



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:32 PM UTC

PDB ID : 4Q5Y / pdb_00004q5y
Title : Crystal structure of extended-Tudor 10-11 of Drosophila melanogaster
Authors : Liu, H.; Ren, R.; Wang, W.; Wang, M.; Yang, N.; Dong, Y.; Gong, W.;
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Deposited on : 2014-04-18
Resolution : 3.00 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

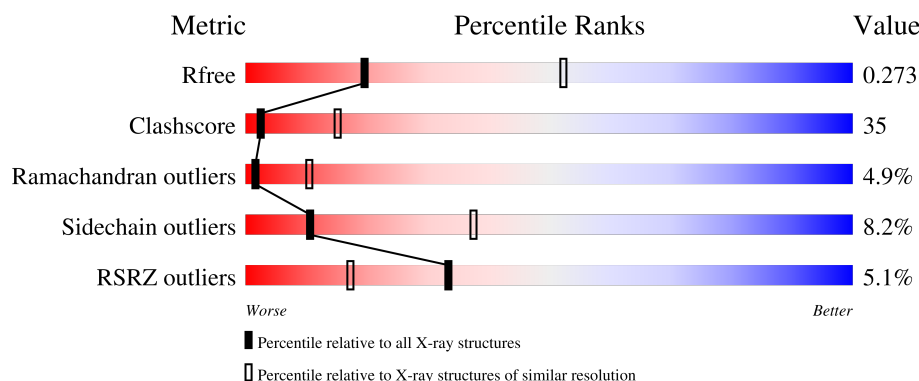
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	355	5% 46% 45% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2729 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 Maternal protein tudor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2673	1695	437	527	14	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2161	SER	-	expression tag	UNP P25823
A	2162	GLU	-	expression tag	UNP P25823
A	2163	PHE	-	expression tag	UNP P25823

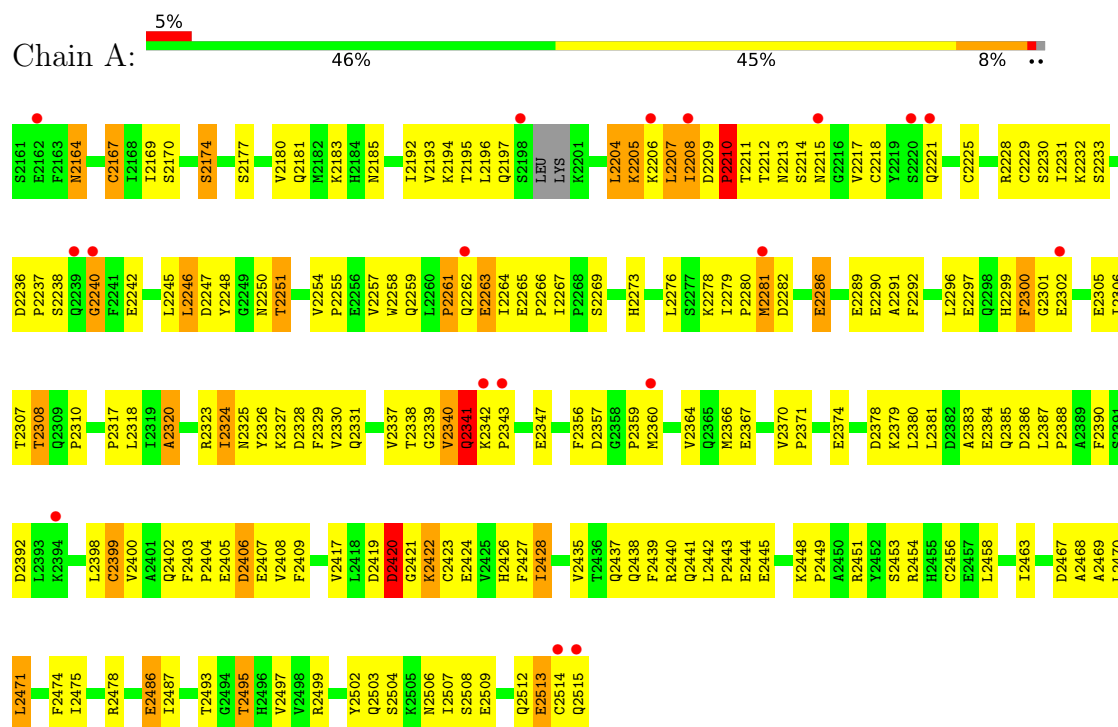
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		

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: Maternal protein tudor



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.25Å 125.44Å 151.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 97.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.271 0.240 , 0.273	Depositor DCC
R_{free} test set	676 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	86.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2729	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.53	0/2726	1.04	18/3715 (0.5%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2497	VAL	N-CA-C	-8.04	96.25	107.99
1	A	2246	LEU	N-CA-C	6.51	118.38	111.28
1	A	2286	GLU	N-CA-C	-6.46	104.24	111.28
1	A	2183	LYS	N-CA-C	-6.06	105.14	112.54
1	A	2486	GLU	N-CA-C	-5.87	99.68	109.24
1	A	2453	SER	N-CA-C	-5.84	100.19	109.59
1	A	2420	ASP	N-CA-C	5.83	123.22	110.80
1	A	2499	ARG	N-CA-C	-5.64	99.98	109.07
1	A	2421	GLY	N-CA-C	-5.54	100.05	113.18
1	A	2424	GLU	N-CA-C	-5.49	100.29	109.24
1	A	2221	GLN	N-CA-C	-5.49	105.20	111.07
1	A	2456	CYS	N-CA-C	5.49	117.32	109.14
1	A	2167	CYS	N-CA-C	5.38	115.22	108.45
1	A	2263	GLU	N-CA-C	-5.36	99.39	110.80
1	A	2320	ALA	N-CA-C	5.25	118.12	109.72
1	A	2279	ILE	CA-C-N	5.24	126.39	119.84
1	A	2279	ILE	C-N-CA	5.24	126.39	119.84
1	A	2232	LYS	N-CA-C	-5.03	106.84	113.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2673	0	2473	179	0
2	A	56	0	0	10	0
All	All	2729	0	2473	179	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 35.

All (179) 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:A:2306:ILE:HD11	1:A:2320:ALA:HB1	1.25	1.08
1:A:2342:LYS:HG3	1:A:2343:PRO:HD2	1.34	1.03
1:A:2506:ASN:HB3	1:A:2509:GLU:HG3	1.49	0.95
1:A:2205:LYS:HD3	1:A:2259:GLN:CB	2.00	0.91
1:A:2428:ILE:HB	1:A:2451:ARG:HH12	1.39	0.88
1:A:2419:ASP:O	1:A:2420:ASP:HB3	1.74	0.86
1:A:2328:ASP:HB3	1:A:2331:GLN:HG2	1.62	0.81
1:A:2300:PHE:O	1:A:2302:GLU:N	2.14	0.80
1:A:2506:ASN:HD22	1:A:2507:ILE:N	1.80	0.80
1:A:2419:ASP:O	1:A:2420:ASP:CB	2.29	0.79
1:A:2230:SER:HB2	1:A:2246:LEU:HD21	1.64	0.78
1:A:2205:LYS:CG	1:A:2206:LYS:H	1.96	0.77
1:A:2428:ILE:HB	1:A:2451:ARG:NH1	2.00	0.77
1:A:2205:LYS:HG2	1:A:2206:LYS:H	1.47	0.76
1:A:2207:LEU:HD22	1:A:2208:ILE:HG12	1.69	0.73
1:A:2342:LYS:CG	1:A:2343:PRO:HD2	2.16	0.73
1:A:2340:VAL:HG12	1:A:2341:GLN:O	1.88	0.72
1:A:2245:LEU:HD12	1:A:2250:ASN:HB2	1.73	0.71
1:A:2402:GLN:HB2	1:A:2409:PHE:CE1	2.26	0.70
1:A:2264:ILE:C	1:A:2266:PRO:HD2	2.17	0.69
1:A:2474:PHE:O	1:A:2478:ARG:HD2	1.91	0.69
1:A:2493:THR:OG1	1:A:2495:THR:HG23	1.93	0.69
1:A:2266:PRO:HG2	1:A:2267:ILE:HD12	1.75	0.69
1:A:2390:PHE:HB3	1:A:2439:PHE:HB3	1.72	0.69
1:A:2205:LYS:HG2	1:A:2206:LYS:N	2.08	0.68
1:A:2403:PHE:CD2	1:A:2406:ASP:HB2	2.29	0.67
1:A:2286:GLU:O	1:A:2290:GLU:HG3	1.95	0.67
1:A:2209:ASP:O	1:A:2211:THR:HG23	1.95	0.67
1:A:2324:ILE:C	1:A:2324:ILE:HD13	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2359:PRO:HG3	1:A:2471:LEU:HD12	1.76	0.66
1:A:2192:ILE:HG23	1:A:2228:ARG:HD2	1.78	0.65
1:A:2192:ILE:O	1:A:2196:LEU:HB2	1.96	0.65
1:A:2194:LYS:C	1:A:2196:LEU:H	2.04	0.64
1:A:2502:TYR:CD2	1:A:2503:GLN:HG3	2.32	0.63
1:A:2342:LYS:HG3	1:A:2343:PRO:CD	2.20	0.62
1:A:2423:CYS:HB2	1:A:2439:PHE:HZ	1.64	0.62
1:A:2423:CYS:O	1:A:2435:VAL:HG13	1.99	0.62
1:A:2192:ILE:CG2	1:A:2228:ARG:HD2	2.30	0.62
1:A:2218:CYS:HB2	1:A:2254:VAL:HG21	1.81	0.62
1:A:2228:ARG:NH2	1:A:2267:ILE:O	2.33	0.62
1:A:2327:LYS:HD2	2:A:2649:HOH:O	2.00	0.61
1:A:2426:HIS:HE1	1:A:2451:ARG:HH22	1.47	0.61
1:A:2217:VAL:HG12	1:A:2218:CYS:N	2.15	0.61
1:A:2512:GLN:O	1:A:2513:GLU:CB	2.49	0.61
1:A:2207:LEU:HB2	1:A:2210:PRO:HG3	1.81	0.60
1:A:2292:PHE:CE2	1:A:2296:LEU:HD11	2.36	0.60
1:A:2276:LEU:HD11	1:A:2329:PHE:HD2	1.67	0.60
1:A:2403:PHE:HD2	1:A:2406:ASP:HB2	1.65	0.60
1:A:2324:ILE:HD13	1:A:2325:ASN:HB2	1.84	0.59
1:A:2170:SER:OG	1:A:2181:GLN:HG3	2.03	0.59
1:A:2512:GLN:O	1:A:2512:GLN:HG3	2.04	0.58
1:A:2338:THR:C	1:A:2340:VAL:H	2.11	0.58
1:A:2267:ILE:HD12	1:A:2267:ILE:H	1.68	0.58
1:A:2205:LYS:CG	1:A:2206:LYS:N	2.60	0.57
1:A:2169:ILE:HD12	1:A:2296:LEU:HD22	1.87	0.56
1:A:2276:LEU:HD11	1:A:2329:PHE:CD2	2.41	0.56
1:A:2380:LEU:O	1:A:2384:GLU:N	2.38	0.56
1:A:2444:GLU:HG2	2:A:2636:HOH:O	2.04	0.56
1:A:2212:THR:HG22	1:A:2213:ASN:CG	2.30	0.56
1:A:2420:ASP:C	1:A:2420:ASP:OD1	2.49	0.56
1:A:2448:LYS:HB2	1:A:2449:PRO:HD3	1.86	0.55
1:A:2356:PHE:HZ	1:A:2471:LEU:HD13	1.71	0.55
1:A:2356:PHE:CZ	1:A:2471:LEU:HD13	2.40	0.55
1:A:2326:TYR:CE1	1:A:2366:MET:HG3	2.42	0.55
1:A:2423:CYS:HB2	1:A:2439:PHE:CZ	2.42	0.55
1:A:2325:ASN:HA	2:A:2629:HOH:O	2.06	0.54
1:A:2225:CYS:CB	2:A:2640:HOH:O	2.56	0.54
1:A:2240:GLY:HA3	1:A:2254:VAL:O	2.07	0.54
1:A:2259:GLN:O	1:A:2261:PRO:HD3	2.07	0.54
1:A:2398:LEU:O	1:A:2399:CYS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2470:LEU:HD12	1:A:2470:LEU:H	1.72	0.54
1:A:2208:ILE:HG13	1:A:2208:ILE:O	2.08	0.54
1:A:2228:ARG:HD3	1:A:2247:ASP:OD2	2.08	0.53
1:A:2228:ARG:HE	1:A:2264:ILE:HG23	1.73	0.53
1:A:2204:LEU:O	1:A:2205:LYS:HB2	2.08	0.52
1:A:2402:GLN:HA	1:A:2408:VAL:O	2.10	0.52
1:A:2207:LEU:CB	1:A:2210:PRO:HG3	2.39	0.52
1:A:2267:ILE:HD12	1:A:2267:ILE:N	2.23	0.52
1:A:2400:VAL:HG12	1:A:2409:PHE:HB3	1.91	0.52
1:A:2388:PRO:HB2	1:A:2441:GLN:NE2	2.25	0.52
1:A:2478:ARG:HG2	1:A:2478:ARG:HH11	1.74	0.52
1:A:2370:VAL:O	1:A:2374:GLU:HG3	2.09	0.52
1:A:2383:ALA:O	1:A:2387:LEU:HG	2.09	0.52
1:A:2420:ASP:OD1	1:A:2437:GLN:NE2	2.43	0.51
1:A:2193:VAL:O	1:A:2196:LEU:HB3	2.11	0.51
1:A:2487:ILE:HD12	1:A:2487:ILE:N	2.26	0.51
1:A:2324:ILE:HD13	1:A:2325:ASN:N	2.24	0.51
1:A:2236:ASP:OD2	1:A:2238:SER:HB3	2.12	0.50
1:A:2342:LYS:CG	1:A:2343:PRO:CD	2.86	0.50
1:A:2167:CYS:HB2	1:A:2180:VAL:HG13	1.94	0.49
1:A:2403:PHE:HB2	1:A:2427:PHE:CZ	2.47	0.49
1:A:2408:VAL:HG12	1:A:2409:PHE:N	2.28	0.49
1:A:2471:LEU:O	1:A:2475:ILE:HG12	2.12	0.49
1:A:2230:SER:CB	1:A:2246:LEU:HD21	2.38	0.49
1:A:2422:LYS:HG3	1:A:2437:GLN:HE22	1.76	0.49
1:A:2177:SER:OG	1:A:2273:HIS:HE1	1.95	0.49
1:A:2265:GLU:N	1:A:2266:PRO:HD2	2.27	0.49
1:A:2261:PRO:O	1:A:2263:GLU:N	2.41	0.49
1:A:2328:ASP:HB3	1:A:2331:GLN:CG	2.40	0.49
1:A:2209:ASP:O	1:A:2210:PRO:C	2.56	0.49
1:A:2251:THR:O	1:A:2251:THR:HG22	2.12	0.48
1:A:2502:TYR:CE2	1:A:2503:GLN:HG3	2.48	0.48
1:A:2506:ASN:HD22	1:A:2506:ASN:C	2.17	0.48
1:A:2385:GLN:HG2	2:A:2634:HOH:O	2.13	0.48
1:A:2228:ARG:NH1	1:A:2247:ASP:OD1	2.47	0.48
1:A:2310:PRO:HA	1:A:2318:LEU:HD23	1.95	0.48
1:A:2164:ASN:HD21	1:A:2323:ARG:NH2	2.12	0.48
1:A:2417:VAL:HA	1:A:2423:CYS:SG	2.54	0.48
1:A:2281:MET:HG2	1:A:2282:ASP:N	2.28	0.47
1:A:2470:LEU:H	1:A:2470:LEU:CD1	2.26	0.47
1:A:2194:LYS:C	1:A:2196:LEU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2208:ILE:O	1:A:2209:ASP:C	2.56	0.47
1:A:2370:VAL:HB	1:A:2371:PRO:HD3	1.97	0.47
1:A:2378:ASP:O	1:A:2379:LYS:C	2.56	0.47
1:A:2364:VAL:HG23	1:A:2366:MET:HE2	1.96	0.47
1:A:2444:GLU:N	1:A:2444:GLU:OE1	2.48	0.47
1:A:2360:MET:HG2	2:A:2618:HOH:O	2.15	0.47
1:A:2402:GLN:HE21	1:A:2407:GLU:C	2.24	0.46
1:A:2454:ARG:HA	1:A:2454:ARG:HD3	1.71	0.46
1:A:2164:ASN:HB2	2:A:2639:HOH:O	2.14	0.46
1:A:2470:LEU:HD12	1:A:2470:LEU:N	2.31	0.46
1:A:2308:THR:CG2	1:A:2318:LEU:HB3	2.46	0.46
1:A:2445:GLU:H	1:A:2445:GLU:CD	2.23	0.46
1:A:2338:THR:C	1:A:2340:VAL:N	2.69	0.46
1:A:2194:LYS:O	1:A:2196:LEU:N	2.47	0.46
1:A:2237:PRO:O	1:A:2238:SER:C	2.59	0.46
1:A:2233:SER:HB2	1:A:2242:GLU:HB3	1.98	0.45
1:A:2506:ASN:HD22	1:A:2507:ILE:H	1.59	0.45
1:A:2442:LEU:HD12	1:A:2443:PRO:HD2	1.98	0.45
1:A:2207:LEU:HD13	1:A:2214:SER:HB3	1.99	0.45
1:A:2247:ASP:C	1:A:2248:TYR:CD2	2.95	0.45
1:A:2273:HIS:NE2	1:A:2317:PRO:HG3	2.32	0.45
1:A:2276:LEU:HD13	1:A:2330:VAL:CG1	2.47	0.45
1:A:2205:LYS:H	1:A:2258:TRP:HD1	1.65	0.44
1:A:2214:SER:HB2	1:A:2231:ILE:HD12	1.99	0.44
1:A:2217:VAL:HG12	1:A:2218:CYS:H	1.80	0.44
1:A:2257:VAL:HG23	1:A:2258:TRP:N	2.30	0.44
1:A:2451:ARG:HH11	1:A:2451:ARG:HB3	1.81	0.44
1:A:2467:ASP:CB	1:A:2470:LEU:HD13	2.48	0.44
1:A:2324:ILE:C	1:A:2324:ILE:CD1	2.89	0.44
1:A:2471:LEU:HD23	1:A:2471:LEU:HA	1.88	0.44
1:A:2246:LEU:HB3	1:A:2269:SER:HB3	1.98	0.43
1:A:2254:VAL:HG13	1:A:2255:PRO:HD2	1.99	0.43
1:A:2387:LEU:O	1:A:2440:ARG:HD3	2.18	0.43
1:A:2507:ILE:HG23	1:A:2508:SER:N	2.33	0.43
1:A:2212:THR:HG22	1:A:2213:ASN:ND2	2.33	0.43
1:A:2440:ARG:NH1	2:A:2643:HOH:O	2.50	0.43
1:A:2276:LEU:HD23	1:A:2276:LEU:HA	1.85	0.43
1:A:2194:LYS:HA	1:A:2197:GLN:OE1	2.18	0.43
1:A:2217:VAL:CG1	1:A:2218:CYS:N	2.80	0.43
1:A:2428:ILE:O	1:A:2451:ARG:HB2	2.19	0.43
1:A:2339:GLY:O	1:A:2340:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2400:VAL:CG1	1:A:2409:PHE:HB3	2.49	0.43
1:A:2356:PHE:CD1	1:A:2356:PHE:C	2.97	0.43
1:A:2174:SER:CB	1:A:2289:GLU:HG2	2.49	0.42
1:A:2276:LEU:HD13	1:A:2330:VAL:HG13	2.01	0.42
1:A:2257:VAL:O	1:A:2258:TRP:CD2	2.73	0.42
1:A:2340:VAL:C	1:A:2341:GLN:O	2.60	0.42
1:A:2422:LYS:CG	1:A:2437:GLN:HE22	2.33	0.42
1:A:2337:VAL:O	1:A:2337:VAL:CG1	2.68	0.42
1:A:2467:ASP:O	1:A:2468:ALA:C	2.62	0.42
1:A:2185:ASN:HA	2:A:2638:HOH:O	2.18	0.42
1:A:2215:ASN:OD1	1:A:2230:SER:HB2	2.19	0.41
1:A:2422:LYS:CG	1:A:2437:GLN:NE2	2.83	0.41
1:A:2438:GLN:C	1:A:2439:PHE:CD1	2.98	0.41
1:A:2467:ASP:C	1:A:2469:ALA:N	2.77	0.41
1:A:2514:CYS:O	1:A:2515:GLN:O	2.37	0.41
1:A:2338:THR:O	1:A:2340:VAL:N	2.40	0.41
1:A:2297:GLU:C	1:A:2299:HIS:H	2.27	0.41
1:A:2426:HIS:HE1	1:A:2451:ARG:NH2	2.17	0.41
1:A:2503:GLN:HG2	2:A:2601:HOH:O	2.20	0.41
1:A:2291:ALA:O	1:A:2292:PHE:C	2.62	0.41
1:A:2426:HIS:CE1	1:A:2451:ARG:HH22	2.34	0.41
1:A:2267:ILE:H	1:A:2267:ILE:CD1	2.33	0.40
1:A:2278:LYS:O	1:A:2330:VAL:HG11	2.21	0.40
1:A:2458:LEU:HB2	1:A:2463:ILE:HG13	2.03	0.40
1:A:2305:GLU:OE1	1:A:2323:ARG:NH2	2.50	0.40
1:A:2347:GLU:O	1:A:2486:GLU:HA	2.21	0.40
1:A:2402:GLN:HB3	1:A:2438:GLN:HB2	2.02	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	349/355 (98%)	286 (82%)	46 (13%)	17 (5%)	1	10

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2240	GLY
1	A	2262	GLN
1	A	2301	GLY
1	A	2513	GLU
1	A	2195	THR
1	A	2204	LEU
1	A	2205	LYS
1	A	2340	VAL
1	A	2392	ASP
1	A	2420	ASP
1	A	2210	PRO
1	A	2341	GLN
1	A	2404	PRO
1	A	2399	CYS
1	A	2208	ILE
1	A	2207	LEU
1	A	2280	PRO

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	279/322 (87%)	256 (92%)	23 (8%)	10	37

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

Mol	Chain	Res	Type
1	A	2164	ASN
1	A	2174	SER
1	A	2210	PRO
1	A	2229	CYS

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Mol	Chain	Res	Type
1	A	2251	THR
1	A	2261	PRO
1	A	2281	MET
1	A	2300	PHE
1	A	2307	THR
1	A	2308	THR
1	A	2324	ILE
1	A	2341	GLN
1	A	2357	ASP
1	A	2367	GLU
1	A	2381	LEU
1	A	2386	ASP
1	A	2405	GLU
1	A	2406	ASP
1	A	2422	LYS
1	A	2428	ILE
1	A	2471	LEU
1	A	2495	THR
1	A	2504	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2164	ASN
1	A	2250	ASN
1	A	2273	HIS
1	A	2275	GLN
1	A	2299	HIS
1	A	2355	GLN
1	A	2365	GLN
1	A	2402	GLN
1	A	2426	HIS
1	A	2432	ASN
1	A	2441	GLN
1	A	2472	GLN
1	A	2506	ASN
1	A	2512	GLN

5.3.3 RNA ⓘ

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	353/355 (99%)	0.30	18 (5%)	33 17	53, 88, 121, 136	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2198	SER	4.6
1	A	2239	GLN	3.8
1	A	2220	SER	3.6
1	A	2515	GLN	3.4
1	A	2343	PRO	3.2
1	A	2208	ILE	3.1
1	A	2281	MET	3.0
1	A	2514	CYS	3.0
1	A	2162	GLU	2.7
1	A	2240	GLY	2.7
1	A	2394	LYS	2.6
1	A	2342	LYS	2.6
1	A	2221	GLN	2.5
1	A	2262	GLN	2.4
1	A	2215	ASN	2.3
1	A	2206	LYS	2.2
1	A	2360	MET	2.2
1	A	2302	GLU	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.