



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:09 PM UTC

PDB ID : 6R9P / pdb_00006r9p
Title : Structure of *Saccharomyces cerevisiae* apo Pan2 pseudoubiquitin hydrolase-RNA exonuclease (UCH-Exo) module in complex with AAUUA RNA
Authors : Tang, T.T.L.; Stowell, J.A.W.; Hill, C.H.; Passmore, L.A.
Deposited on : 2019-04-03
Resolution : 2.98 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

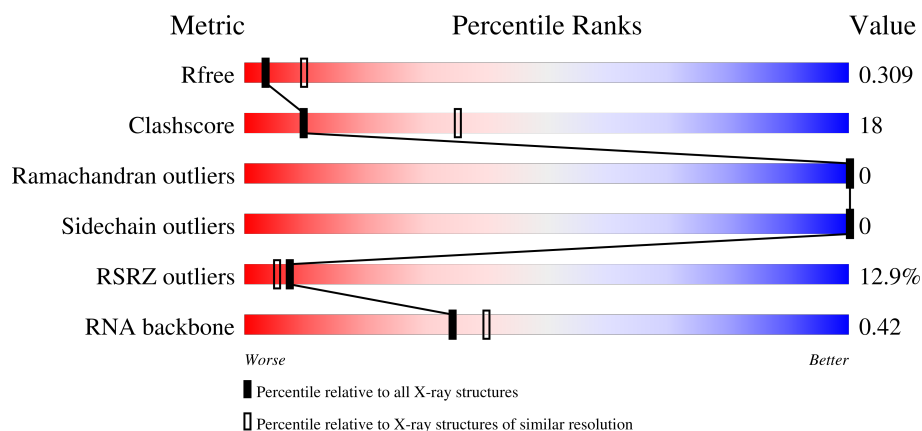
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)
RNA backbone	3983	1013 (3.18-2.78)

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	672	12% 63% 27% 10%
2	B	6	67% 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4631 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 PAN2-PAN3 deadenylation complex catalytic subunit PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4550	2900	751	882	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	MET	-	initiating methionine	UNP P53010
A	445	HIS	-	expression tag	UNP P53010
A	446	HIS	-	expression tag	UNP P53010
A	447	HIS	-	expression tag	UNP P53010
A	448	HIS	-	expression tag	UNP P53010
A	449	HIS	-	expression tag	UNP P53010
A	450	HIS	-	expression tag	UNP P53010
A	451	HIS	-	expression tag	UNP P53010
A	452	HIS	-	expression tag	UNP P53010
A	453	LEU	-	expression tag	UNP P53010
A	454	GLU	-	expression tag	UNP P53010
A	455	VAL	-	expression tag	UNP P53010
A	456	LEU	-	expression tag	UNP P53010
A	457	PHE	-	expression tag	UNP P53010
A	458	GLN	-	expression tag	UNP P53010
A	459	GLY	-	expression tag	UNP P53010
A	460	PRO	-	expression tag	UNP P53010
A	912	ALA	GLU	engineered mutation	UNP P53010

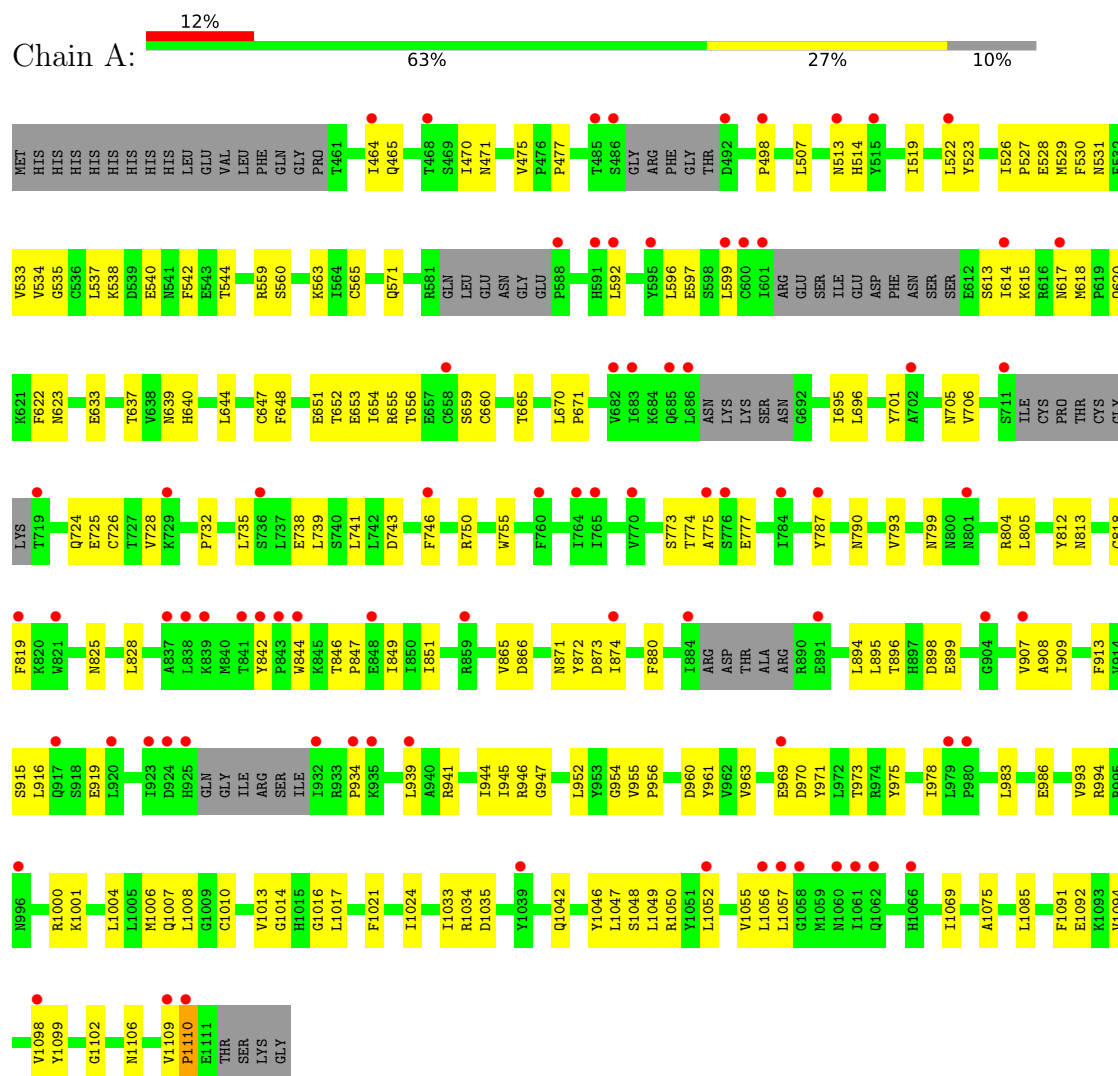
- Molecule 2 is a RNA chain called AAUUAA RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	P	0	0	0
			81	38	14	26	3			

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: PAN2-PAN3 deadenylation complex catalytic subunit PAN2



- Molecule 2: AAUUAA RNA



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.89Å 117.09Å 255.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.48 – 2.98 86.48 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.48-2.98) 99.8 (86.48-2.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.261 , 0.309 0.273 , 0.309	Depositor DCC
R_{free} test set	1462 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	113.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4631	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	0.20	0/4645	0.49	1/6351 (0.0%)
2	B	0.07	0/90	0.21	0/138
All	All	0.20	0/4735	0.49	1/6489 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	PRO	CA-N-CD	-9.02	99.37	112.00

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	4550	0	4096	153	0
2	B	81	0	44	2	0
All	All	4631	0	4140	154	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 (154) 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:1109:VAL:CG1	1:A:1110:PRO:HD3	1.30	1.58
1:A:1109:VAL:HG12	1:A:1110:PRO:CD	1.31	1.57
1:A:907:VAL:HG12	1:A:947:GLY:H	1.35	0.91
1:A:1109:VAL:HG12	1:A:1110:PRO:HD2	1.53	0.90
1:A:1109:VAL:HG13	1:A:1110:PRO:HD3	1.54	0.86
1:A:971:TYR:HD2	1:A:978:ILE:HD13	1.40	0.85
1:A:790:ASN:HB3	1:A:851:ILE:HD11	1.61	0.83
1:A:560:SER:HB3	1:A:563:LYS:HB3	1.63	0.81
1:A:1091:PHE:HD1	1:A:1092:GLU:H	1.28	0.78
1:A:1017:LEU:HB2	1:A:1033:ILE:HD11	1.66	0.77
1:A:655:ARG:O	1:A:725:GLU:N	2.21	0.72
1:A:945:ILE:HA	1:A:956:PRO:HA	1.70	0.72
1:A:1085:LEU:HD13	1:A:1094:VAL:HG21	1.72	0.72
1:A:880:PHE:HA	1:A:993:VAL:HG12	1.72	0.71
1:A:529:MET:HG3	1:A:644:LEU:HD21	1.72	0.71
1:A:559:ARG:HH22	1:A:1007:GLN:NE2	1.92	0.68
1:A:652:THR:O	1:A:654:ILE:HD12	1.94	0.68
1:A:523:TYR:HB3	1:A:529:MET:HE1	1.76	0.67
1:A:513:ASN:OD1	1:A:571:GLN:NE2	2.28	0.67
1:A:825:ASN:HB3	1:A:828:LEU:HB3	1.76	0.67
1:A:960:ASP:OD1	1:A:1001:LYS:NZ	2.27	0.66
1:A:971:TYR:CD2	1:A:978:ILE:HD13	2.28	0.66
1:A:614:ILE:HD11	1:A:618:MET:HB3	1.78	0.65
1:A:656:THR:HG22	1:A:724:GLN:HG3	1.78	0.65
1:A:978:ILE:HD12	1:A:978:ILE:O	1.97	0.65
1:A:519:ILE:HD13	1:A:622:PHE:HD2	1.60	0.64
1:A:652:THR:HG21	1:A:670:LEU:HD12	1.81	0.62
1:A:1110:PRO:HD2	1:A:1110:PRO:O	2.00	0.62
1:A:909:ILE:HD13	1:A:944:ILE:HG12	1.82	0.62
1:A:1109:VAL:CG1	1:A:1110:PRO:CD	2.20	0.61
1:A:750:ARG:HH21	1:A:846:THR:HG22	1.64	0.61
1:A:1014:GLY:HA3	1:A:1017:LEU:HD21	1.81	0.61
1:A:530:PHE:O	1:A:534:VAL:HG22	2.01	0.61
1:A:1048:SER:O	1:A:1052:LEU:HD13	2.00	0.61
1:A:523:TYR:OH	1:A:623:ASN:OD1	2.19	0.60
1:A:537:LEU:O	1:A:1000:ARG:NH1	2.35	0.60
1:A:544:THR:OG1	1:A:633:GLU:HB3	2.01	0.60
1:A:939:LEU:HD13	1:A:1024:ILE:HG22	1.82	0.60
1:A:1013:VAL:HG12	1:A:1034:ARG:HB2	1.83	0.60
1:A:654:ILE:HD12	1:A:654:ILE:N	2.16	0.60
1:A:1052:LEU:HA	1:A:1055:VAL:HG12	1.83	0.59
1:A:1109:VAL:HG12	1:A:1110:PRO:HD3	0.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:TYR:O	2:B:3:U:O2'	2.21	0.58
1:A:652:THR:O	1:A:654:ILE:CD1	2.52	0.58
1:A:946:ARG:HH11	1:A:955:VAL:HG23	1.68	0.58
1:A:739:LEU:HD21	1:A:741:LEU:HG	1.84	0.58
1:A:620:GLN:HB3	1:A:738:GLU:HB3	1.84	0.58
1:A:919:GLU:HA	1:A:934:PRO:HB3	1.86	0.57
1:A:523:TYR:CB	1:A:529:MET:HE1	2.35	0.57
1:A:804:ARG:HH21	1:A:804:ARG:HB3	1.68	0.57
1:A:915:SER:HB3	1:A:970:ASP:HB3	1.87	0.57
1:A:945:ILE:HG22	1:A:956:PRO:HB3	1.86	0.56
1:A:465:GLN:HG2	1:A:828:LEU:HD21	1.86	0.56
1:A:946:ARG:O	1:A:954:GLY:N	2.39	0.56
1:A:540:GLU:HB2	1:A:542:PHE:CZ	2.41	0.55
1:A:874:ILE:HD11	1:A:1004:LEU:HD12	1.89	0.55
1:A:535:GLY:O	1:A:538:LYS:HG3	2.07	0.54
1:A:894:LEU:HD23	1:A:895:LEU:O	2.07	0.54
1:A:614:ILE:HG21	1:A:805:LEU:HD11	1.89	0.54
1:A:739:LEU:HD13	1:A:847:PRO:HG2	1.89	0.54
1:A:773:SER:O	1:A:774:THR:OG1	2.22	0.54
1:A:813:ASN:HB3	1:A:818:CYS:SG	2.47	0.54
1:A:559:ARG:HH22	1:A:1007:GLN:HE22	1.55	0.54
1:A:790:ASN:HB3	1:A:851:ILE:CD1	2.36	0.54
1:A:1048:SER:OG	1:A:1049:LEU:N	2.40	0.53
1:A:526:ILE:HD11	1:A:851:ILE:HD13	1.90	0.53
1:A:915:SER:C	1:A:916:LEU:HD23	2.33	0.53
1:A:871:ASN:O	1:A:1000:ARG:NH2	2.42	0.53
2:B:4:U:H3'	2:B:5:A:C8	2.44	0.53
1:A:654:ILE:HG23	1:A:724:GLN:OE1	2.09	0.53
1:A:963:VAL:HG22	1:A:994:ARG:HA	1.90	0.52
1:A:1008:LEU:HD11	1:A:1010:CYS:SG	2.50	0.52
1:A:470:ILE:HD12	1:A:471:ASN:N	2.25	0.52
1:A:623:ASN:HB2	1:A:849:ILE:HD13	1.91	0.52
1:A:866:ASP:HB3	1:A:1007:GLN:OE1	2.10	0.51
1:A:596:LEU:HD23	1:A:596:LEU:O	2.11	0.51
1:A:941:ARG:NH1	1:A:961:TYR:OH	2.44	0.51
1:A:529:MET:O	1:A:533:VAL:HG23	2.10	0.51
1:A:946:ARG:HD2	1:A:952:LEU:HB3	1.93	0.51
1:A:701:TYR:O	1:A:705:ASN:HB3	2.11	0.50
1:A:1016:GLY:N	1:A:1035:ASP:OD1	2.42	0.50
1:A:528:GLU:OE2	1:A:647:CYS:HB3	2.12	0.50
1:A:743:ASP:HA	1:A:746:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:TYR:HB3	1:A:844:TRP:CE2	2.46	0.50
1:A:659:SER:OG	1:A:660:CYS:N	2.45	0.50
1:A:804:ARG:HB3	1:A:804:ARG:NH2	2.27	0.50
1:A:706:VAL:HG12	1:A:725:GLU:HA	1.94	0.50
1:A:946:ARG:HH11	1:A:946:ARG:HG3	1.75	0.49
1:A:973:THR:HG23	1:A:978:ILE:HD12	1.94	0.49
1:A:639:ASN:O	1:A:639:ASN:ND2	2.45	0.48
1:A:973:THR:HG22	1:A:978:ILE:H	1.77	0.48
1:A:739:LEU:CD2	1:A:741:LEU:HG	2.42	0.48
1:A:973:THR:HG22	1:A:978:ILE:N	2.29	0.48
1:A:614:ILE:HD12	1:A:615:LYS:H	1.78	0.47
1:A:874:ILE:HD13	1:A:1001:LYS:HG2	1.96	0.47
1:A:696:LEU:H	1:A:696:LEU:HD22	1.79	0.47
1:A:654:ILE:O	1:A:665:THR:HA	2.15	0.47
1:A:1013:VAL:C	1:A:1017:LEU:HD11	2.40	0.47
1:A:945:ILE:HD12	1:A:954:GLY:HA2	1.97	0.47
1:A:559:ARG:NH1	1:A:1006:MET:SD	2.89	0.46
1:A:1056:LEU:O	1:A:1057:LEU:HG	2.16	0.46
1:A:647:CYS:O	1:A:732:PRO:HB2	2.15	0.46
1:A:735:LEU:HD11	1:A:787:TYR:CZ	2.51	0.46
1:A:907:VAL:HB	1:A:945:ILE:O	2.16	0.46
1:A:523:TYR:CG	1:A:529:MET:HE1	2.50	0.45
1:A:648:PHE:O	1:A:671:PRO:HA	2.15	0.45
1:A:773:SER:C	1:A:775:ALA:H	2.23	0.45
1:A:507:LEU:HD23	1:A:565:CYS:HB2	1.97	0.45
1:A:896:THR:OG1	1:A:898:ASP:OD1	2.29	0.45
1:A:637:THR:OG1	1:A:640:HIS:HA	2.17	0.45
1:A:973:THR:C	1:A:975:TYR:N	2.73	0.45
1:A:913:PHE:HB3	1:A:939:LEU:HA	1.97	0.45
1:A:983:LEU:CD1	1:A:986:GLU:H	2.29	0.45
1:A:1042:GLN:HB3	1:A:1099:TYR:CE2	2.52	0.45
1:A:617:ASN:HA	1:A:620:GLN:OE1	2.17	0.45
1:A:1052:LEU:HD12	1:A:1052:LEU:N	2.32	0.45
1:A:522:LEU:HD22	1:A:793:VAL:HG23	1.99	0.44
1:A:526:ILE:HG22	1:A:529:MET:H	1.82	0.44
1:A:896:THR:O	1:A:899:GLU:N	2.45	0.44
1:A:651:GLU:O	1:A:728:VAL:HA	2.17	0.44
1:A:941:ARG:HH21	1:A:1069:ILE:HG23	1.83	0.44
1:A:1102:GLY:O	1:A:1106:ASN:N	2.51	0.44
1:A:464:ILE:HA	1:A:477:PRO:HB2	1.99	0.44
1:A:812:TYR:HB2	1:A:819:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:PRO:CD	1:A:1110:PRO:O	2.66	0.43
1:A:969:GLU:HG3	1:A:970:ASP:N	2.31	0.43
1:A:1021:PHE:HA	1:A:1024:ILE:HG12	2.00	0.43
1:A:1098:VAL:O	1:A:1102:GLY:N	2.52	0.43
1:A:592:LEU:H	1:A:592:LEU:HD12	1.84	0.42
1:A:1021:PHE:HE2	1:A:1033:ILE:HD12	1.83	0.42
1:A:1048:SER:OG	1:A:1050:ARG:N	2.52	0.42
1:A:465:GLN:NE2	1:A:498:PRO:O	2.39	0.42
1:A:537:LEU:HB2	1:A:865:VAL:HG21	2.00	0.42
1:A:514:HIS:CD2	1:A:613:SER:HB3	2.55	0.42
1:A:1047:LEU:CB	1:A:1052:LEU:HD11	2.49	0.42
1:A:775:ALA:O	1:A:777:GLU:N	2.51	0.42
1:A:653:GLU:O	1:A:726:CYS:HA	2.19	0.42
1:A:908:ALA:HB3	1:A:945:ILE:HG12	2.02	0.41
1:A:946:ARG:HG3	1:A:946:ARG:NH1	2.35	0.41
1:A:1042:GLN:N	1:A:1042:GLN:OE1	2.54	0.41
1:A:475:VAL:HG12	1:A:799:ASN:OD1	2.20	0.41
1:A:913:PHE:HA	1:A:939:LEU:HA	2.01	0.41
1:A:871:ASN:OD1	1:A:873:ASP:HB2	2.21	0.41
1:A:913:PHE:CB	1:A:939:LEU:HA	2.50	0.41
1:A:983:LEU:HD12	1:A:986:GLU:H	1.86	0.41
1:A:1014:GLY:HA2	1:A:1075:ALA:HB1	2.02	0.41
1:A:851:ILE:C	1:A:851:ILE:HD12	2.46	0.41
1:A:872:TYR:HA	1:A:1004:LEU:HD13	2.03	0.41
1:A:597:GLU:C	1:A:599:LEU:H	2.29	0.41
1:A:1006:MET:HE2	1:A:1006:MET:HB2	1.91	0.41
1:A:1091:PHE:HD1	1:A:1092:GLU:N	2.06	0.41
1:A:527:PRO:O	1:A:531:ASN:ND2	2.54	0.41
1:A:655:ARG:HB3	1:A:725:GLU:CB	2.51	0.40
1:A:695:ILE:HA	1:A:755:TRP:CZ2	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	591/672 (88%)	540 (91%)	51 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	456/617 (74%)	456 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN
1	A	966	ASN
1	A	996	ASN
1	A	1007	GLN
1	A	1015	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	3/6 (50%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	A

There are no RNA pucker outliers to report.

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	607/672 (90%)	0.89	79 (13%) 7 5	66, 131, 191, 228	0
2	B	4/6 (66%)	0.61	0 100 100	246, 250, 267, 273	0
All	All	611/678 (90%)	0.89	79 (12%) 7 5	66, 131, 194, 273	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	841	THR	5.1
1	A	1062	GLN	4.3
1	A	884	ILE	4.0
1	A	515	TYR	4.0
1	A	801	ASN	3.8
1	A	923	ILE	3.7
1	A	599	LEU	3.7
1	A	1110	PRO	3.6
1	A	775	ALA	3.6
1	A	1109	VAL	3.5
1	A	592	LEU	3.5
1	A	595	TYR	3.5
1	A	765	ILE	3.4
1	A	682	VAL	3.3
1	A	1060	ASN	3.3
1	A	821	TRP	3.2
1	A	1061	ILE	3.2
1	A	719	THR	3.1
1	A	711	SER	3.0
1	A	838	LEU	3.0
1	A	907	VAL	3.0
1	A	614	ILE	2.9
1	A	934	PRO	2.9
1	A	842	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	924	ASP	2.9
1	A	925	HIS	2.8
1	A	492	ASP	2.8
1	A	1057	LEU	2.8
1	A	736	SER	2.8
1	A	702	ALA	2.7
1	A	685	GLN	2.7
1	A	848	GLU	2.7
1	A	770	VAL	2.7
1	A	996	ASN	2.7
1	A	600	CYS	2.7
1	A	939	LEU	2.7
1	A	935	LYS	2.7
1	A	468	THR	2.7
1	A	1058	GLY	2.7
1	A	513	ASN	2.6
1	A	932	ILE	2.6
1	A	837	ALA	2.6
1	A	588	PRO	2.5
1	A	776	SER	2.5
1	A	485	THR	2.5
1	A	464	ILE	2.5
1	A	917	GLN	2.5
1	A	1052	LEU	2.5
1	A	874	ILE	2.5
1	A	686	LEU	2.4
1	A	658	CYS	2.4
1	A	486	SER	2.4
1	A	617	ASN	2.4
1	A	969	GLU	2.4
1	A	522	LEU	2.3
1	A	729	LYS	2.3
1	A	843	PRO	2.3
1	A	1056	LEU	2.3
1	A	764	ILE	2.3
1	A	844	TRP	2.3
1	A	859	ARG	2.3
1	A	1098	VAL	2.3
1	A	498	PRO	2.2
1	A	760	PHE	2.2
1	A	920	LEU	2.2
1	A	601	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	787	TYR	2.2
1	A	784	ILE	2.1
1	A	819	PHE	2.1
1	A	1039	TYR	2.1
1	A	891	GLU	2.1
1	A	1066	HIS	2.1
1	A	904	GLY	2.1
1	A	683	ILE	2.1
1	A	591	HIS	2.1
1	A	980	PRO	2.1
1	A	979	LEU	2.1
1	A	746	PHE	2.0
1	A	839	LYS	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.