Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:04 am BST

PDB ID	:	3SQN
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 following versions of software and data (see references ①) were used in the production of this report:

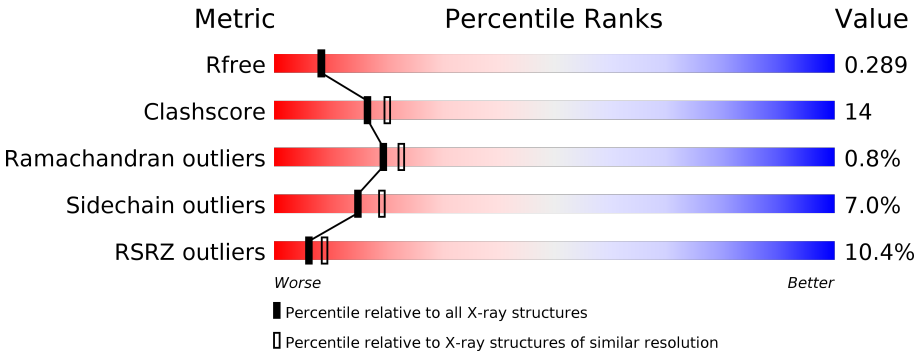
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.31 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 on 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 <=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	9% 72% 22%
1	B	485	8% 52% 23% 21%

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.

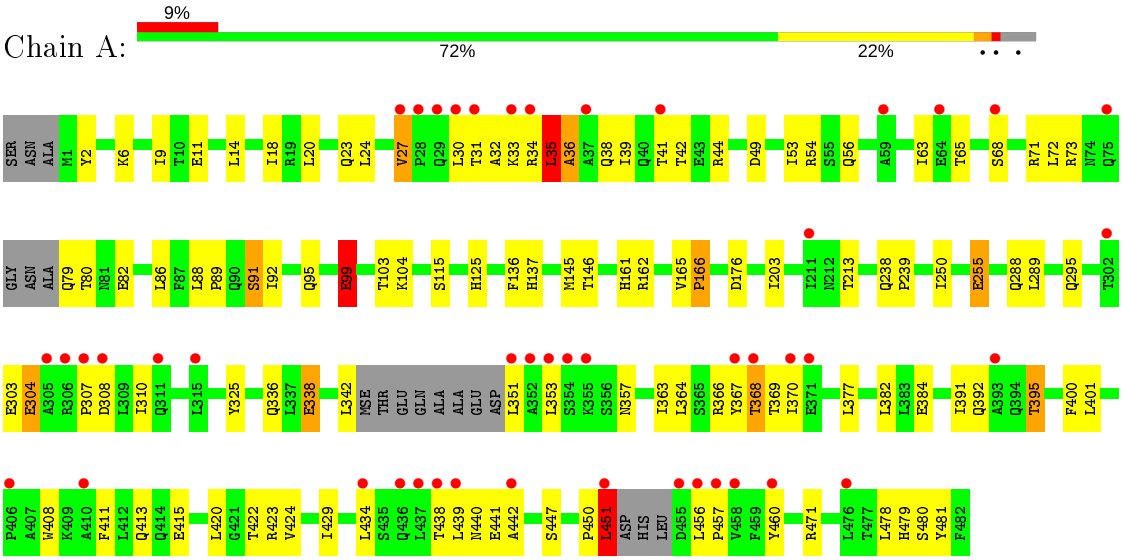
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	13	Total	O	0	0
			13	13		

3 Residue-property plots (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 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.

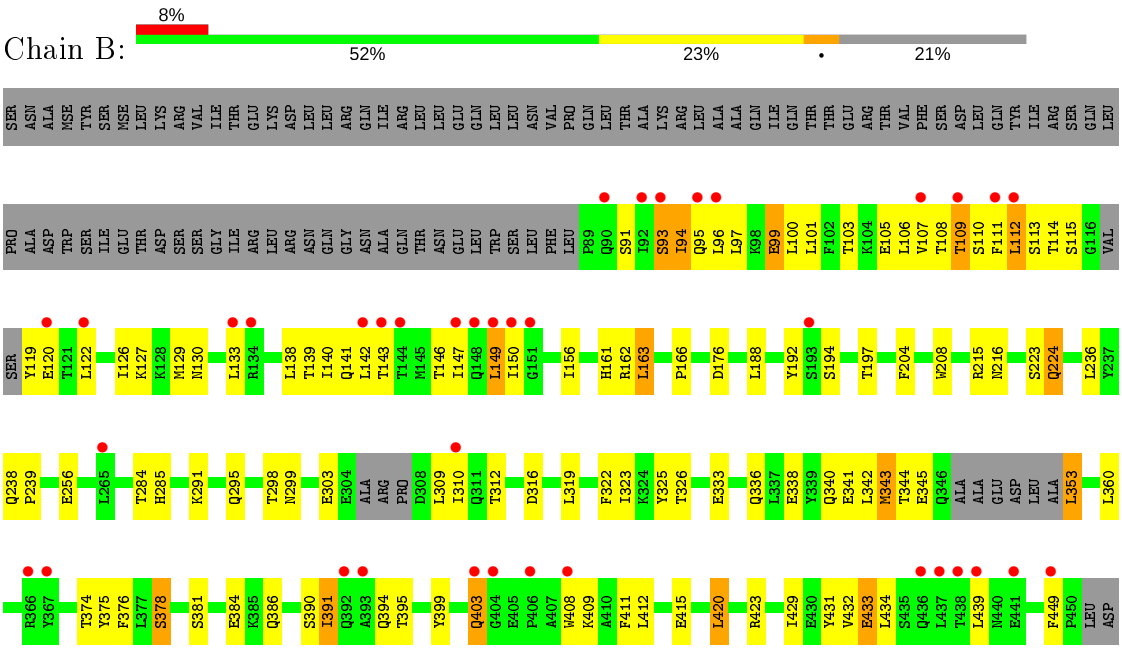
- Molecule 1: Conserved domain protein

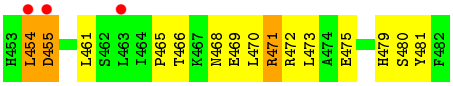
Chain A:



- Molecule 1: Conserved domain protein

Chain B:




H453
L454
D455
L461
S462
L463
I464
P465
T466
K467
N468
E469
L470
R471
R472
L473
A474
E475
H479
S480
Y481
F482

4 Data and refinement statistics (i)

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) 97.2 (36.17-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.282 0.227 , 0.289	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)	0.36 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.87	3/3965 (0.1%)	0.81	2/5365 (0.0%)
1	B	0.90	0/3260	0.84	1/4408 (0.0%)
All	All	0.88	3/7225 (0.0%)	0.83	3/9773 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE2	5.81	1.32	1.25
1	A	255	GLU	CG-CD	-5.28	1.44	1.51
1	A	338	GLU	CG-CD	5.03	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	316	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	162	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	451	LEU	CA-CB-CG	5.26	127.39	115.30

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	86	0
1	B	3181	0	3130	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	26	0	0	0	0
2	B	13	0	0	1	0
All	All	7103	0	7006	200	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 (200) 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:O	1:B:163:LEU:HD23	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:HE2	1:A:145:MSE:HA	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: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
1:B:403:GLN:HB3	1:B:449:PHE:CE2	2.26	0.71
1:A:35:LEU:C	1:A:35:LEU:HD12	2.12	0.70
1:B:408[A]:TRP:CZ3	1:B:411:PHE:CD2	2.80	0.70
1:A:434:LEU:HD23	1:A:434:LEU:O	1.92	0.69
1:A:408:TRP:CD1	1:B:342:LEU:HD21	2.29	0.67
1:A:420:LEU:HD23	1:A:424:VAL:HG11	1.77	0.67
1:B:114:THR:CG2	1:B:114:THR:O	2.39	0.66
1:A:63:ILE:HG12	1:A:72:LEU:HD12	1.79	0.65
1:B:129:MSE:HE2	1:B:140:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:CD2	1:B:163:LEU:O	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:CD2	1:A:451:LEU:O	2.46	0.63
1:B:122:LEU:HD21	1:B:147:ILE:HD11	1.80	0.63
1:B:163:LEU:CD2	1:B:163:LEU:C	2.66	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:B:108:THR:HG22	1:B:146:THR:C	2.21	0.60
1:A:481:TYR:O	1:B:415:GLU:OE1	2.19	0.60
1:B:163:LEU:HD23	1:B:163:LEU:C	2.16	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:B:108:THR:CG2	1:B:146:THR:C	2.71	0.58
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:A:65:THR:HG23	1:A:65:THR:O	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
1:B:408[B]:TRP:CD1	1:B:412:LEU:HD22	2.41	0.56
1:A:145:MSE:CE	1:A:145:MSE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:341:GLU:O	1:B:342:LEU:C	2.47	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:OE1	1:A:23:GLN:HA	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:N	1:B:149:LEU:HD23	2.24	0.51
1:B:408[A]:TRP:HA	1:B:408[A]:TRP:CE3	2.45	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:B:295:GLN:HG3	1:B:299:ASN:HD21	1.75	0.50
1:A:478:LEU:HD22	1:B:470:LEU:HD13	1.94	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
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:HE3	1:B:343:MSE:N	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:111:PHE:O	1:B:112:LEU:C	2.51	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:108:THR:HG22	1:B:147:ILE:N	2.30	0.47
1:B:386:GLN:NE2	2:B:483:HOH:O	2.12	0.47
1:A:49:ASP:O	1:A:53:ILE:HG13	2.15	0.47
1:A:401:LEU:O	1:A:447:SER:HA	2.15	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:HA	1:B:391:ILE:HD12	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:451:LEU:C	1:A:451:LEU:HD23	2.35	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: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:B:113:SER:C	1:B:115:SER:H	2.18	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:434:LEU:HD23	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: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: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:343:MSE:O	1:B:345:GLU:N	2.52	0.42
1:A:165:VAL:CG1	1:A:166:PRO:HD3	2.38	0.42
1:A:31:THR:HG22	1:A:35:LEU:HB3	2.00	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
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:138:LEU:O	1:B:139:THR:CG2	2.64	0.41
1:B:96:LEU:HD11	1:B:147:ILE:HG21	2.02	0.41
1:A:35:LEU:C	1:A:35:LEU:CD1	2.83	0.41
1:B:454:LEU:HD23	1:B:455:ASP:CB	2.50	0.41
1:B:433:GLU:HG2	1:B:433:GLU:H	1.64	0.41
1:B:420:LEU:HD11	1:B:473:LEU:HG	2.03	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:B:91:SER:OG	1:B:94:ILE:HG12	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:THR:HG22	1:B:105:GLU:O	2.22	0.40
1:B:95:GLN:HE22	1:B:115:SER:HB3	1.86	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	461/485 (95%)	434 (94%)	24 (5%)	3 (1%)	22	26
1	B	374/485 (77%)	348 (93%)	22 (6%)	4 (1%)	14	15
All	All	835/970 (86%)	782 (94%)	46 (6%)	7 (1%)	19	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ALA
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 (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	434/439 (99%)	410 (94%)	24 (6%)	21 29
1	B	356/439 (81%)	325 (91%)	31 (9%)	10 12
All	All	790/878 (90%)	735 (93%)	55 (7%)	15 19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	146	THR
1	A	166	PRO
1	A	176	ASP
1	A	255	GLU
1	A	288	GLN
1	A	295	GLN
1	A	304	GLU
1	A	342	LEU
1	A	351	LEU
1	A	368	THR
1	A	392	GLN
1	A	395	THR
1	A	422	THR
1	A	439	LEU
1	A	440	ASN
1	A	451	LEU
1	B	93	SER
1	B	99	GLU
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

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Mol	Chain	Res	Type
1	B	176	ASP
1	B	194	SER
1	B	204	PHE
1	B	236	LEU
1	B	291	LYS
1	B	303	GLU
1	B	343	MSE
1	B	353	LEU
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
1	B	433	GLU
1	B	454	LEU
1	B	455	ASP
1	B	468	ASN
1	B	471	ARG
1	B	479	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	336	GLN
1	B	95	GLN
1	B	169	HIS
1	B	295	GLN
1	B	299	ASN
1	B	386	GLN
1	B	394	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	463/485 (95%)	0.60	46 (9%)	7	10	28, 53, 90, 105	0
1	B	377/485 (77%)	0.76	41 (10%)	5	8	29, 59, 91, 110	0
All	All	840/970 (86%)	0.67	87 (10%)	6	9	28, 55, 90, 110	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	LEU	10.7
1	B	92	ILE	9.9
1	A	437	LEU	8.1
1	A	438	THR	7.3
1	B	393	ALA	7.3
1	B	149	LEU	5.8
1	A	456	LEU	5.7
1	B	122	LEU	5.6
1	B	133	LEU	5.5
1	A	307	PRO	5.4
1	A	28	PRO	5.2
1	B	150	ILE	5.2
1	A	29	GLN	5.1
1	A	458	VAL	5.0
1	A	439	LEU	4.9
1	B	143	THR	4.8
1	B	107	VAL	4.7
1	A	355	LYS	4.6
1	A	34	ARG	4.6
1	B	142	LEU	4.6
1	A	302	THR	4.5
1	A	353	LEU	4.4
1	B	193	SER	4.3
1	A	354	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	371	GLU	4.2
1	A	436	GLN	4.1
1	B	438	THR	4.1
1	A	306	ARG	3.9
1	B	437	LEU	3.9
1	A	352	ALA	3.9
1	B	111	PHE	3.9
1	A	33	LYS	3.8
1	A	393	ALA	3.8
1	B	439	LEU	3.8
1	B	449	PHE	3.6
1	B	120	GLU	3.6
1	B	147	ILE	3.5
1	B	436	GLN	3.4
1	B	148	GLN	3.4
1	B	151	GLY	3.3
1	A	476	LEU	3.2
1	A	434	LEU	3.2
1	A	455	ASP	3.1
1	B	392	GLN	3.1
1	A	31	THR	3.1
1	B	95	GLN	3.0
1	A	406	PRO	3.0
1	B	366	ARG	3.0
1	A	460	TYR	2.9
1	B	93	SER	2.9
1	A	451	LEU	2.9
1	A	457	PRO	2.9
1	A	27	VAL	2.9
1	A	305	ALA	2.8
1	A	367	TYR	2.8
1	A	59	ALA	2.7
1	A	370	ILE	2.7
1	B	109	THR	2.7
1	B	408[A]	TRP	2.6
1	A	64	GLU	2.6
1	B	406	PRO	2.5
1	A	410	ALA	2.5
1	B	96	LEU	2.5
1	B	367	TYR	2.4
1	B	454	LEU	2.4
1	A	37	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	112	LEU	2.4
1	B	404	GLY	2.4
1	A	30	LEU	2.3
1	B	134	ARG	2.3
1	B	90	GLN	2.3
1	B	463	LEU	2.3
1	A	308	ASP	2.3
1	B	441	GLU	2.2
1	A	211	ILE	2.2
1	A	68	SER	2.2
1	A	41	THR	2.1
1	A	442	ALA	2.1
1	B	310	ILE	2.1
1	B	455	ASP	2.1
1	A	311	GLN	2.1
1	B	265	LEU	2.1
1	A	368	THR	2.1
1	B	403	GLN	2.1
1	A	315	LEU	2.1
1	A	75	GLN	2.0
1	B	144	THR	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.