	expression tag	UNP Q82ZN7
B	-2	SER	-	expression tag	UNP Q82ZN7
B	-1	ASN	-	expression tag	UNP Q82ZN7
B	0	ALA	-	expression tag	UNP Q82ZN7

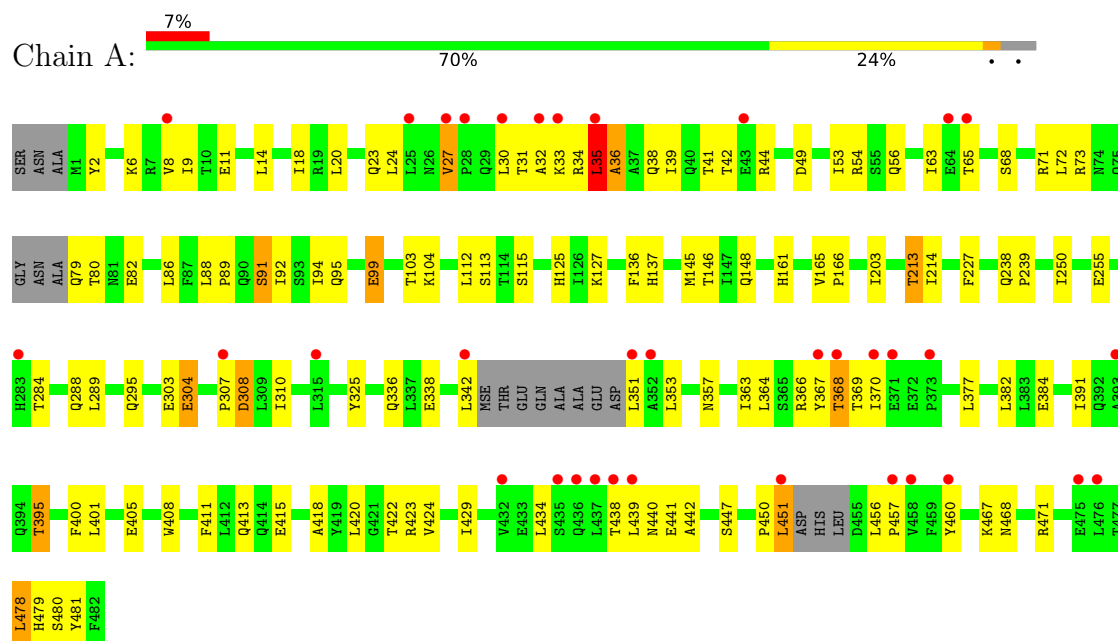
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	13	Total	O	0	0
			13	13		

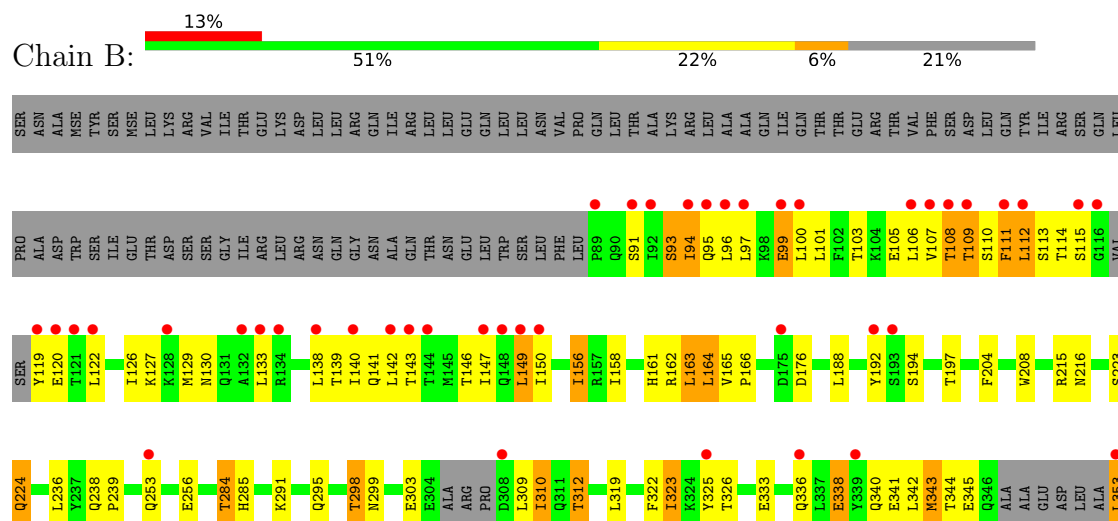
3 Residue-property plots

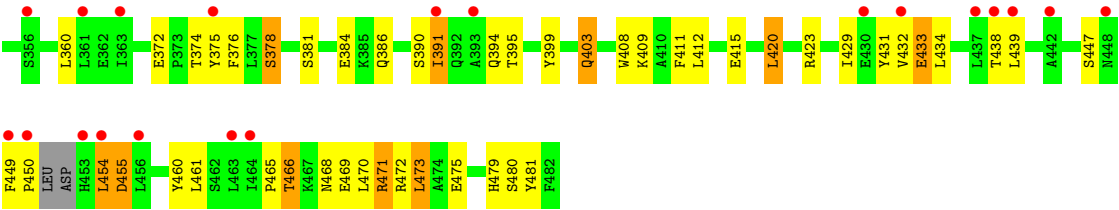
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Conserved domain protein



• Molecule 1: Conserved domain protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.80Å 101.76Å 89.90Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	36.17 – 2.31 36.17 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.17-2.31) 94.8 (36.17-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.282 (Not available) , 0.286	Depositor DCC
R_{free} test set	2439 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7103	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	5/3965 (0.1%)	1.05	5/5365 (0.1%)
1	B	1.10	2/3260 (0.1%)	1.09	5/4408 (0.1%)
All	All	1.08	7/7225 (0.1%)	1.07	10/9773 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	PHE	CA-C	7.28	1.62	1.52
1	A	213	THR	N-CA	-5.43	1.39	1.46
1	A	418	ALA	C-O	-5.41	1.17	1.24
1	A	112	LEU	N-CA	5.13	1.52	1.46
1	B	156	ILE	CA-CB	5.11	1.60	1.54
1	A	227	PHE	C-O	-5.09	1.18	1.23
1	A	214	ILE	N-CA	-5.03	1.40	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	SER	N-CA-C	6.75	118.45	108.60
1	B	312	THR	N-CA-C	-5.70	101.56	110.17
1	B	164	LEU	N-CA-C	5.54	121.81	114.12
1	B	338	GLU	N-CA-C	5.52	117.30	111.28
1	A	113	SER	N-CA-C	5.46	117.67	111.11
1	A	405	GLU	CA-C-N	5.45	124.91	119.24
1	A	405	GLU	C-N-CA	5.45	124.91	119.24
1	B	158	ILE	CB-CA-C	-5.23	105.08	112.14
1	A	284	THR	N-CA-C	5.18	118.76	112.23
1	A	478	LEU	N-CA-C	5.03	117.49	111.71

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	3883	0	3876	87	0
1	B	3181	0	3130	126	0
2	A	26	0	0	0	0
2	B	13	0	0	1	0
All	All	7103	0	7006	204	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 14.

All (204) 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:114:THR:HG22	1:B:114:THR:O	1.68	0.92
1:B:112:LEU:HD11	1:B:119:TYR:HA	1.53	0.90
1:B:340:GLN:O	1:B:344:THR:HG23	1.72	0.90
1:A:451:LEU:HD23	1:A:451:LEU:O	1.73	0.88
1:B:133:LEU:HD11	1:B:140:ILE:CD1	2.05	0.87
1:B:163:LEU:HD23	1:B:163:LEU:O	1.76	0.86
1:A:165:VAL:HG13	1:A:166:PRO:HD3	1.58	0.85
1:A:23:GLN:O	1:A:27:VAL:HG13	1.79	0.82
1:B:112:LEU:HD21	1:B:119:TYR:HB2	1.61	0.82
1:A:145:MSE:HA	1:A:145:MSE:HE2	1.62	0.81
1:A:27:VAL:O	1:A:27:VAL:HG22	1.81	0.80
1:B:133:LEU:CD1	1:B:140:ILE:HD12	2.13	0.79
1:B:126:ILE:HG23	1:B:140:ILE:HB	1.64	0.79
1:B:133:LEU:HD11	1:B:140:ILE:HD11	1.65	0.79
1:B:133:LEU:HD12	1:B:140:ILE:HD12	1.65	0.77
1:B:95:GLN:NE2	1:B:115:SER:OG	2.19	0.76
1:A:35:LEU:C	1:A:35:LEU:HD12	2.12	0.75
1:B:138:LEU:O	1:B:139:THR:HG23	1.86	0.75
1:B:133:LEU:CD1	1:B:140:ILE:CD1	2.63	0.75
1:B:423:ARG:HG3	1:B:481:TYR:CE2	2.21	0.75
1:A:20:LEU:HA	1:A:39:ILE:HD11	1.70	0.73
1:B:192:TYR:HA	1:B:197:THR:HG23	1.72	0.71
1:B:112:LEU:HD11	1:B:119:TYR:CA	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLN:HB3	1:B:449:PHE:CE2	2.26	0.71
1:B:408[A]:TRP:CZ3	1:B:411:PHE:CD2	2.80	0.70
1:A:434:LEU:O	1:A:434:LEU:HD23	1.92	0.69
1:B:163:LEU:C	1:B:163:LEU:CD2	2.66	0.68
1:A:408:TRP:CD1	1:B:342:LEU:HD21	2.29	0.67
1:B:163:LEU:HD23	1:B:163:LEU:C	2.16	0.67
1:A:420:LEU:HD23	1:A:424:VAL:HG11	1.77	0.67
1:B:114:THR:O	1:B:114:THR:CG2	2.39	0.66
1:A:63:ILE:HG12	1:A:72:LEU:HD12	1.79	0.65
1:B:108:THR:HG22	1:B:146:THR:C	2.21	0.65
1:B:129:MSE:HE2	1:B:140:ILE:HD11	1.78	0.65
1:B:163:LEU:O	1:B:163:LEU:CD2	2.44	0.64
1:A:450:PRO:O	1:A:460:TYR:OH	2.13	0.64
1:A:456:LEU:HB3	1:A:457:PRO:HD2	1.77	0.64
1:A:451:LEU:O	1:A:451:LEU:CD2	2.46	0.63
1:B:108:THR:CG2	1:B:146:THR:C	2.71	0.63
1:B:122:LEU:HD21	1:B:147:ILE:HD11	1.80	0.63
1:B:298:THR:OG1	1:B:310:ILE:HD11	1.99	0.62
1:A:88:LEU:N	1:A:89:PRO:HD2	2.14	0.62
1:A:368:THR:CG2	1:A:369:THR:N	2.62	0.62
1:B:140:ILE:HG13	1:B:149:LEU:HD22	1.82	0.62
1:B:454:LEU:HD23	1:B:455:ASP:N	2.15	0.61
1:A:27:VAL:O	1:A:27:VAL:CG2	2.47	0.61
1:B:95:GLN:HE22	1:B:115:SER:CB	2.14	0.61
1:B:408[B]:TRP:NE1	1:B:412:LEU:HD22	2.15	0.60
1:B:466:THR:OG1	1:B:469:GLU:HG2	2.02	0.60
1:B:162:ARG:HB2	1:B:338:GLU:HG3	1.82	0.60
1:B:126:ILE:HD11	1:B:142:LEU:HD13	1.82	0.60
1:A:481:TYR:O	1:B:415:GLU:OE1	2.19	0.60
1:B:110:SER:O	1:B:114:THR:N	2.32	0.59
1:A:161:HIS:ND1	1:A:338:GLU:OE1	2.24	0.59
1:B:319:LEU:O	1:B:323:ILE:HG13	2.03	0.59
1:A:165:VAL:HG13	1:A:166:PRO:CD	2.31	0.58
1:B:99:GLU:O	1:B:103:THR:N	2.36	0.58
1:A:429:ILE:HD11	1:A:434:LEU:HD12	1.85	0.58
1:B:341:GLU:O	1:B:342:LEU:C	2.47	0.58
1:A:65:THR:O	1:A:65:THR:HG23	2.02	0.57
1:A:203:ILE:HD11	1:B:431:TYR:HB2	1.86	0.57
1:A:36:ALA:HB1	1:A:41:THR:O	2.05	0.57
1:A:65:THR:O	1:A:65:THR:CG2	2.53	0.57
1:B:126:ILE:CG2	1:B:140:ILE:HB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408[B]:TRP:CD1	1:B:412:LEU:HD22	2.41	0.56
1:A:145:MSE:HA	1:A:145:MSE:CE	2.34	0.56
1:B:343:MSE:HG2	1:B:378:SER:HB2	1.87	0.56
1:B:336:GLN:HB3	1:B:375:TYR:CD2	2.41	0.56
1:A:353:LEU:HD22	1:A:384:GLU:OE1	2.06	0.55
1:A:429:ILE:CD1	1:A:434:LEU:HD12	2.35	0.55
1:A:42:THR:HG21	1:A:44:ARG:NH1	2.21	0.55
1:B:94:ILE:O	1:B:97:LEU:N	2.39	0.55
1:A:325:TYR:OH	1:A:336:GLN:NE2	2.38	0.54
1:A:35:LEU:HD12	1:A:36:ALA:N	2.22	0.54
1:B:97:LEU:O	1:B:101:LEU:N	2.38	0.54
1:A:54:ARG:NH1	1:A:63:ILE:O	2.39	0.54
1:B:188:LEU:O	1:B:192:TYR:N	2.28	0.54
1:A:95:GLN:O	1:A:99:GLU:HG2	2.07	0.54
1:B:111:PHE:O	1:B:112:LEU:C	2.51	0.53
1:B:471:ARG:HG2	1:B:472:ARG:N	2.23	0.53
1:A:303:GLU:HG2	1:A:304:GLU:OE1	2.08	0.53
1:B:99:GLU:HB2	1:B:106:LEU:HD21	1.91	0.53
1:B:138:LEU:HD11	1:B:156:ILE:HA	1.91	0.53
1:A:32:ALA:O	1:A:35:LEU:HB3	2.09	0.52
1:B:108:THR:HG21	1:B:143:THR:O	2.08	0.52
1:B:375:TYR:O	1:B:378:SER:N	2.43	0.52
1:A:23:GLN:HA	1:A:23:GLN:OE1	2.08	0.52
1:A:42:THR:HG21	1:A:44:ARG:HH12	1.75	0.51
1:A:23:GLN:NE2	1:A:38:GLN:OE1	2.42	0.51
1:A:35:LEU:O	1:A:38:GLN:N	2.40	0.51
1:A:79:GLN:O	1:A:82:GLU:HG2	2.11	0.51
1:B:149:LEU:HD23	1:B:149:LEU:N	2.24	0.51
1:B:408[A]:TRP:HA	1:B:408[A]:TRP:CE3	2.45	0.51
1:A:451:LEU:HD23	1:A:451:LEU:C	2.35	0.51
1:A:308:ASP:HB2	1:A:391:ILE:HD12	1.92	0.51
1:B:238:GLN:HB3	1:B:239:PRO:HD3	1.93	0.50
1:A:39:ILE:HG22	1:A:41:THR:HG22	1.93	0.50
1:A:478:LEU:HD22	1:B:470:LEU:HD13	1.94	0.50
1:B:295:GLN:HG3	1:B:299:ASN:HD21	1.75	0.50
1:B:113:SER:C	1:B:115:SER:H	2.18	0.50
1:B:129:MSE:HE2	1:B:140:ILE:CD1	2.40	0.50
1:A:71:ARG:HB2	1:A:73:ARG:NH2	2.27	0.50
1:A:411:PHE:CZ	1:A:415:GLU:OE2	2.65	0.50
1:B:408[B]:TRP:HE1	1:B:412:LEU:HD22	1.75	0.50
1:B:399:TYR:CE2	1:B:439:LEU:HD12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TRP:CG	1:B:342:LEU:HD21	2.46	0.50
1:A:23:GLN:O	1:A:27:VAL:CG1	2.56	0.50
1:B:110:SER:O	1:B:114:THR:OG1	2.23	0.50
1:B:343:MSE:N	1:B:343:MSE:HE3	2.26	0.49
1:B:216:ASN:ND2	1:B:256:GLU:OE2	2.40	0.49
1:A:2:TYR:O	1:A:6:LYS:HG2	2.11	0.49
1:A:307:PRO:O	1:A:310:ILE:HD12	2.12	0.49
1:B:461:LEU:HG	1:B:465:PRO:HG3	1.94	0.49
1:B:353:LEU:HD13	1:B:384:GLU:OE1	2.13	0.48
1:B:390:SER:O	1:B:391:ILE:HD12	2.14	0.48
1:A:395:THR:OG1	1:A:480:SER:OG	2.05	0.48
1:B:141:GLN:OE1	1:B:150:ILE:HG13	2.14	0.48
1:A:14:LEU:HD23	1:A:91:SER:HB2	1.96	0.48
1:B:122:LEU:HD23	1:B:142:LEU:HD11	1.96	0.48
1:B:333:GLU:O	1:B:336:GLN:HG2	2.14	0.48
1:A:30:LEU:HD22	1:A:68:SER:OG	2.14	0.48
1:B:142:LEU:HD12	1:B:147:ILE:HG12	1.96	0.47
1:A:56:GLN:O	1:A:86:LEU:HD21	2.13	0.47
1:B:295:GLN:HG3	1:B:299:ASN:ND2	2.30	0.47
1:B:342:LEU:HG	1:B:343:MSE:HE1	1.96	0.47
1:A:49:ASP:O	1:A:53:ILE:HG13	2.15	0.47
1:B:386:GLN:NE2	2:B:483:HOH:O	2.12	0.47
1:A:401:LEU:O	1:A:447:SER:HA	2.15	0.47
1:B:108:THR:HG22	1:B:147:ILE:N	2.30	0.47
1:B:429:ILE:HB	1:B:433:GLU:HG3	1.96	0.47
1:B:162:ARG:HD2	1:B:338:GLU:O	2.15	0.46
1:B:336:GLN:CB	1:B:375:TYR:CD2	2.97	0.46
1:B:391:ILE:HD12	1:B:391:ILE:HA	1.74	0.46
1:A:203:ILE:HD11	1:B:431:TYR:CB	2.44	0.46
1:A:382:LEU:HD22	1:B:408[A]:TRP:CZ3	2.50	0.46
1:B:223:SER:OG	1:B:224:GLN:N	2.47	0.46
1:B:395:THR:OG1	1:B:480[A]:SER:OG	2.25	0.46
1:A:364:LEU:CD2	1:A:370:ILE:HG21	2.45	0.46
1:A:411:PHE:HD1	1:B:386:GLN:HB3	1.81	0.46
1:A:35:LEU:C	1:A:35:LEU:CD1	2.83	0.46
1:A:88:LEU:N	1:A:89:PRO:CD	2.78	0.46
1:B:107:VAL:O	1:B:110:SER:HB2	2.16	0.46
1:A:213:THR:HG23	1:A:250:ILE:HD11	1.98	0.45
1:A:165:VAL:CG1	1:A:166:PRO:CD	2.94	0.45
1:B:126:ILE:CD1	1:B:142:LEU:HD13	2.46	0.45
1:A:238:GLN:HB3	1:A:239:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:GLN:HB2	1:B:375:TYR:CG	2.51	0.45
1:A:442:ALA:HB1	1:A:479:HIS:NE2	2.31	0.45
1:B:122:LEU:HD21	1:B:147:ILE:CD1	2.44	0.45
1:B:309:LEU:O	1:B:312:THR:HG23	2.17	0.45
1:B:399:TYR:HE2	1:B:439:LEU:HD12	1.80	0.45
1:B:100:LEU:O	1:B:215:ARG:NH1	2.46	0.45
1:A:9:ILE:HD13	1:A:18:ILE:HD12	1.99	0.45
1:A:363:ILE:HA	1:A:366:ARG:HD2	1.99	0.45
1:A:11:GLU:HG3	1:A:125:HIS:HE1	1.82	0.45
1:A:30:LEU:HD22	1:A:68:SER:O	2.17	0.44
1:A:423:ARG:CD	1:A:481:TYR:CE2	3.01	0.44
1:B:110:SER:O	1:B:114:THR:CB	2.66	0.44
1:B:336:GLN:CB	1:B:375:TYR:CG	3.00	0.44
1:B:399:TYR:CE2	1:B:439:LEU:CD1	3.00	0.44
1:B:122:LEU:CD2	1:B:147:ILE:HD11	2.46	0.44
1:B:408[A]:TRP:CZ3	1:B:411:PHE:HD2	2.34	0.43
1:B:434:LEU:HD23	1:B:434:LEU:O	2.18	0.43
1:B:95:GLN:NE2	1:B:115:SER:CB	2.78	0.43
1:B:322:PHE:CE1	1:B:360:LEU:HD22	2.53	0.43
1:A:368:THR:HG23	1:A:369:THR:N	2.33	0.43
1:B:450:PRO:C	1:B:460:TYR:OH	2.61	0.43
1:B:161:HIS:NE2	1:B:208:TRP:CD1	2.87	0.43
1:A:18:ILE:HD11	1:A:88:LEU:HD23	2.00	0.43
1:B:164:LEU:O	1:B:165:VAL:C	2.59	0.42
1:A:400:PHE:CD2	1:A:413:GLN:HG3	2.54	0.42
1:A:438:THR:HG22	1:A:438:THR:O	2.19	0.42
1:B:94:ILE:O	1:B:95:GLN:C	2.61	0.42
1:B:343:MSE:O	1:B:345:GLU:N	2.52	0.42
1:A:31:THR:HG22	1:A:35:LEU:HB3	2.00	0.42
1:A:94:ILE:O	1:A:95:GLN:C	2.61	0.42
1:A:165:VAL:CG1	1:A:166:PRO:HD3	2.38	0.42
1:B:126:ILE:HG22	1:B:130:ASN:ND2	2.33	0.42
1:B:322:PHE:O	1:B:326:THR:HG23	2.20	0.42
1:A:456:LEU:HB3	1:A:457:PRO:CD	2.46	0.42
1:B:100:LEU:HA	1:B:103:THR:O	2.20	0.42
1:A:92:ILE:HD12	1:A:115:SER:HB2	2.02	0.42
1:A:79:GLN:CG	1:A:80:THR:N	2.83	0.42
1:B:343:MSE:HE3	1:B:343:MSE:CA	2.49	0.42
1:A:289:LEU:HD13	1:A:367:TYR:CE2	2.55	0.42
1:A:471:ARG:HD2	1:B:475:GLU:OE2	2.20	0.42
1:A:450:PRO:O	1:A:451:LEU:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ARG:HG3	1:B:481:TYR:HE2	1.78	0.41
1:A:357:ASN:HB3	1:A:377:LEU:HD22	2.02	0.41
1:B:96:LEU:HD11	1:B:147:ILE:HG21	2.02	0.41
1:B:138:LEU:O	1:B:139:THR:CG2	2.64	0.41
1:B:454:LEU:HD23	1:B:455:ASP:CB	2.50	0.41
1:B:433:GLU:H	1:B:433:GLU:HG2	1.64	0.41
1:B:420:LEU:HD11	1:B:473:LEU:HG	2.03	0.41
1:B:91:SER:OG	1:B:94:ILE:HG12	2.21	0.41
1:B:109:THR:HA	1:B:112:LEU:HB2	2.03	0.41
1:B:284:THR:HG22	1:B:285:HIS:CE1	2.56	0.41
1:A:20:LEU:CD2	1:A:24:LEU:HD11	2.50	0.40
1:B:342:LEU:HG	1:B:343:MSE:CE	2.52	0.40
1:B:454:LEU:HD23	1:B:455:ASP:CA	2.51	0.40
1:B:325:TYR:CE1	1:B:376:PHE:HB2	2.57	0.40
1:A:136:PHE:O	1:A:137:HIS:HB2	2.22	0.40
1:B:95:GLN:HE22	1:B:115:SER:HB3	1.86	0.40
1:B:103:THR:HG22	1:B:105:GLU:O	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	461/485 (95%)	434 (94%)	24 (5%)	3 (1%)	18	22
1	B	374/485 (77%)	348 (93%)	22 (6%)	4 (1%)	11	12
All	All	835/970 (86%)	782 (94%)	46 (6%)	7 (1%)	16	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ALA

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Mol	Chain	Res	Type
1	B	94	ILE
1	A	35	LEU
1	B	432	VAL
1	B	93	SER
1	B	224	GLN
1	A	441	GLU

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	434/439 (99%)	407 (94%)	27 (6%)	16	23
1	B	356/439 (81%)	315 (88%)	41 (12%)	5	6
All	All	790/878 (90%)	722 (91%)	68 (9%)	9	12

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	27	VAL
1	A	33	LYS
1	A	34	ARG
1	A	35	LEU
1	A	91	SER
1	A	99	GLU
1	A	103	THR
1	A	104	LYS
1	A	127	LYS
1	A	146	THR
1	A	148	GLN
1	A	255	GLU
1	A	288	GLN
1	A	295	GLN
1	A	304	GLU
1	A	308	ASP

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	351	LEU
1	A	368	THR
1	A	395	THR
1	A	422	THR
1	A	439	LEU
1	A	440	ASN
1	A	451	LEU
1	A	467	LYS
1	A	468	ASN
1	B	93	SER
1	B	99	GLU
1	B	108	THR
1	B	109	THR
1	B	112	LEU
1	B	120	GLU
1	B	127	LYS
1	B	149	LEU
1	B	163	LEU
1	B	166	PRO
1	B	176	ASP
1	B	194	SER
1	B	204	PHE
1	B	236	LEU
1	B	253	GLN
1	B	284	THR
1	B	291	LYS
1	B	298	THR
1	B	303	GLU
1	B	310	ILE
1	B	323	ILE
1	B	343	MSE
1	B	353	LEU
1	B	372	GLU
1	B	374	THR
1	B	378	SER
1	B	381	SER
1	B	391	ILE
1	B	394	GLN
1	B	403	GLN
1	B	409	LYS
1	B	420	LEU

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Mol	Chain	Res	Type
1	B	433	GLU
1	B	438	THR
1	B	454	LEU
1	B	455	ASP
1	B	466	THR
1	B	468	ASN
1	B	471	ARG
1	B	473	LEU
1	B	479	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	141	GLN
1	A	336	GLN
1	B	95	GLN
1	B	131	GLN
1	B	299	ASN
1	B	386	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](#)

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

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	463/485 (95%)	0.59	35 (7%) 20 22	26, 53, 90, 105	1 (0%)
1	B	377/485 (77%)	1.03	63 (16%) 4 5	29, 59, 91, 110	3 (0%)
All	All	840/970 (86%)	0.79	98 (11%) 9 10	26, 55, 90, 110	4 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	LEU	5.4
1	B	393	ALA	5.3
1	B	147	ILE	5.2
1	B	92	ILE	5.2
1	A	351	LEU	4.9
1	B	89	PRO	4.7
1	A	458	VAL	4.6
1	B	107	VAL	4.6
1	B	116	GLY	4.6
1	B	133	LEU	4.5
1	B	453	HIS	4.5
1	A	437	LEU	4.3
1	B	142	LEU	4.3
1	A	342	LEU	4.3
1	B	353	LEU	4.3
1	A	370	ILE	4.3
1	A	438	THR	4.2
1	A	439	LEU	4.1
1	B	95	GLN	4.0
1	A	367	TYR	3.9
1	B	449	PHE	3.9
1	B	94	ILE	3.8
1	A	30	LEU	3.7
1	B	99	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	120	GLU	3.6
1	B	97	LEU	3.6
1	B	456	LEU	3.6
1	A	27	VAL	3.6
1	A	28	PRO	3.5
1	B	375	TYR	3.4
1	B	122	LEU	3.3
1	A	32	ALA	3.3
1	B	193	SER	3.3
1	A	436	GLN	3.3
1	B	464	ILE	3.2
1	A	352	ALA	3.2
1	B	192	TYR	3.1
1	B	112	LEU	3.0
1	B	454	LEU	3.0
1	B	463	LEU	3.0
1	A	451	LEU	2.9
1	B	106	LEU	2.9
1	B	138	LEU	2.9
1	B	109	THR	2.9
1	B	143	THR	2.9
1	A	475	GLU	2.8
1	B	308	ASP	2.8
1	B	91	SER	2.8
1	B	100	LEU	2.7
1	B	437	LEU	2.7
1	A	432	VAL	2.7
1	B	121	THR	2.6
1	B	128	LYS	2.6
1	B	115	SER	2.5
1	B	148	GLN	2.5
1	B	96	LEU	2.5
1	B	391	ILE	2.5
1	B	175	ASP	2.5
1	B	119	TYR	2.5
1	A	43	GLU	2.4
1	A	25	LEU	2.4
1	A	368	THR	2.4
1	B	108	THR	2.4
1	B	442	ALA	2.4
1	B	111	PHE	2.3
1	B	134	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	64	GLU	2.3
1	A	460	TYR	2.3
1	A	435	SER	2.3
1	B	361	LEU	2.3
1	A	307	PRO	2.3
1	B	132	ALA	2.3
1	B	150	ILE	2.3
1	A	315	LEU	2.3
1	A	393	ALA	2.3
1	B	356	SER	2.3
1	A	33	LYS	2.3
1	B	144	THR	2.2
1	B	430	GLU	2.2
1	B	439	LEU	2.2
1	A	373	PRO	2.2
1	B	438	THR	2.2
1	B	432	VAL	2.2
1	A	35	LEU	2.2
1	A	476	LEU	2.1
1	B	363	ILE	2.1
1	A	457	PRO	2.1
1	B	253	GLN	2.1
1	B	450	PRO	2.1
1	A	371	GLU	2.1
1	A	283	HIS	2.1
1	B	336	GLN	2.1
1	B	448	ASN	2.1
1	B	339	TYR	2.1
1	A	65	THR	2.0
1	B	140	ILE	2.0
1	B	325	TYR	2.0
1	A	8	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.