



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:37 AM UTC

PDB ID : 3DQQ / pdb_00003dqq
Title : The crystal structure of the putative tRNA synthase from *Salmonella typhimurium* LT2
Authors : Zhang, R.; Gu, M.; Zhou, M.; Anderson, W.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2008-07-09
Resolution : 2.70 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

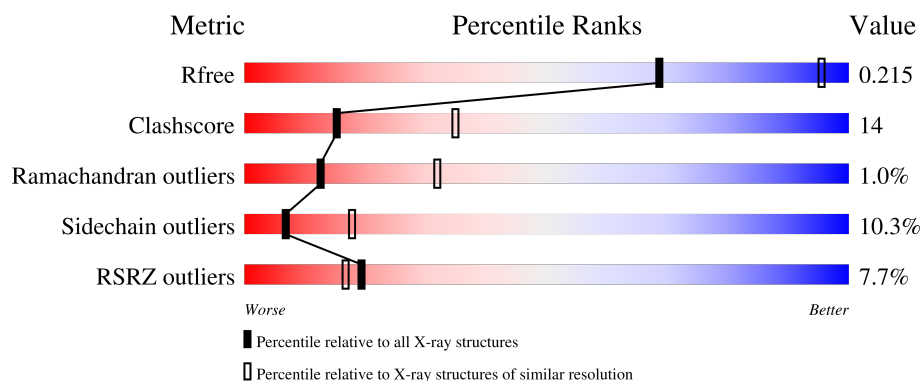
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	421	7% 78% 19% .
1	B	421	9% 67% 24% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6264 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 Putative tRNA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3134	1966	550	600	18			
1	B	412	Total	C	N	O	S	0	0	0
			3085	1937	538	592	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8ZMG5
B	0	GLY	-	expression tag	UNP Q8ZMG5

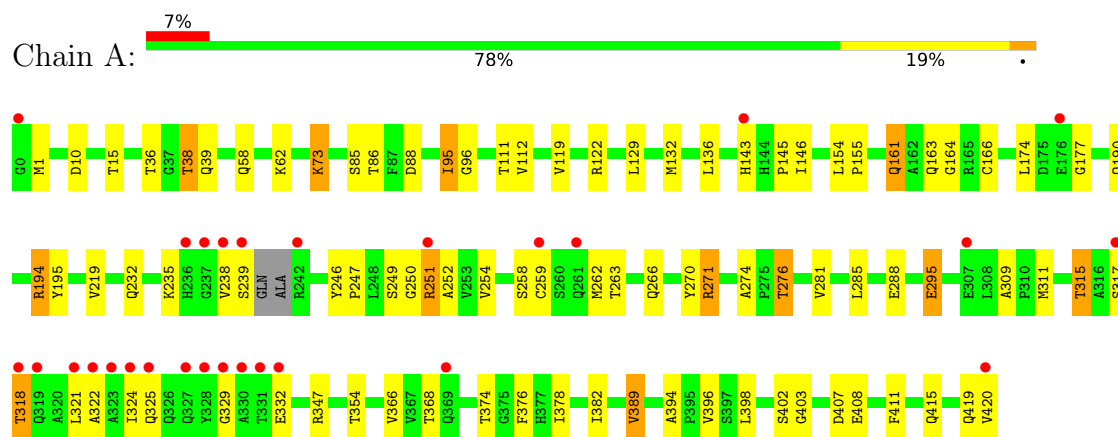
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	14	Total	O	0	0
			14	14		

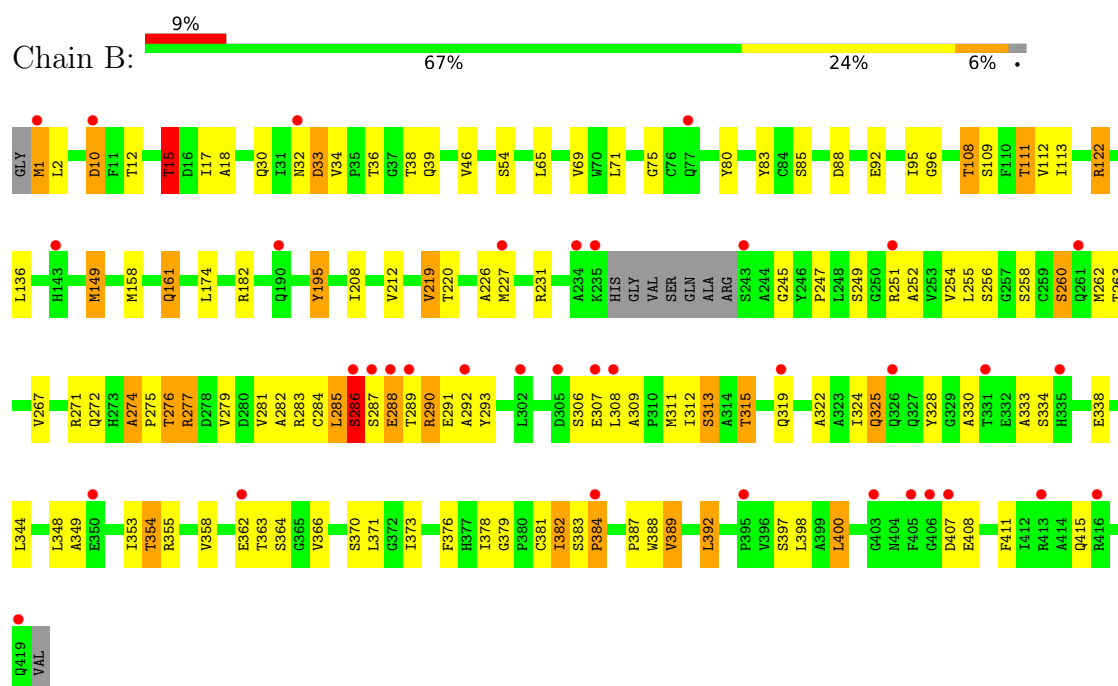
3 Residue-property plots [i](#)

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: Putative tRNA synthase



• Molecule 1: Putative tRNA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	254.54Å 254.54Å 94.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	127.00 – 2.70 127.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (127.00-2.70) 99.8 (127.00-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.210 0.194 , 0.215	Depositor DCC
R_{free} test set	2515 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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

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	1.23	4/3193 (0.1%)	1.12	11/4341 (0.3%)
1	B	0.96	1/3143 (0.0%)	1.03	4/4274 (0.1%)
All	All	1.10	5/6336 (0.1%)	1.08	15/8615 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	THR	CA-CB	5.63	1.62	1.53
1	A	73	LYS	C-O	-5.17	1.17	1.24
1	A	132	MET	C-O	-5.17	1.19	1.24
1	A	166	CYS	C-O	-5.07	1.18	1.24
1	A	190	GLN	CG-CD	5.04	1.64	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ILE	N-CA-C	-9.18	103.92	111.81
1	B	382	ILE	N-CA-C	-7.27	103.38	110.72
1	B	274	ALA	N-CA-C	6.49	114.06	108.22
1	B	161	GLN	N-CA-CB	-6.17	102.36	110.88
1	A	288	GLU	N-CA-C	-5.96	104.86	111.36
1	A	194	ARG	CB-CA-C	-5.91	98.33	110.38
1	A	36	THR	N-CA-C	-5.84	106.49	113.97
1	B	108	THR	CB-CA-C	-5.77	100.29	109.80
1	A	95	ILE	N-CA-C	5.51	115.71	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH2	5.38	124.05	119.20
1	A	161	GLN	N-CA-CB	-5.27	102.90	110.65
1	A	394	ALA	N-CA-C	-5.16	101.17	109.58
1	A	163	GLN	N-CA-C	5.15	118.72	112.23
1	A	177	GLY	N-CA-C	5.15	118.29	111.70
1	A	194	ARG	CD-NE-CZ	-5.13	117.22	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	GLN	Peptide

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	3134	0	3105	55	0
1	B	3085	0	3056	113	1
2	A	31	0	0	1	0
2	B	14	0	0	0	0
All	All	6264	0	6161	168	1

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 (168) 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:284:CYS:C	1:B:285:LEU:HD23	1.40	1.45
1:B:285:LEU:HD23	1:B:285:LEU:N	1.50	1.05
1:B:284:CYS:C	1:B:285:LEU:CD2	2.36	0.98
1:B:282:ALA:HB2	1:B:328:TYR:OH	1.63	0.97
1:B:1:MET:O	1:B:1:MET:HE3	1.63	0.96
1:B:287:SER:O	1:B:291:GLU:HG2	1.70	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:SER:O	1:B:291:GLU:CG	2.18	0.91
1:B:283:ARG:HD2	1:B:293:TYR:CD2	2.06	0.89
1:A:309:ALA:H	1:A:415:GLN:HE22	1.19	0.87
1:A:143:HIS:HB2	2:A:426:HOH:O	1.76	0.86
1:A:259:CYS:HA	1:A:318:THR:HG21	1.60	0.84
1:B:286:SER:OG	1:B:288:GLU:HB2	1.77	0.84
1:B:252:ALA:HB3	1:B:309:ALA:HB2	1.58	0.82
1:B:283:ARG:HD2	1:B:293:TYR:CG	2.13	0.81
1:B:309:ALA:H	1:B:415:GLN:HE22	1.28	0.79
1:B:284:CYS:O	1:B:285:LEU:HD23	1.82	0.79
1:B:1:MET:HE3	1:B:1:MET:C	2.09	0.77
1:A:376:PHE:HB2	1:A:389:VAL:HG13	1.68	0.76
1:B:283:ARG:O	1:B:283:ARG:HG2	1.88	0.73
1:B:254:VAL:HG11	1:B:311:MET:HE3	1.71	0.73
1:B:289:THR:O	1:B:290:ARG:C	2.30	0.72
1:B:2:LEU:HD11	1:B:46:VAL:HG23	1.72	0.72
1:A:254:VAL:HG11	1:A:311:MET:CE	2.19	0.72
1:B:289:THR:O	1:B:291:GLU:N	2.23	0.72
1:B:289:THR:O	1:B:292:ALA:N	2.24	0.71
1:B:287:SER:O	1:B:291:GLU:HG3	1.90	0.70
1:A:254:VAL:HG11	1:A:311:MET:HE3	1.72	0.70
1:B:338:GLU:HB2	1:B:366:VAL:HG21	1.74	0.69
1:B:319:GLN:O	1:B:322:ALA:HB3	1.93	0.69
1:A:311:MET:HE1	1:A:411:PHE:CE2	2.28	0.68
1:B:262:MET:CE	1:B:407:ASP:C	2.66	0.68
1:B:283:ARG:CD	1:B:293:TYR:CG	2.77	0.67
1:B:85:SER:HB3	1:B:122:ARG:HG3	1.77	0.66
1:B:283:ARG:O	1:B:283:ARG:CG	2.43	0.66
1:A:96:GLY:H	1:A:161:GLN:NE2	1.94	0.66
1:B:15:THR:HG22	1:B:30:GLN:OE1	1.96	0.66
1:A:309:ALA:N	1:A:415:GLN:HE22	1.93	0.65
1:B:262:MET:HE1	1:B:408:GLU:N	2.11	0.65
1:B:272:GLN:HE21	1:B:272:GLN:HA	1.61	0.65
1:B:256:SER:OG	1:B:315:THR:HG22	1.96	0.64
1:B:267:VAL:HG21	1:B:315:THR:HG21	1.80	0.64
1:B:325:GLN:HE21	1:B:330:ALA:HA	1.64	0.63
1:B:256:SER:OG	1:B:315:THR:CG2	2.47	0.63
1:B:283:ARG:CD	1:B:293:TYR:CD2	2.80	0.62
1:A:376:PHE:CG	1:A:389:VAL:CG1	2.82	0.62
1:A:376:PHE:CB	1:A:389:VAL:HG13	2.29	0.62
1:A:376:PHE:CG	1:A:389:VAL:HG13	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:VAL:HG11	1:B:311:MET:CE	2.30	0.62
1:B:258:SER:O	1:B:315:THR:HB	2.00	0.61
1:B:227:MET:HE2	1:B:231:ARG:NH2	2.16	0.61
1:A:250:GLY:HA3	1:A:354:THR:HG21	1.82	0.61
1:B:344:LEU:O	1:B:348:LEU:HD13	2.01	0.61
1:B:309:ALA:N	1:B:415:GLN:HE22	1.97	0.60
1:B:1:MET:C	1:B:1:MET:CE	2.75	0.60
1:B:2:LEU:HD13	1:B:39:GLN:NE2	2.16	0.60
1:B:364:SER:HB3	1:B:400:LEU:HG	1.84	0.59
1:B:10:ASP:OD1	1:B:10:ASP:C	2.44	0.59
1:B:397:SER:O	1:B:398:LEU:HD12	2.03	0.59
1:A:322:ALA:HB2	1:A:329:GLY:O	2.01	0.59
1:B:311:MET:HE1	1:B:411:PHE:CE2	2.38	0.57
1:A:145:PRO:HB2	1:A:146:ILE:HD12	1.86	0.57
1:B:289:THR:C	1:B:291:GLU:N	2.63	0.56
1:B:18:ALA:HB1	1:B:378:ILE:HG13	1.86	0.56
1:B:271:ARG:HA	1:B:276:THR:HG21	1.87	0.56
1:B:376:PHE:HA	1:B:392:LEU:HD13	1.88	0.55
1:A:164:GLY:HA3	1:A:194:ARG:HG3	1.88	0.55
1:B:376:PHE:HB2	1:B:389:VAL:HG13	1.89	0.55
1:A:376:PHE:CD2	1:A:389:VAL:CG1	2.90	0.54
1:A:249:SER:O	1:A:354:THR:HG21	2.07	0.54
1:A:262:MET:HE1	1:A:408:GLU:HA	1.90	0.54
1:B:258:SER:HG	1:B:260:SER:HG	1.55	0.53
1:A:259:CYS:SG	1:A:332:GLU:HA	2.48	0.53
1:A:311:MET:HE1	1:A:411:PHE:CD2	2.42	0.53
1:B:376:PHE:CG	1:B:389:VAL:HG13	2.44	0.53
1:B:208:ILE:O	1:B:212:VAL:HG23	2.09	0.52
1:B:262:MET:HE2	1:B:407:ASP:CA	2.40	0.52
1:B:15:THR:HG22	1:B:30:GLN:HE22	1.74	0.51
1:B:254:VAL:C	1:B:255:LEU:HD23	2.36	0.51
1:B:267:VAL:HG21	1:B:315:THR:CG2	2.40	0.51
1:B:383:SER:O	1:B:384:PRO:C	2.53	0.51
1:B:286:SER:O	1:B:287:SER:C	2.53	0.51
1:A:95:ILE:HB	1:A:161:GLN:HE22	1.76	0.50
1:B:283:ARG:HD2	1:B:293:TYR:CE2	2.46	0.50
1:B:382:ILE:H	1:B:382:ILE:HD12	1.76	0.50
1:A:258:SER:HB3	1:A:263:THR:HG21	1.92	0.50
1:B:262:MET:HE2	1:B:407:ASP:HA	1.92	0.50
1:B:287:SER:O	1:B:288:GLU:O	2.30	0.50
1:A:376:PHE:CD2	1:A:389:VAL:HG13	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:HG12	1:A:398:LEU:HD13	1.94	0.50
1:A:396:VAL:HG12	1:A:398:LEU:CD1	2.41	0.49
1:B:83:TYR:OH	1:B:113:ILE:HG23	2.11	0.49
1:B:247:PRO:HG3	1:B:388:TRP:CG	2.48	0.49
1:A:262:MET:CE	1:A:408:GLU:HA	2.43	0.49
1:B:252:ALA:HB3	1:B:309:ALA:CB	2.37	0.49
1:B:272:GLN:HA	1:B:272:GLN:NE2	2.27	0.49
1:B:306:SER:OG	1:B:307:GLU:N	2.46	0.49
1:B:251:ARG:O	1:B:353:ILE:HG23	2.13	0.48
1:B:284:CYS:O	1:B:285:LEU:CD2	2.51	0.48
1:A:58:GLN:HE21	1:A:62:LYS:HE2	1.78	0.48
1:A:251:ARG:HG3	1:A:252:ALA:N	2.27	0.48
1:B:15:THR:HG22	1:B:30:GLN:NE2	2.28	0.48
1:B:333:ALA:O	1:B:334:SER:C	2.56	0.48
1:A:378:ILE:HD13	1:A:389:VAL:HG22	1.96	0.47
1:B:381:CYS:HA	1:B:387:PRO:HA	1.96	0.47
1:B:285:LEU:N	1:B:285:LEU:CD2	2.30	0.47
1:B:309:ALA:CB	1:B:415:GLN:HE22	2.27	0.47
1:A:86:THR:OG1	1:A:88:ASP:OD1	2.25	0.47
1:A:232:GLN:HE22	1:A:235:LYS:NZ	2.13	0.47
1:A:376:PHE:CD2	1:A:389:VAL:HG11	2.50	0.47
1:A:376:PHE:CG	1:A:389:VAL:HG11	2.49	0.47
1:B:376:PHE:CB	1:B:389:VAL:HG13	2.45	0.47
1:A:254:VAL:HG11	1:A:311:MET:HE2	1.97	0.47
1:A:10:ASP:OD1	1:A:10:ASP:C	2.58	0.46
1:B:286:SER:C	1:B:288:GLU:N	2.70	0.46
1:A:111:THR:HG22	1:A:112:VAL:N	2.31	0.46
1:B:80:TYR:CD1	1:B:219:VAL:HG12	2.50	0.46
1:B:15:THR:HG22	1:B:30:GLN:CD	2.40	0.46
1:B:149:MET:CE	1:B:149:MET:HA	2.45	0.46
1:B:32:ASN:O	1:B:33:ASP:HB2	2.15	0.45
1:A:311:MET:CE	1:A:411:PHE:CE2	2.98	0.45
1:B:149:MET:HA	1:B:149:MET:HE2	1.98	0.45
1:A:250:GLY:CA	1:A:354:THR:HG21	2.45	0.45
1:A:274:ALA:O	1:A:276:THR:HG23	2.16	0.44
1:B:262:MET:HE1	1:B:407:ASP:C	2.38	0.44
1:B:33:ASP:O	1:B:34:VAL:C	2.60	0.44
1:A:154:LEU:N	1:A:155:PRO:CD	2.80	0.44
1:B:344:LEU:HD11	1:B:348:LEU:HD11	2.00	0.44
1:B:17:ILE:HD11	1:B:226:ALA:HB2	1.99	0.44
1:B:376:PHE:CG	1:B:389:VAL:CG1	3.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:CE	1:A:266:GLN:HG3	2.48	0.44
1:A:38:THR:O	1:A:39:GLN:C	2.60	0.43
1:B:349:ALA:HB2	1:B:371:LEU:HD21	1.99	0.43
1:B:113:ILE:HD11	1:B:158:MET:HE2	2.01	0.43
1:B:254:VAL:O	1:B:255:LEU:HD23	2.18	0.43
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.87	0.43
1:B:312:ILE:HG13	1:B:344:LEU:HD21	1.99	0.43
1:B:277:ARG:NH1	1:B:277:ARG:HG2	2.33	0.43
1:B:288:GLU:O	1:B:289:THR:C	2.60	0.43
1:A:295:GLU:HG3	1:A:347:ARG:CZ	2.49	0.43
1:A:262:MET:HE2	1:A:407:ASP:C	2.44	0.43
1:B:344:LEU:CD1	1:B:348:LEU:HD11	2.49	0.42
1:A:96:GLY:H	1:A:161:GLN:HE21	1.67	0.42
1:B:111:THR:O	1:B:195:TYR:HA	2.20	0.42
1:A:271:ARG:HA	1:A:276:THR:HG21	2.02	0.42
1:A:315:THR:HA	1:A:318:THR:HB	2.02	0.42
1:B:279:VAL:HG23	1:B:313:SER:O	2.19	0.42
1:B:258:SER:HB3	1:B:263:THR:HG21	2.00	0.42
1:A:270:TYR:OH	1:A:309:ALA:O	2.33	0.42
1:B:95:ILE:N	1:B:161:GLN:NE2	2.67	0.42
1:B:111:THR:HG22	1:B:112:VAL:H	1.84	0.42
1:B:283:ARG:HG2	1:B:293:TYR:CD2	2.55	0.42
1:B:309:ALA:CB	1:B:415:GLN:NE2	2.83	0.42
1:B:88:ASP:OD1	1:B:88:ASP:N	2.52	0.42
1:B:400:LEU:HD12	1:B:400:LEU:HA	1.91	0.42
1:A:259:CYS:CA	1:A:318:THR:HG21	2.38	0.41
1:B:262:MET:HE2	1:B:407:ASP:C	2.44	0.41
1:B:354:THR:HG22	1:B:355:ARG:HG3	2.01	0.41
1:A:276:THR:HB	1:A:311:MET:HB3	2.02	0.41
1:B:281:VAL:HG21	1:B:324:ILE:HD13	2.01	0.41
1:A:281:VAL:CG2	1:A:317:SER:HB2	2.51	0.41
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.90	0.41
1:B:245:GLY:O	1:B:379:GLY:HA3	2.21	0.41
1:A:246:TYR:CG	1:A:247:PRO:HD2	2.55	0.41
1:B:96:GLY:H	1:B:161:GLN:NE2	2.19	0.41
1:B:287:SER:O	1:B:288:GLU:C	2.64	0.41
1:B:271:ARG:HA	1:B:276:THR:CG2	2.49	0.40
1:A:86:THR:HA	1:A:129:LEU:HD21	2.04	0.40
1:B:274:ALA:HB1	1:B:275:PRO:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:NH1	1:B:283:ARG:NH2[12_565]	2.16	0.04

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	415/421 (99%)	397 (96%)	16 (4%)	2 (0%)	24	48
1	B	408/421 (97%)	366 (90%)	36 (9%)	6 (2%)	8	22
All	All	823/842 (98%)	763 (93%)	52 (6%)	8 (1%)	12	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASP
1	B	288	GLU
1	B	286	SER
1	B	290	ARG
1	B	384	PRO
1	A	403	GLY
1	A	238	VAL
1	B	75	GLY

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	329/330 (100%)	302 (92%)	27 (8%)	10	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	324/330 (98%)	284 (88%)	40 (12%)	4	12
All	All	653/660 (99%)	586 (90%)	67 (10%)	7	18

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	THR
1	A	38	THR
1	A	85	SER
1	A	119	VAL
1	A	122	ARG
1	A	136	LEU
1	A	174	LEU
1	A	195	TYR
1	A	219	VAL
1	A	239	SER
1	A	251	ARG
1	A	271	ARG
1	A	276	THR
1	A	285	LEU
1	A	295	GLU
1	A	315	THR
1	A	318	THR
1	A	321	LEU
1	A	324	ILE
1	A	325	GLN
1	A	366	VAL
1	A	368	THR
1	A	374	THR
1	A	389	VAL
1	A	402	SER
1	A	420	VAL
1	B	1	MET
1	B	10	ASP
1	B	12	THR
1	B	15	THR
1	B	36	THR
1	B	38	THR
1	B	54	SER
1	B	69	VAL
1	B	71	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	GLU
1	B	108	THR
1	B	109	SER
1	B	111	THR
1	B	122	ARG
1	B	136	LEU
1	B	149	MET
1	B	174	LEU
1	B	182	ARG
1	B	195	TYR
1	B	219	VAL
1	B	220	THR
1	B	249	SER
1	B	260	SER
1	B	276	THR
1	B	277	ARG
1	B	285	LEU
1	B	286	SER
1	B	308	LEU
1	B	313	SER
1	B	315	THR
1	B	325	GLN
1	B	354	THR
1	B	358	VAL
1	B	362	GLU
1	B	363	THR
1	B	370	SER
1	B	373	ILE
1	B	389	VAL
1	B	392	LEU
1	B	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	58	GLN
1	A	147	ASN
1	A	161	GLN
1	A	190	GLN
1	A	232	GLN
1	A	261	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	ASN
1	A	272	GLN
1	A	319	GLN
1	A	369	GLN
1	A	415	GLN
1	B	58	GLN
1	B	120	ASN
1	B	161	GLN
1	B	265	GLN
1	B	272	GLN
1	B	299	GLN
1	B	325	GLN
1	B	377	HIS
1	B	415	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	419/421 (99%)	0.23	28 (6%) 24 21	26, 39, 61, 81	0
1	B	412/421 (97%)	0.44	36 (8%) 16 13	27, 50, 82, 86	0
All	All	831/842 (98%)	0.33	64 (7%) 19 17	26, 42, 78, 86	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	VAL	8.9
1	B	288	GLU	6.4
1	A	329	GLY	5.5
1	A	331	THR	5.3
1	A	328	TYR	5.2
1	A	321	LEU	4.7
1	A	330	ALA	4.7
1	B	235	LYS	4.1
1	B	289	THR	3.8
1	A	322	ALA	3.7
1	A	332	GLU	3.5
1	A	239	SER	3.5
1	A	324	ILE	3.5
1	B	331	THR	3.3
1	B	234	ALA	3.3
1	B	287	SER	3.3
1	B	384	PRO	3.1
1	A	318	THR	3.1
1	A	327	GLN	3.1
1	A	251	ARG	3.0
1	A	0	GLY	2.9
1	A	261	GLN	2.9
1	B	251	ARG	2.9
1	A	307	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	419	GLN	2.8
1	B	308	LEU	2.8
1	B	416	ARG	2.8
1	A	236	HIS	2.7
1	B	243	SER	2.7
1	B	292	ALA	2.7
1	B	319	GLN	2.7
1	A	242	ARG	2.6
1	B	302	LEU	2.6
1	B	307	GLU	2.6
1	B	407	ASP	2.6
1	B	326	GLN	2.5
1	B	286	SER	2.5
1	B	405	PHE	2.5
1	B	305	ASP	2.4
1	B	335	HIS	2.4
1	B	143	HIS	2.4
1	A	238	VAL	2.4
1	B	395	PRO	2.3
1	B	406	GLY	2.3
1	B	77	GLN	2.2
1	B	403	GLY	2.2
1	B	1	MET	2.2
1	A	369	GLN	2.2
1	A	323	ALA	2.2
1	A	319	GLN	2.2
1	B	190	GLN	2.2
1	B	261	GLN	2.2
1	A	259	CYS	2.1
1	B	227	MET	2.1
1	B	362	GLU	2.1
1	B	32	ASN	2.1
1	B	10	ASP	2.1
1	B	350	GLU	2.1
1	A	143	HIS	2.1
1	A	176	GLU	2.0
1	B	413	ARG	2.0
1	A	317	SER	2.0
1	A	325	GLN	2.0
1	A	237	GLY	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.