



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:42 PM UTC

PDB ID : 3NOW / pdb_00003now
Title : UNC-45 from *Drosophila melanogaster*
Authors : Lee, C.F.; Hauenstein, A.V.; Fleming, J.K.; Gasper, W.C.; Engelke, V.; Banumathi, S.; Bernstein, S.I.; Huxford, T.
Deposited on : 2010-06-25
Resolution : 2.99 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

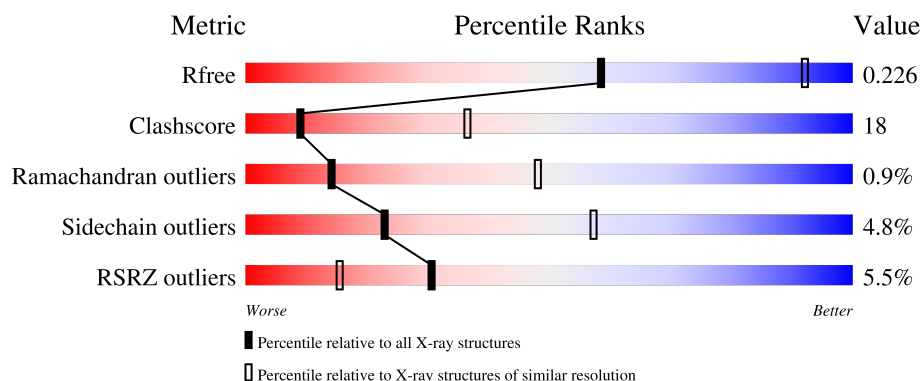
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	810	5% 64% 30% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6077 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.

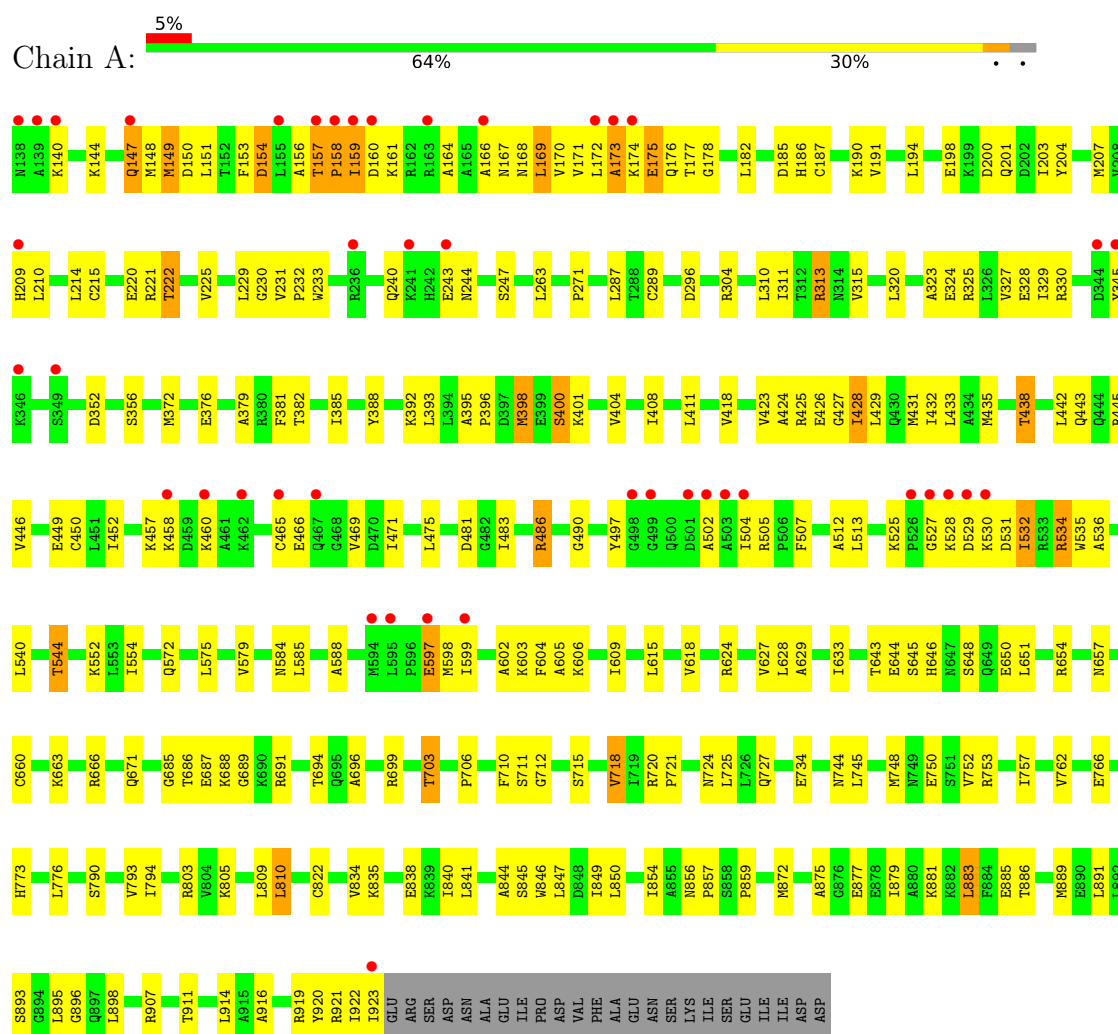
- Molecule 1 is a protein called UNC-45 protein, SD10334p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	786	6077	3805	1059	1166	47	0	0	0

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: UNC-45 protein, SD10334p



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	184.08Å 184.08Å 184.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.99 49.20 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.20-2.99) 93.3 (49.20-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.201 , 0.235 0.193 , 0.226	Depositor DCC
R_{free} test set	1999 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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	0.68	6/6145 (0.1%)	0.96	14/8296 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	LYS	CG-CD	6.05	1.70	1.52
1	A	149	MET	SD-CE	5.97	1.94	1.79
1	A	185	ASP	CG-OD2	5.82	1.36	1.25
1	A	147	GLN	CD-OE1	5.61	1.34	1.23
1	A	147	GLN	CG-CD	5.58	1.66	1.52
1	A	140	LYS	CD-CE	5.07	1.67	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	CA-C-N	8.20	127.88	119.19
1	A	525	LYS	C-N-CA	8.20	127.88	119.19
1	A	505	ARG	CA-C-N	7.53	127.46	119.85
1	A	505	ARG	C-N-CA	7.53	127.46	119.85
1	A	609	ILE	CA-C-N	6.94	128.51	119.84
1	A	609	ILE	C-N-CA	6.94	128.51	119.84
1	A	615	LEU	N-CA-C	6.36	119.03	111.71
1	A	597	GLU	N-CA-C	-6.17	101.15	110.28
1	A	428	ILE	N-CA-C	-5.94	104.31	113.16
1	A	159	ILE	N-CA-C	-5.62	105.96	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	THR	CA-C-N	5.51	126.73	119.84
1	A	157	THR	C-N-CA	5.51	126.73	119.84
1	A	898	LEU	CA-C-N	5.25	125.31	119.32
1	A	898	LEU	C-N-CA	5.25	125.31	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	529	ASP	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	6077	0	6234	226	0
All	All	6077	0	6234	226	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 18.

All (226) 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:425:ARG:HA	1:A:426:GLU:HB2	1.50	0.94
1:A:465:CYS:HA	1:A:469:VAL:HG23	1.51	0.92
1:A:148:MET:HE3	1:A:164:ALA:HA	1.56	0.88
1:A:400:SER:O	1:A:404:VAL:HG23	1.74	0.87
1:A:715:SER:HB2	1:A:748:MET:HE1	1.56	0.86
1:A:187:CYS:O	1:A:191:VAL:HG23	1.76	0.85
1:A:424:ALA:O	1:A:426:GLU:HA	1.77	0.84
1:A:889:MET:HE3	1:A:914:LEU:HD23	1.59	0.83
1:A:229:LEU:HD23	1:A:233:TRP:CD2	2.14	0.82
1:A:457:LYS:HD3	1:A:460:LYS:HG2	1.60	0.82
1:A:530:LYS:HG3	1:A:531:ASP:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD12	1:A:172:LEU:H	1.45	0.80
1:A:666:ARG:NH1	1:A:699:ARG:HB3	1.97	0.80
1:A:382:THR:HG22	1:A:418:VAL:HG13	1.64	0.79
1:A:173:ALA:O	1:A:175:GLU:N	2.15	0.79
1:A:544:THR:HG22	1:A:584:ASN:CB	2.13	0.79
1:A:147:GLN:O	1:A:151:LEU:HD13	1.83	0.78
1:A:645:SER:HB3	1:A:648:SER:HB2	1.65	0.77
1:A:530:LYS:HG3	1:A:531:ASP:N	1.97	0.76
1:A:534:ARG:HG2	1:A:534:ARG:HH11	1.50	0.76
1:A:686:THR:HG22	1:A:688:LYS:H	1.50	0.75
1:A:572:GLN:HE22	1:A:643:THR:HB	1.52	0.75
1:A:385:ILE:HG21	1:A:411:LEU:HD21	1.69	0.74
1:A:544:THR:HG22	1:A:584:ASN:HB3	1.67	0.74
1:A:502:ALA:C	1:A:504:ILE:H	1.97	0.73
1:A:660:CYS:O	1:A:666:ARG:NH1	2.22	0.73
1:A:431:MET:O	1:A:435:MET:HG3	1.89	0.73
1:A:745:LEU:HD23	1:A:748:MET:HE2	1.71	0.72
1:A:720:ARG:HB3	1:A:721:PRO:HD3	1.69	0.72
1:A:423:VAL:HA	1:A:428:ILE:HD11	1.72	0.71
1:A:599:ILE:HD12	1:A:599:ILE:H	1.56	0.70
1:A:182:LEU:O	1:A:187:CYS:HB2	1.92	0.69
1:A:404:VAL:O	1:A:408:ILE:HG12	1.92	0.69
1:A:850:LEU:O	1:A:854:ILE:HG13	1.93	0.69
1:A:544:THR:CG2	1:A:584:ASN:CB	2.70	0.69
1:A:840:ILE:HD12	1:A:872:MET:HE2	1.75	0.69
1:A:186:HIS:O	1:A:190:LYS:HG3	1.93	0.68
1:A:172:LEU:O	1:A:173:ALA:C	2.35	0.68
1:A:840:ILE:CD1	1:A:872:MET:HE2	2.24	0.68
1:A:172:LEU:HD23	1:A:214:LEU:HD21	1.76	0.67
1:A:393:LEU:O	1:A:396:PRO:HG3	1.95	0.67
1:A:231:VAL:N	1:A:232:PRO:HD2	2.10	0.66
1:A:324:GLU:O	1:A:327:VAL:HG12	1.95	0.66
1:A:345:TYR:CE2	1:A:442:LEU:HD13	2.31	0.66
1:A:544:THR:CG2	1:A:584:ASN:HB3	2.25	0.66
1:A:840:ILE:HG21	1:A:872:MET:HE1	1.76	0.66
1:A:745:LEU:HD23	1:A:748:MET:CE	2.26	0.65
1:A:168:ASN:O	1:A:171:VAL:HG12	1.96	0.65
1:A:540:LEU:O	1:A:544:THR:HB	1.96	0.65
1:A:686:THR:HG22	1:A:688:LYS:N	2.13	0.64
1:A:435:MET:O	1:A:438:THR:HG23	1.98	0.64
1:A:148:MET:CE	1:A:164:ALA:HA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:LEU:HD12	1:A:734:GLU:HB3	1.80	0.63
1:A:154:ASP:OD2	1:A:156:ALA:HB3	1.98	0.62
1:A:534:ARG:HH11	1:A:534:ARG:CG	2.12	0.62
1:A:304:ARG:NH1	1:A:352:ASP:O	2.31	0.62
1:A:164:ALA:O	1:A:168:ASN:N	2.31	0.62
1:A:229:LEU:HD23	1:A:233:TRP:CG	2.34	0.62
1:A:376:GLU:O	1:A:379:ALA:HB3	2.00	0.62
1:A:425:ARG:O	1:A:425:ARG:HG3	2.00	0.61
1:A:710:PHE:O	1:A:715:SER:HB3	2.00	0.60
1:A:449:GLU:OE2	1:A:486:ARG:NH1	2.34	0.60
1:A:896:GLY:O	1:A:907:ARG:HD3	2.01	0.60
1:A:229:LEU:N	1:A:229:LEU:HD12	2.17	0.60
1:A:748:MET:HE3	1:A:752:VAL:HG21	1.84	0.59
1:A:172:LEU:HG	1:A:182:LEU:HD13	1.85	0.58
1:A:423:VAL:HA	1:A:428:ILE:CD1	2.34	0.58
1:A:178:GLY:O	1:A:182:LEU:HD12	2.05	0.57
1:A:395:ALA:N	1:A:396:PRO:HD3	2.20	0.57
1:A:229:LEU:HD23	1:A:233:TRP:CE2	2.39	0.57
1:A:663:LYS:HA	1:A:666:ARG:HG3	1.86	0.57
1:A:172:LEU:HD12	1:A:172:LEU:N	2.18	0.56
1:A:877:GLU:HA	1:A:920:TYR:CE1	2.40	0.56
1:A:172:LEU:HD23	1:A:214:LEU:CD2	2.36	0.55
1:A:401:LYS:HE2	1:A:431:MET:HG3	1.88	0.55
1:A:172:LEU:HD22	1:A:210:LEU:HD12	1.89	0.55
1:A:169:LEU:HD13	1:A:209:HIS:HB3	1.89	0.55
1:A:544:THR:HG22	1:A:584:ASN:HD22	1.72	0.55
1:A:602:ALA:O	1:A:606:LYS:HE3	2.07	0.55
1:A:243:GLU:O	1:A:244:ASN:HB2	2.05	0.55
1:A:544:THR:CG2	1:A:584:ASN:HB2	2.37	0.54
1:A:194:LEU:O	1:A:198:GLU:HB2	2.08	0.54
1:A:287:LEU:HD23	1:A:325:ARG:HG3	1.90	0.54
1:A:445:ARG:HH11	1:A:445:ARG:HG2	1.73	0.54
1:A:554:ILE:HG12	1:A:624:ARG:HG2	1.89	0.53
1:A:215:CYS:HB3	1:A:222:THR:OG1	2.07	0.53
1:A:544:THR:HG22	1:A:584:ASN:ND2	2.23	0.53
1:A:465:CYS:O	1:A:466:GLU:C	2.51	0.53
1:A:167:ASN:O	1:A:170:VAL:HB	2.08	0.53
1:A:857:PRO:O	1:A:859:PRO:HD3	2.09	0.52
1:A:507:PHE:HB2	1:A:512:ALA:HB2	1.91	0.52
1:A:881:LYS:O	1:A:885:GLU:HG3	2.09	0.52
1:A:356:SER:HB3	1:A:572:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LEU:HD12	1:A:575:LEU:C	2.35	0.52
1:A:328:GLU:C	1:A:330:ARG:H	2.17	0.52
1:A:650:GLU:OE1	1:A:686:THR:HG21	2.09	0.52
1:A:176:GLN:C	1:A:178:GLY:N	2.68	0.52
1:A:172:LEU:H	1:A:172:LEU:CD1	2.20	0.51
1:A:773:HIS:HB3	1:A:776:LEU:HB2	1.91	0.51
1:A:502:ALA:C	1:A:504:ILE:N	2.61	0.51
1:A:606:LYS:HB2	1:A:773:HIS:CD2	2.45	0.51
1:A:753:ARG:O	1:A:757:ILE:HG13	2.11	0.51
1:A:597:GLU:O	1:A:598:MET:HB2	2.10	0.51
1:A:838:GLU:HG3	1:A:879:ILE:HD11	1.93	0.50
1:A:313:ARG:NH1	1:A:644:GLU:OE2	2.42	0.50
1:A:544:THR:CG2	1:A:544:THR:O	2.58	0.50
1:A:834:VAL:HG13	1:A:875:ALA:HB1	1.94	0.50
1:A:426:GLU:HG2	1:A:427:GLY:N	2.27	0.50
1:A:176:GLN:C	1:A:178:GLY:H	2.19	0.50
1:A:445:ARG:HG2	1:A:445:ARG:NH1	2.26	0.50
1:A:757:ILE:HD11	1:A:793:VAL:HG23	1.93	0.50
1:A:182:LEU:O	1:A:187:CYS:CB	2.60	0.50
1:A:544:THR:HG21	1:A:584:ASN:HB2	1.93	0.49
1:A:657:ASN:HA	1:A:696:ALA:HB2	1.93	0.49
1:A:424:ALA:C	1:A:426:GLU:HA	2.38	0.49
1:A:148:MET:HE2	1:A:167:ASN:OD1	2.13	0.48
1:A:426:GLU:O	1:A:427:GLY:C	2.54	0.48
1:A:372:MET:HE2	1:A:372:MET:HA	1.96	0.48
1:A:157:THR:HB	1:A:160:ASP:HB2	1.94	0.48
1:A:166:ALA:O	1:A:170:VAL:HG23	2.14	0.48
1:A:724:ASN:O	1:A:727:GLN:HG2	2.14	0.48
1:A:296:ASP:OD1	1:A:296:ASP:C	2.57	0.47
1:A:164:ALA:O	1:A:168:ASN:HB2	2.14	0.47
1:A:200:ASP:OD2	1:A:203:ILE:HG13	2.13	0.47
1:A:481:ASP:HB3	1:A:532:ILE:HD11	1.96	0.47
1:A:604:PHE:O	1:A:605:ALA:HB3	2.14	0.47
1:A:840:ILE:HD13	1:A:872:MET:HE2	1.96	0.47
1:A:231:VAL:N	1:A:232:PRO:CD	2.76	0.47
1:A:315:VAL:HG13	1:A:323:ALA:HB2	1.96	0.47
1:A:694:THR:HB	1:A:725:LEU:HD21	1.97	0.47
1:A:263:LEU:HD13	1:A:271:PRO:HG3	1.96	0.47
1:A:207:MET:O	1:A:210:LEU:HB3	2.14	0.47
1:A:575:LEU:HD12	1:A:575:LEU:O	2.14	0.47
1:A:846:TRP:H	1:A:846:TRP:CD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:O	1:A:225:VAL:HG23	2.15	0.47
1:A:311:ILE:O	1:A:315:VAL:HG23	2.15	0.47
1:A:603:LYS:O	1:A:773:HIS:HD2	1.97	0.47
1:A:527:GLY:O	1:A:528:LYS:HD3	2.14	0.47
1:A:229:LEU:CD2	1:A:233:TRP:CD2	2.93	0.46
1:A:745:LEU:HA	1:A:748:MET:HE2	1.97	0.46
1:A:204:TYR:O	1:A:207:MET:HB2	2.14	0.46
1:A:810:LEU:HB3	1:A:822:CYS:SG	2.55	0.46
1:A:579:VAL:HG12	1:A:651:LEU:HB3	1.97	0.46
1:A:629:ALA:HA	1:A:633:ILE:HG22	1.96	0.46
1:A:176:GLN:O	1:A:178:GLY:N	2.49	0.46
1:A:168:ASN:O	1:A:172:LEU:HD12	2.16	0.46
1:A:432:ILE:CD1	1:A:450:CYS:SG	3.04	0.46
1:A:585:LEU:O	1:A:624:ARG:HD2	2.16	0.46
1:A:650:GLU:HG3	1:A:689:GLY:CA	2.46	0.46
1:A:706:PRO:CG	1:A:744:ASN:HB3	2.46	0.45
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.64	0.45
1:A:356:SER:CB	1:A:572:GLN:HB2	2.46	0.45
1:A:426:GLU:C	1:A:428:ILE:N	2.74	0.45
1:A:711:SER:HA	1:A:712:GLY:HA2	1.65	0.45
1:A:201:GLN:HE22	1:A:240:GLN:HE22	1.63	0.45
1:A:172:LEU:CD2	1:A:210:LEU:HD11	2.47	0.45
1:A:168:ASN:O	1:A:172:LEU:CD1	2.65	0.45
1:A:426:GLU:O	1:A:428:ILE:N	2.50	0.45
1:A:599:ILE:H	1:A:599:ILE:CD1	2.27	0.45
1:A:922:ILE:O	1:A:922:ILE:HG22	2.16	0.45
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.65	0.45
1:A:847:LEU:HD22	1:A:886:THR:HG21	1.98	0.44
1:A:230:GLY:O	1:A:231:VAL:C	2.60	0.44
1:A:835:LYS:HB2	1:A:835:LYS:HE3	1.69	0.44
1:A:921:ARG:C	1:A:923:ILE:H	2.25	0.44
1:A:452:ILE:HG12	1:A:490:GLY:HA2	2.00	0.44
1:A:481:ASP:HB3	1:A:532:ILE:CD1	2.47	0.44
1:A:766:GLU:OE1	1:A:803:ARG:NH1	2.51	0.44
1:A:432:ILE:HD11	1:A:450:CYS:SG	2.58	0.44
1:A:686:THR:HB	1:A:689:GLY:H	1.82	0.44
1:A:172:LEU:HD22	1:A:210:LEU:CD1	2.48	0.43
1:A:762:VAL:O	1:A:766:GLU:HG3	2.19	0.43
1:A:750:GLU:OE1	1:A:790:SER:HB2	2.18	0.43
1:A:922:ILE:O	1:A:922:ILE:CG2	2.67	0.43
1:A:230:GLY:C	1:A:232:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:MET:HE2	1:A:435:MET:HB3	1.81	0.43
1:A:157:THR:HA	1:A:158:PRO:HD3	1.64	0.43
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.76	0.43
1:A:628:LEU:HD23	1:A:628:LEU:HA	1.84	0.43
1:A:916:ALA:HA	1:A:919:ARG:HD2	2.00	0.43
1:A:144:LYS:O	1:A:148:MET:HG2	2.19	0.43
1:A:325:ARG:O	1:A:329:ILE:HG12	2.19	0.43
1:A:172:LEU:HD21	1:A:210:LEU:HD11	2.00	0.43
1:A:534:ARG:CG	1:A:534:ARG:NH1	2.76	0.43
1:A:666:ARG:HD2	1:A:703:THR:HB	2.01	0.43
1:A:475:LEU:HD22	1:A:483:ILE:HG21	2.01	0.42
1:A:148:MET:O	1:A:149:MET:C	2.63	0.42
1:A:398:MET:HE3	1:A:443:GLN:NE2	2.34	0.42
1:A:650:GLU:HG3	1:A:689:GLY:HA2	2.01	0.42
1:A:666:ARG:HH11	1:A:699:ARG:HB3	1.78	0.42
1:A:178:GLY:O	1:A:182:LEU:CD1	2.67	0.42
1:A:388:TYR:O	1:A:392:LYS:HG2	2.19	0.42
1:A:554:ILE:CG1	1:A:624:ARG:HG2	2.50	0.42
1:A:458:LYS:HG2	1:A:497:TYR:CE1	2.55	0.42
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.84	0.42
1:A:646:HIS:ND1	1:A:685:GLY:HA2	2.35	0.42
1:A:718:VAL:O	1:A:721:PRO:HD2	2.20	0.42
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.72	0.42
1:A:150:ASP:O	1:A:151:LEU:C	2.62	0.42
1:A:694:THR:HG21	1:A:725:LEU:HD23	2.02	0.42
1:A:535:TRP:O	1:A:536:ALA:C	2.62	0.42
1:A:381:PHE:CD2	1:A:381:PHE:C	2.98	0.41
1:A:883:LEU:HD12	1:A:883:LEU:HA	1.77	0.41
1:A:575:LEU:HD21	1:A:648:SER:HB3	2.02	0.41
1:A:877:GLU:HA	1:A:920:TYR:HE1	1.85	0.41
1:A:877:GLU:HG2	1:A:920:TYR:HE1	1.85	0.41
1:A:544:THR:CG2	1:A:584:ASN:HD22	2.33	0.41
1:A:810:LEU:HD13	1:A:810:LEU:HA	1.75	0.41
1:A:856:ASN:HA	1:A:857:PRO:HD3	1.92	0.41
1:A:718:VAL:C	1:A:721:PRO:HD2	2.45	0.41
1:A:172:LEU:HG	1:A:182:LEU:CD1	2.51	0.41
1:A:809:LEU:HD23	1:A:849:ILE:HD11	2.03	0.41
1:A:893:SER:HA	1:A:914:LEU:HD11	2.02	0.41
1:A:404:VAL:O	1:A:408:ILE:CG1	2.66	0.41
1:A:552:LYS:HD2	1:A:552:LYS:HA	1.88	0.41
1:A:844:ALA:O	1:A:845:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:CD2	1:A:210:LEU:CD1	2.99	0.41
1:A:329:ILE:HG22	1:A:329:ILE:O	2.21	0.41
1:A:597:GLU:O	1:A:598:MET:CB	2.69	0.41
1:A:158:PRO:HB2	1:A:159:ILE:H	1.63	0.40
1:A:203:ILE:O	1:A:207:MET:HG2	2.21	0.40
1:A:588:ALA:O	1:A:654:ARG:HD3	2.21	0.40
1:A:686:THR:HG22	1:A:687:GLU:N	2.36	0.40
1:A:149:MET:O	1:A:153:PHE:CD2	2.74	0.40
1:A:328:GLU:C	1:A:330:ARG:N	2.80	0.40
1:A:877:GLU:HG2	1:A:920:TYR:CE1	2.57	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	784/810 (97%)	718 (92%)	59 (8%)	7 (1%)	14	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	PRO
1	A	174	LYS
1	A	169	LEU
1	A	173	ALA
1	A	175	GLU
1	A	177	THR
1	A	220	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	661/683 (97%)	629 (95%)	32 (5%)	23 57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ASP
1	A	161	LYS
1	A	222	THR
1	A	247	SER
1	A	289	CYS
1	A	313	ARG
1	A	320	LEU
1	A	398	MET
1	A	400	SER
1	A	429	LEU
1	A	433	LEU
1	A	438	THR
1	A	446	VAL
1	A	471	ILE
1	A	486	ARG
1	A	513	LEU
1	A	532	ILE
1	A	534	ARG
1	A	544	THR
1	A	618	VAL
1	A	627	VAL
1	A	671	GLN
1	A	691	ARG
1	A	703	THR
1	A	718	VAL
1	A	794	ILE
1	A	805	LYS
1	A	810	LEU
1	A	883	LEU
1	A	891	LEU

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Mol	Chain	Res	Type
1	A	895	LEU
1	A	911	THR

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	147	GLN
1	A	201	GLN
1	A	250	GLN
1	A	254	GLN
1	A	280	ASN
1	A	314	ASN
1	A	316	HIS
1	A	371	ASN
1	A	443	GLN
1	A	572	GLN
1	A	584	ASN
1	A	607	GLN
1	A	613	HIS
1	A	692	HIS

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	786/810 (97%)	-0.11	43 (5%) 30 15	32, 55, 111, 159	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	GLY	13.1
1	A	528	LYS	7.3
1	A	345	TYR	5.5
1	A	174	LYS	5.5
1	A	159	ILE	5.4
1	A	462	LYS	4.6
1	A	526	PRO	4.4
1	A	139	ALA	4.4
1	A	595	LEU	4.4
1	A	166	ALA	3.9
1	A	923	ILE	3.8
1	A	140	LYS	3.8
1	A	138	ASN	3.6
1	A	236	ARG	3.6
1	A	504	ILE	3.5
1	A	502	ALA	3.5
1	A	467	GLN	3.4
1	A	529	ASP	3.3
1	A	498	GLY	3.1
1	A	594	MET	3.1
1	A	465	CYS	3.0
1	A	460	LYS	3.0
1	A	499	GLY	3.0
1	A	172	LEU	2.8
1	A	346	LYS	2.7
1	A	349	SER	2.6
1	A	344	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	147	GLN	2.4
1	A	157	THR	2.3
1	A	158	PRO	2.3
1	A	530	LYS	2.2
1	A	599	ILE	2.2
1	A	163	ARG	2.2
1	A	209	HIS	2.2
1	A	160	ASP	2.2
1	A	458	LYS	2.2
1	A	503	ALA	2.2
1	A	501	ASP	2.1
1	A	241	LYS	2.1
1	A	243	GLU	2.1
1	A	173	ALA	2.1
1	A	597	GLU	2.1
1	A	155	LEU	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.