



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 6LBS / pdb_00006lbs
Title : Crystal structure of yeast Stn1
Authors : Ge, Y.; Wu, Z.; Wu, J.; Lei, M.
Deposited on : 2019-11-14
Resolution : 2.60 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

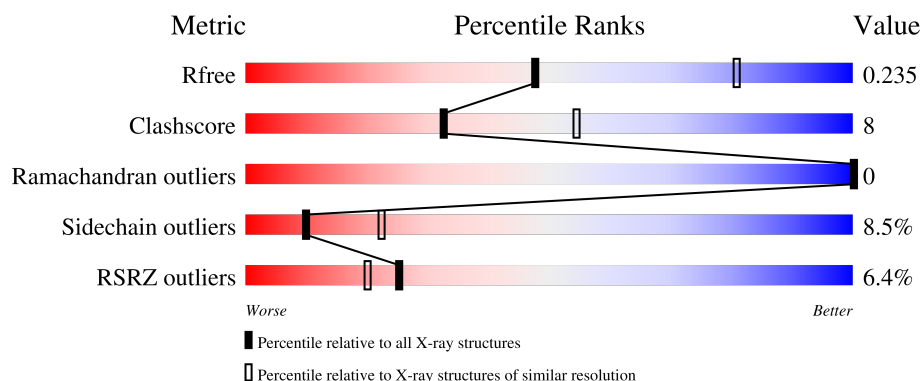
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	166	
1	B	166	
1	C	166	
1	D	166	
1	E	166	

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Mol	Chain	Length	Quality of chain
1	F	166	4% 68% 16% 5% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7463 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 KLLA0C11825p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	Se	0	0	0
			1227	806	199	213	4	5			
1	B	146	Total	C	N	O	S	Se	0	0	0
			1217	799	198	211	4	5			
1	C	144	Total	C	N	O	S	Se	0	0	0
			1191	782	194	206	4	5			
1	D	150	Total	C	N	O	S	Se	0	0	0
			1245	818	203	215	4	5			
1	E	148	Total	C	N	O	S	Se	0	0	0
			1228	806	200	213	4	5			
1	F	148	Total	C	N	O	S	Se	0	0	0
			1229	807	200	213	4	5			

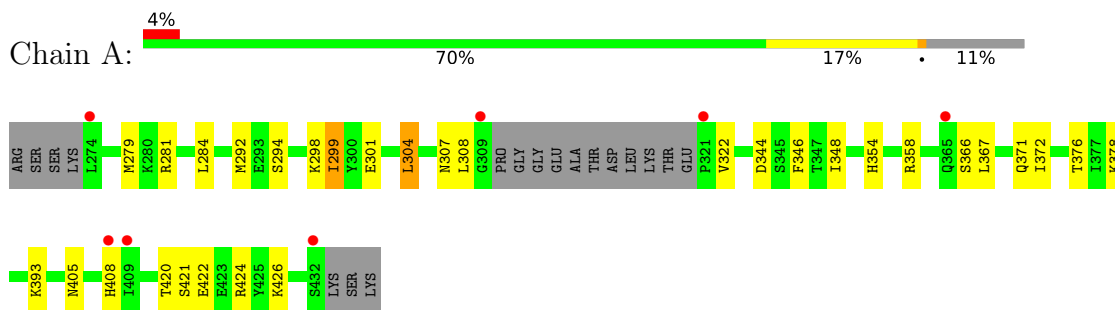
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	13	Total	O	0	0
			13	13		
2	C	10	Total	O	0	0
			10	10		
2	D	29	Total	O	0	0
			29	29		
2	E	25	Total	O	0	0
			25	25		
2	F	36	Total	O	0	0
			36	36		

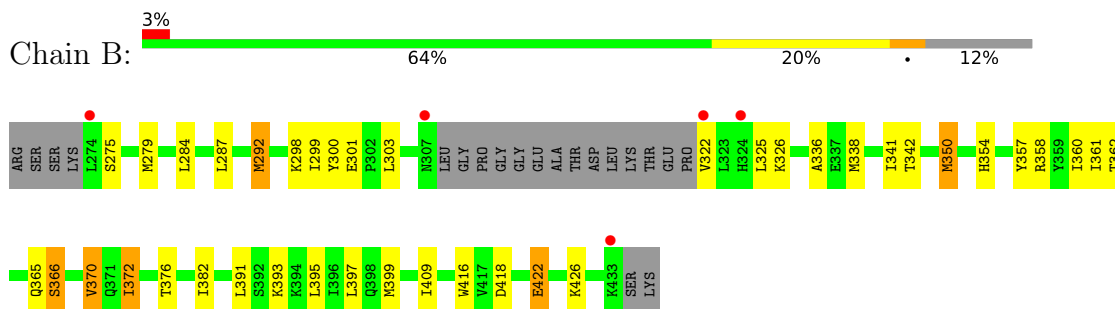
3 Residue-property plots

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.

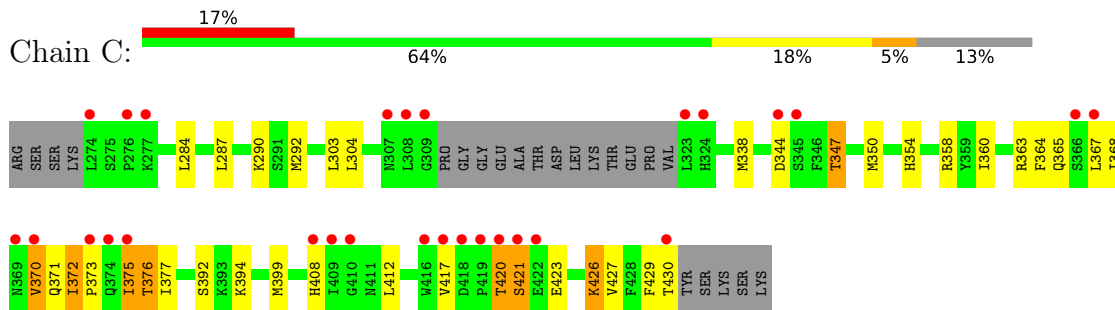
- Molecule 1: KLLA0C11825p



- Molecule 1: KLLA0C11825p

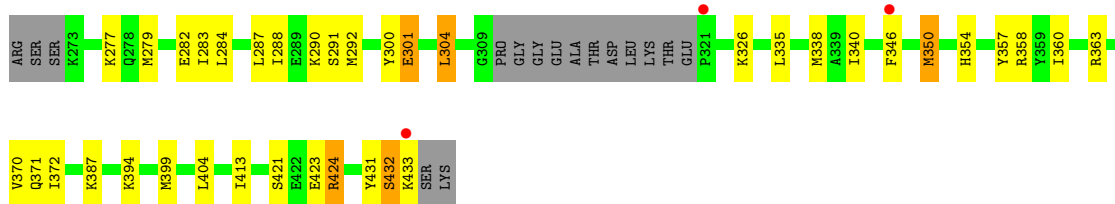


- Molecule 1: KLLA0C11825p

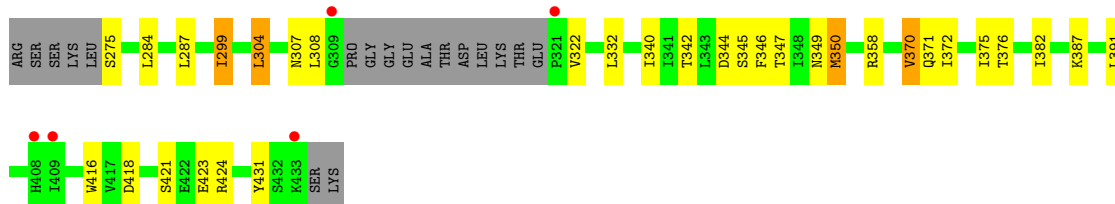


- Molecule 1: KLLA0C11825p

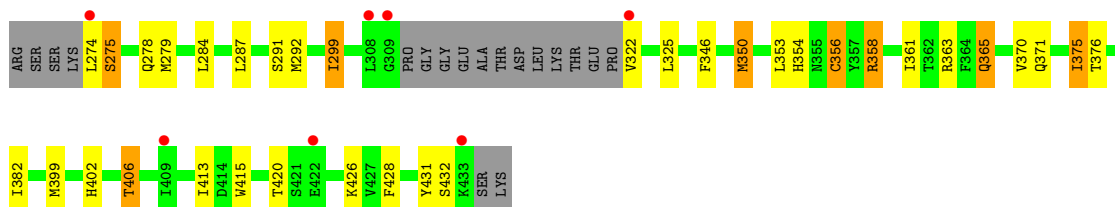




● Molecule 1: KLLA0C11825p



● Molecule 1: KLLA0C11825p



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.43Å 94.75Å 97.50Å 90.00° 96.26° 90.00°	Depositor
Resolution (Å)	37.95 – 2.60 37.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.95-2.60) 97.1 (37.95-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.183 , 0.235 0.184 , 0.235	Depositor DCC
R_{free} test set	2114 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.9	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	7463	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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	0.35	0/1249	0.57	0/1678
1	B	0.37	0/1238	0.61	0/1662
1	C	0.36	0/1211	0.80	4/1626 (0.2%)
1	D	0.40	0/1267	0.56	0/1700
1	E	0.36	0/1250	0.65	2/1678 (0.1%)
1	F	0.42	0/1250	0.61	0/1678
All	All	0.38	0/7465	0.64	6/10022 (0.1%)

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	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	THR	N-CA-C	12.35	126.47	111.40
1	E	308	LEU	N-CA-C	8.70	122.46	111.24
1	C	370	VAL	CB-CA-C	7.92	118.54	110.70
1	C	420	THR	CB-CA-C	-6.69	99.55	110.79
1	C	421	SER	N-CA-C	-6.62	100.15	110.42
1	E	308	LEU	CB-CA-C	-5.59	101.64	110.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	432	SER	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	1227	0	1277	18	0
1	B	1217	0	1268	23	0
1	C	1191	0	1240	21	0
1	D	1245	0	1303	26	0
1	E	1228	0	1279	17	0
1	F	1229	0	1282	18	0
2	A	13	0	0	1	0
2	B	13	0	0	1	0
2	C	10	0	0	3	0
2	D	29	0	0	0	0
2	E	25	0	0	0	0
2	F	36	0	0	0	0
All	All	7463	0	7649	118	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 8.

All (118) 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:F:292:MSE:HE1	1:F:354:HIS:HA	1.56	0.88
1:D:292:MSE:HE1	1:D:354:HIS:HA	1.65	0.79
1:B:292:MSE:HE1	1:B:354:HIS:HA	1.65	0.78
1:C:360:ILE:HD12	1:C:399:MSE:HE2	1.69	0.74
1:B:287:LEU:HD22	1:B:350:MSE:HE1	1.69	0.73
1:E:287:LEU:HD22	1:E:350:MSE:HE1	1.77	0.66
1:E:344:ASP:HB3	1:E:346:PHE:H	1.61	0.66
1:D:421:SER:HB2	1:D:424:ARG:H	1.64	0.63
1:A:393:LYS:NZ	1:A:422:GLU:OE1	2.34	0.61
1:D:360:ILE:HD12	1:D:399:MSE:HE2	1.83	0.60
1:B:382:ILE:H	1:B:382:ILE:HD12	1.66	0.60
1:D:432:SER:O	1:D:433:LYS:HB2	2.03	0.59
1:D:287:LEU:HB3	1:D:350:MSE:HE1	1.85	0.59
1:D:300:TYR:HD1	1:D:304:LEU:HD22	1.68	0.58
1:F:299:ILE:HG13	1:F:346:PHE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:SER:OG	1:F:292:MSE:HE2	2.06	0.56
1:C:363:ARG:HH21	1:C:377:ILE:HG12	1.70	0.56
1:C:290:LYS:NZ	2:C:502:HOH:O	2.39	0.55
1:F:287:LEU:HB3	1:F:350:MSE:HE1	1.89	0.55
1:C:376:THR:HG23	1:C:426:LYS:HG2	1.88	0.55
1:F:356:CYS:HB3	1:F:399:MSE:HE1	1.89	0.55
1:D:290:LYS:HE3	1:D:301:GLU:OE2	2.06	0.54
1:A:304:LEU:HD12	1:B:300:TYR:HB3	1.89	0.54
1:C:287:LEU:HD22	1:C:350:MSE:CE	2.38	0.54
1:A:299:ILE:HD11	1:A:344:ASP:O	2.08	0.53
1:B:393:LYS:NZ	1:B:422:GLU:O	2.27	0.53
1:A:304:LEU:HD11	1:B:299:ILE:HG22	1.91	0.53
1:D:413:ILE:HG21	1:D:432:SER:HB3	1.91	0.52
1:B:370:VAL:HG12	1:B:372:ILE:HG12	1.91	0.52
1:A:298:LYS:HB2	1:A:301:GLU:HG3	1.91	0.52
1:A:367:LEU:HD23	1:A:372:ILE:HD13	1.92	0.52
1:C:303:LEU:HD23	1:D:304:LEU:HD21	1.92	0.51
1:E:344:ASP:HB3	1:E:347:THR:H	1.76	0.51
1:E:342:THR:OG1	1:E:349:ASN:HB3	2.11	0.51
1:A:421:SER:HB3	1:A:424:ARG:HB2	1.93	0.50
1:D:288:ILE:HD11	1:D:399:MSE:HG2	1.93	0.50
1:C:338:MSE:SE	1:C:392:SER:HB3	2.61	0.50
1:B:365:GLN:NE2	1:B:409:ILE:HB	2.26	0.50
1:C:292:MSE:HE1	1:C:354:HIS:HA	1.93	0.50
1:C:367:LEU:HD21	1:C:375:ILE:HD13	1.94	0.49
1:E:421:SER:HB2	1:E:424:ARG:H	1.77	0.49
1:B:416:TRP:CZ3	1:B:418:ASP:HB2	2.47	0.49
1:D:287:LEU:HD22	1:D:350:MSE:HE1	1.94	0.48
1:D:413:ILE:HD13	1:D:432:SER:HB3	1.95	0.48
1:A:292:MSE:HE1	1:A:354:HIS:HA	1.94	0.48
1:B:391:LEU:HD22	1:B:395:LEU:HD23	1.95	0.48
1:E:340:ILE:HD12	1:E:391:LEU:HD21	1.95	0.48
1:C:368:ILE:C	1:C:370:VAL:H	2.21	0.48
1:F:415:TRP:HA	1:F:428:PHE:O	2.13	0.48
1:C:417:VAL:HA	1:C:427:VAL:HG12	1.96	0.48
1:A:420:THR:OG1	1:A:421:SER:N	2.46	0.48
1:F:375:ILE:HG13	1:F:376:THR:N	2.29	0.48
1:C:430:THR:C	2:C:505:HOH:O	2.57	0.47
1:F:371:GLN:HA	1:F:431:TYR:CZ	2.49	0.47
1:D:292:MSE:HE3	1:D:357:TYR:HB3	1.96	0.47
1:A:307:ASN:O	1:A:308:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ILE:HD12	1:E:382:ILE:H	1.78	0.47
1:F:275:SER:HB3	1:F:278:GLN:OE1	2.15	0.47
1:D:291:SER:OG	1:D:292:MSE:HE2	2.15	0.47
1:E:299:ILE:HD11	1:E:345:SER:C	2.39	0.47
1:F:402:HIS:O	1:F:406:THR:HB	2.16	0.46
1:E:416:TRP:CZ3	1:E:418:ASP:HB2	2.51	0.46
1:C:344:ASP:HB2	1:C:347:THR:OG1	2.14	0.46
1:A:299:ILE:HG13	1:A:346:PHE:C	2.40	0.46
1:B:322:VAL:N	2:B:501:HOH:O	2.49	0.46
1:B:336:ALA:HA	1:B:341:ILE:O	2.16	0.46
1:A:299:ILE:HD13	1:A:299:ILE:HG21	1.59	0.46
1:B:350:MSE:HE2	1:B:350:MSE:HB3	1.81	0.46
1:C:304:LEU:HD12	1:C:304:LEU:HA	1.74	0.45
1:A:378:LYS:HE3	1:A:424:ARG:HH21	1.81	0.45
1:C:412:LEU:CD1	1:C:429:PHE:HB3	2.46	0.45
1:E:307:ASN:OD1	1:E:322:VAL:HB	2.15	0.45
1:E:375:ILE:HG13	1:E:376:THR:N	2.32	0.45
1:E:421:SER:HB3	1:E:423:GLU:H	1.82	0.45
1:C:412:LEU:HD11	1:C:429:PHE:HB3	1.98	0.45
1:B:360:ILE:HD12	1:B:399:MSE:HE2	2.00	0.44
1:F:358:ARG:HH21	1:F:361:ILE:HG21	1.82	0.44
1:C:363:ARG:NH2	1:C:377:ILE:HG12	2.32	0.44
1:D:421:SER:HB2	1:D:423:GLU:H	1.83	0.44
1:F:420:THR:HG21	1:F:426:LYS:HE3	2.00	0.44
1:A:376:THR:OG1	1:A:426:LYS:HG2	2.18	0.44
1:D:300:TYR:CD1	1:D:304:LEU:HD22	2.51	0.44
1:B:372:ILE:HD13	1:B:372:ILE:HA	1.72	0.43
1:D:371:GLN:HA	1:D:431:TYR:CZ	2.53	0.43
1:F:361:ILE:O	1:F:365:GLN:HB2	2.17	0.43
1:E:287:LEU:HB3	1:E:350:MSE:HE1	2.00	0.43
1:C:364:PHE:HE2	1:C:427:VAL:HG21	1.83	0.43
1:C:421:SER:C	1:C:423:GLU:H	2.26	0.43
1:D:292:MSE:CE	1:D:354:HIS:HA	2.42	0.43
1:F:350:MSE:HE2	1:F:350:MSE:HB3	1.93	0.43
1:E:371:GLN:HA	1:E:431:TYR:CZ	2.54	0.43
1:E:304:LEU:HB3	1:F:325:LEU:CD1	2.49	0.43
1:B:298:LYS:HB2	1:B:301:GLU:HG3	2.00	0.42
1:B:338:MSE:CE	1:B:395:LEU:HD22	2.49	0.42
1:F:279:MSE:HE1	1:F:322:VAL:HG12	2.00	0.42
1:F:350:MSE:HE2	1:F:353:LEU:HD23	2.00	0.42
1:D:421:SER:HB2	1:D:424:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LEU:HD21	1:B:325:LEU:HD23	2.00	0.42
1:D:287:LEU:CB	1:D:350:MSE:HE1	2.49	0.42
1:D:350:MSE:HE2	1:D:350:MSE:HB3	1.72	0.42
1:A:279:MSE:HE1	1:A:322:VAL:HG12	2.01	0.42
1:B:357:TYR:CE2	1:B:361:ILE:HD11	2.55	0.42
1:F:299:ILE:HG13	1:F:299:ILE:H	1.46	0.41
1:B:376:THR:OG1	1:B:426:LYS:HE2	2.19	0.41
1:C:372:ILE:HG23	1:C:373:PRO:HD2	2.03	0.41
1:E:370:VAL:HG12	1:E:372:ILE:HG12	2.02	0.41
1:D:279:MSE:O	1:D:283:ILE:HG13	2.20	0.41
1:E:332:LEU:HD23	1:E:332:LEU:HA	1.84	0.41
1:D:404:LEU:HA	1:D:404:LEU:HD23	1.78	0.41
1:D:304:LEU:HD12	1:D:304:LEU:HA	1.82	0.41
1:B:362:THR:O	1:B:366:SER:HB3	2.20	0.41
1:A:344:ASP:HB3	2:A:512:HOH:O	2.21	0.40
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.81	0.40
1:D:290:LYS:HE3	1:D:301:GLU:CD	2.46	0.40
1:A:299:ILE:HA	1:A:348:ILE:HG13	2.04	0.40
1:A:308:LEU:HD11	1:B:303:LEU:HD21	2.02	0.40
1:D:335:LEU:HA	1:D:338:MSE:HE3	2.04	0.40
1:C:371:GLN:OE1	2:C:501:HOH:O	2.22	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	144/166 (87%)	138 (96%)	6 (4%)	0	100	100
1	B	142/166 (86%)	135 (95%)	7 (5%)	0	100	100
1	C	140/166 (84%)	128 (91%)	12 (9%)	0	100	100
1	D	146/166 (88%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	144/166 (87%)	140 (97%)	4 (3%)	0	100	100
1	F	144/166 (87%)	138 (96%)	6 (4%)	0	100	100
All	All	860/996 (86%)	820 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	142/152 (93%)	132 (93%)	10 (7%)	14	31
1	B	141/152 (93%)	129 (92%)	12 (8%)	10	22
1	C	137/152 (90%)	126 (92%)	11 (8%)	11	25
1	D	144/152 (95%)	128 (89%)	16 (11%)	6	12
1	E	142/152 (93%)	134 (94%)	8 (6%)	19	40
1	F	142/152 (93%)	127 (89%)	15 (11%)	6	14
All	All	848/912 (93%)	776 (92%)	72 (8%)	10	22

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	A	284	LEU
1	A	294	SER
1	A	299	ILE
1	A	304	LEU
1	A	358	ARG
1	A	366	SER
1	A	371	GLN
1	A	405	ASN
1	A	408	HIS
1	B	275	SER
1	B	279	MSE

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	292	MSE
1	B	326	LYS
1	B	342	THR
1	B	350	MSE
1	B	358	ARG
1	B	366	SER
1	B	370	VAL
1	B	372	ILE
1	B	422	GLU
1	C	284	LEU
1	C	347	THR
1	C	358	ARG
1	C	365	GLN
1	C	372	ILE
1	C	375	ILE
1	C	376	THR
1	C	394	LYS
1	C	408	HIS
1	C	420	THR
1	C	426	LYS
1	D	277	LYS
1	D	282	GLU
1	D	284	LEU
1	D	301	GLU
1	D	304	LEU
1	D	326	LYS
1	D	340	ILE
1	D	346	PHE
1	D	350	MSE
1	D	358	ARG
1	D	363	ARG
1	D	370	VAL
1	D	372	ILE
1	D	387	LYS
1	D	394	LYS
1	D	424	ARG
1	E	275	SER
1	E	284	LEU
1	E	299	ILE
1	E	304	LEU
1	E	350	MSE

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Mol	Chain	Res	Type
1	E	358	ARG
1	E	370	VAL
1	E	387	LYS
1	F	274	LEU
1	F	275	SER
1	F	284	LEU
1	F	299	ILE
1	F	350	MSE
1	F	356	CYS
1	F	358	ARG
1	F	363	ARG
1	F	365	GLN
1	F	370	VAL
1	F	375	ILE
1	F	382	ILE
1	F	406	THR
1	F	413	ILE
1	F	432	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	398	GLN
1	D	334	GLN
1	E	334	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 oligosaccharides 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, 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	143/166 (86%)	-0.13	7 (4%) 35 29	24, 43, 83, 114	0
1	B	141/166 (84%)	-0.12	5 (3%) 47 41	25, 41, 82, 123	0
1	C	139/166 (83%)	0.75	28 (20%) 3 2	26, 56, 111, 136	0
1	D	145/166 (87%)	-0.44	3 (2%) 63 58	20, 33, 66, 105	0
1	E	143/166 (86%)	-0.24	5 (3%) 47 41	23, 39, 70, 109	0
1	F	143/166 (86%)	-0.36	7 (4%) 35 29	17, 33, 78, 130	0
All	All	854/996 (85%)	-0.10	55 (6%) 25 20	17, 40, 89, 136	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	LEU	6.5
1	B	274	LEU	5.8
1	D	321	PRO	5.4
1	B	322	VAL	5.3
1	F	308	LEU	5.2
1	C	417	VAL	5.0
1	C	308	LEU	4.7
1	A	274	LEU	4.7
1	F	309	GLY	4.7
1	E	321	PRO	4.3
1	D	433	LYS	4.2
1	B	433	LYS	4.2
1	C	420	THR	4.2
1	C	307	ASN	4.0
1	E	409	ILE	3.8
1	C	345	SER	3.8
1	F	274	LEU	3.8
1	C	370	VAL	3.8
1	C	274	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	309	GLY	3.8
1	C	277	LYS	3.6
1	A	309	GLY	3.5
1	C	409	ILE	3.4
1	F	409	ILE	3.4
1	C	324	HIS	3.1
1	F	322	VAL	3.1
1	C	344	ASP	3.0
1	C	416	TRP	3.0
1	C	421	SER	3.0
1	C	408	HIS	2.9
1	C	276	PRO	2.9
1	C	375	ILE	2.9
1	C	374	GLN	2.8
1	C	418	ASP	2.7
1	E	433	LYS	2.7
1	C	373	PRO	2.6
1	A	408	HIS	2.6
1	A	365	GLN	2.6
1	C	430	THR	2.5
1	E	408	HIS	2.5
1	D	346	PHE	2.5
1	C	410	GLY	2.4
1	C	419	PRO	2.3
1	B	324	HIS	2.3
1	C	422	GLU	2.3
1	F	433	LYS	2.2
1	E	309	GLY	2.2
1	F	422	GLU	2.2
1	C	366	SER	2.2
1	A	432	SER	2.1
1	A	409	ILE	2.1
1	B	307	ASN	2.0
1	A	321	PRO	2.0
1	C	367	LEU	2.0
1	C	369	ASN	2.0

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 [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.