



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 4XVM / pdb_00004xvm
Title : Binary complex of human polymerase nu and DNA with the finger domain closed and thumb domain rotated out
Authors : Lee, Y.-S.; Yang, W.
Deposited on : 2015-01-27
Resolution : 3.20 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

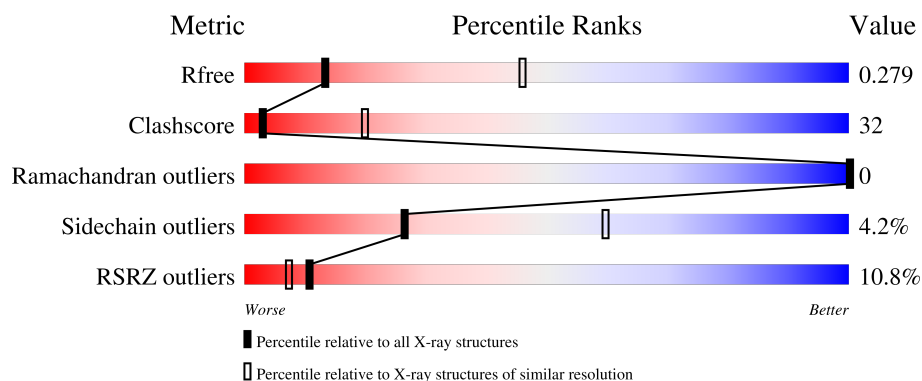
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	666	11% 56% 34% 6%
2	T	9	44% 22% 33%
3	P	13	23% 69% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5401 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 DNA polymerase nu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	627	Total	C	N	O	S	0	0	0
			4952	3155	872	900	25			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*AP*GP*CP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			183	87	33	54	9			

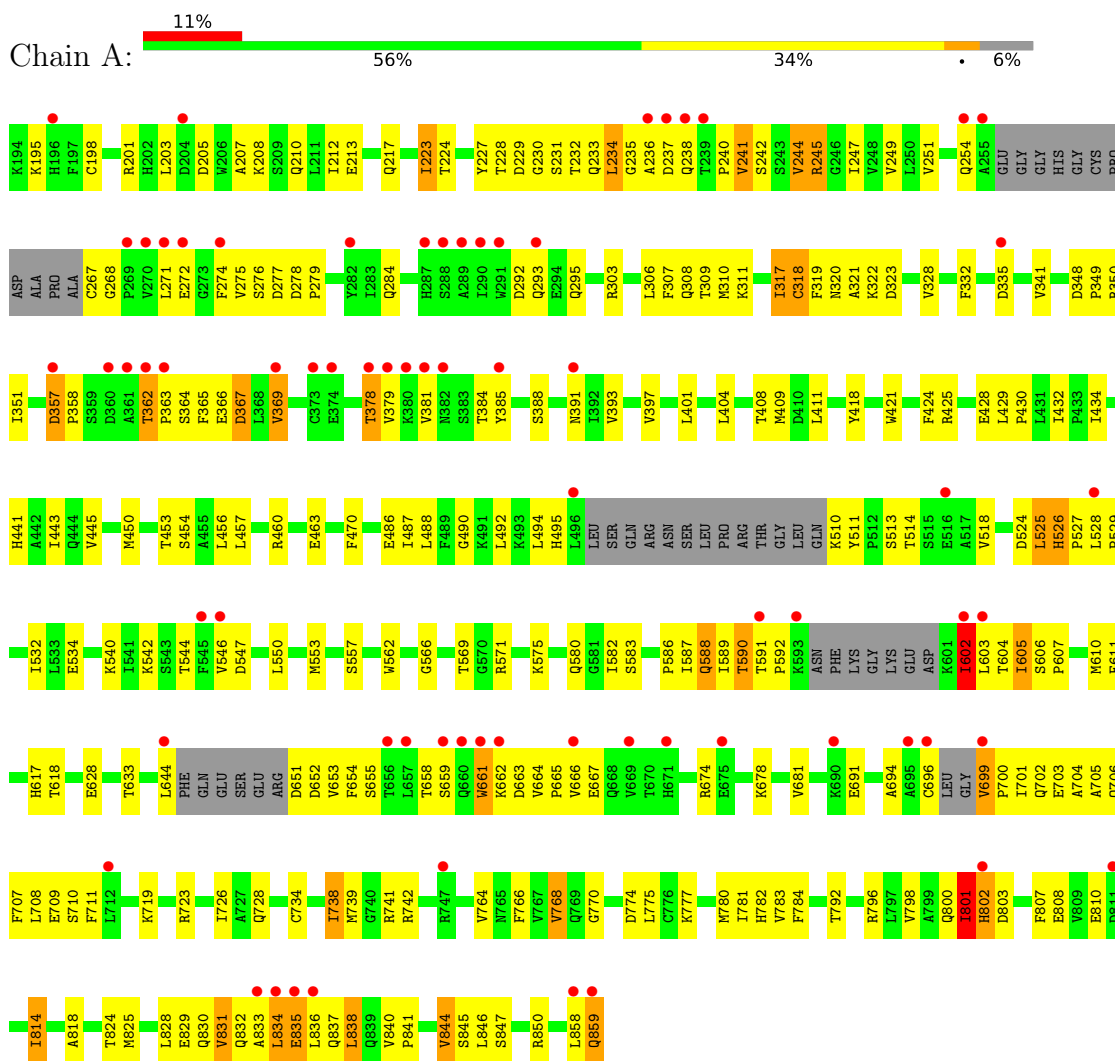
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*TP*CP*TP*GP*AP*CP*GP*CP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			266	128	49	77	12			

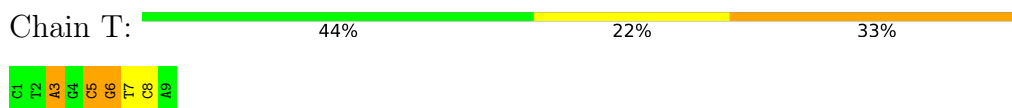
3 Residue-property plots

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: DNA polymerase nu

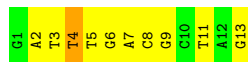


• Molecule 2: DNA (5'-D(*CP*TP*AP*GP*CP*GP*TP*CP*A)-3')



- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*TP*GP*AP*CP*GP*CP*TP*AP*G)-3')

Chain P:  23% 69% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.00Å 110.92Å 277.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 3.20 29.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.70-3.20) 98.5 (29.70-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.242 , 0.281 0.242 , 0.279	Depositor DCC
R_{free} test set	1283 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.5	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	0.91	EDS
Total number of atoms	5401	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.87	7/5045 (0.1%)	1.25	47/6824 (0.7%)
2	T	0.44	0/204	1.19	4/312 (1.3%)
3	P	0.47	0/298	1.25	1/459 (0.2%)
All	All	0.84	7/5547 (0.1%)	1.25	52/7595 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432	ILE	CA-CB	8.44	1.58	1.54
1	A	487	ILE	C-O	-7.22	1.16	1.24
1	A	470	PHE	C-O	-5.78	1.17	1.24
1	A	223	ILE	CA-CB	5.71	1.61	1.54
1	A	699	VAL	C-N	5.65	1.41	1.33
1	A	318	CYS	CA-C	-5.26	1.46	1.52
1	A	249	VAL	CA-CB	5.03	1.60	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	THR	N-CA-C	10.15	121.23	108.45
1	A	205	ASP	N-CA-C	9.55	122.89	111.33
1	A	293	GLN	N-CA-C	8.95	121.85	111.11
1	A	357	ASP	CA-C-N	8.57	128.70	119.28
1	A	357	ASP	C-N-CA	8.57	128.70	119.28
1	A	802	HIS	N-CA-C	8.44	121.23	111.11
1	A	691	GLU	N-CA-C	8.26	119.97	110.97
1	A	524	ASP	N-CA-C	8.22	120.24	111.28
1	A	801	ILE	N-CA-C	-7.69	101.66	110.05
1	A	768	VAL	N-CA-C	7.26	117.34	110.30
1	A	244	VAL	CB-CA-C	-7.19	101.70	111.63
1	A	362	THR	CA-C-N	7.08	127.25	120.31
1	A	362	THR	C-N-CA	7.08	127.25	120.31
1	A	831	VAL	N-CA-C	7.01	119.93	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	835	GLU	N-CA-C	-6.99	103.66	111.28
1	A	526	HIS	N-CA-C	-6.83	100.33	108.25
1	A	268	GLY	CA-C-N	-6.75	113.56	120.85
1	A	268	GLY	C-N-CA	-6.75	113.56	120.85
1	A	369	VAL	CB-CA-C	-6.73	103.20	112.02
1	A	699	VAL	CA-C-N	-6.66	112.90	119.76
1	A	699	VAL	C-N-CA	-6.66	112.90	119.76
1	A	661	TRP	N-CA-C	-6.65	103.96	111.14
1	A	245	ARG	N-CA-C	6.52	122.13	114.04
2	T	6	DG	P-O5'-C5'	-6.42	110.36	120.00
1	A	195	LYS	N-CA-C	-6.39	105.12	113.17
1	A	295	GLN	N-CA-C	-6.37	104.42	111.36
1	A	602	ILE	N-CA-C	6.25	116.88	107.75
1	A	831	VAL	CB-CA-C	-6.16	104.60	110.70
1	A	696	CYS	CB-CA-C	-5.97	98.75	110.10
1	A	566	GLY	N-CA-C	5.86	119.98	112.83
3	P	4	DT	N1-C1'-C2'	5.86	122.29	113.50
1	A	234	LEU	N-CA-C	5.83	119.37	112.72
1	A	768	VAL	CB-CA-C	-5.79	104.57	111.81
2	T	3	DA	P-O5'-C5'	-5.77	111.35	120.00
1	A	388	SER	N-CA-C	5.67	116.56	108.74
1	A	667	GLU	N-CA-C	5.63	118.95	111.75
1	A	198	CYS	N-CA-C	5.61	117.87	108.73
1	A	391	ASN	N-CA-C	5.48	117.25	111.28
1	A	487	ILE	N-CA-C	5.47	115.67	110.53
1	A	367	ASP	N-CA-C	-5.40	104.63	111.11
1	A	824	THR	N-CA-C	5.35	117.54	111.02
1	A	292	ASP	N-CA-C	5.32	116.37	108.86
1	A	208	LYS	N-CA-C	-5.31	105.40	111.14
1	A	557	SER	N-CA-C	5.28	118.16	109.72
2	T	5	DC	O5'-C5'-C4'	-5.23	102.96	110.80
1	A	792	THR	N-CA-C	5.21	116.65	110.97
1	A	814	ILE	CB-CA-C	-5.13	108.83	113.70
1	A	341	VAL	N-CA-C	5.09	117.78	112.90
2	T	3	DA	C5'-C4'-C3'	-5.07	107.29	114.90
1	A	844	VAL	CB-CA-C	-5.06	106.02	111.59
1	A	588	GLN	N-CA-C	5.02	117.16	109.07
1	A	318	CYS	N-CA-C	-5.02	101.44	109.07

There are no chirality outliers.

There are no planarity outliers.

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	4952	0	5050	320	0
2	T	183	0	102	9	0
3	P	266	0	149	21	0
All	All	5401	0	5301	340	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 32.

All (340) 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:703:GLU:O	1:A:706:GLN:HB3	1.28	1.32
1:A:378:THR:CG2	1:A:379:VAL:H	1.41	1.31
1:A:858:LEU:HD12	1:A:858:LEU:O	1.37	1.23
1:A:659:SER:O	1:A:663:ASP:N	1.72	1.21
1:A:831:VAL:C	1:A:833:ALA:HA	1.65	1.19
1:A:832:GLN:HG2	1:A:835:GLU:HB3	1.25	1.19
1:A:453:THR:HG23	1:A:605:ILE:CD1	1.74	1.17
1:A:303:ARG:NH1	1:A:335:ASP:OD2	1.79	1.14
1:A:453:THR:CG2	1:A:605:ILE:CD1	2.26	1.13
1:A:664:VAL:HG13	1:A:665:PRO:HD2	1.19	1.11
1:A:664:VAL:CG1	1:A:665:PRO:HD2	1.80	1.10
1:A:319:PHE:O	1:A:348:ASP:CG	1.98	1.07
1:A:832:GLN:N	1:A:833:ALA:HA	1.68	1.06
1:A:378:THR:HG22	1:A:379:VAL:N	1.54	1.03
1:A:739:MET:HE2	1:A:836:LEU:CD1	1.87	1.03
1:A:453:THR:CG2	1:A:605:ILE:HD13	1.88	1.01
1:A:739:MET:HE2	1:A:836:LEU:HD13	1.38	1.00
1:A:378:THR:HG22	1:A:379:VAL:H	0.85	0.99
1:A:488:LEU:HD23	1:A:528:LEU:HD23	1.44	0.99
1:A:453:THR:HG23	1:A:605:ILE:HD13	1.39	0.98
1:A:700:PRO:HG2	1:A:703:GLU:HB3	1.46	0.94
1:A:703:GLU:O	1:A:706:GLN:CB	2.15	0.94
1:A:829:GLU:HB2	1:A:830:GLN:OE1	1.68	0.94
1:A:739:MET:CE	1:A:836:LEU:CD1	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:GLU:OE1	1:A:841:PRO:HA	1.69	0.93
1:A:739:MET:CE	1:A:836:LEU:HD13	1.99	0.92
1:A:830:GLN:OE1	1:A:830:GLN:N	2.03	0.91
1:A:780:MET:SD	1:A:800:GLN:NE2	2.44	0.91
1:A:618:THR:HG23	1:A:814:ILE:HD11	1.53	0.91
1:A:662:LYS:HB3	1:A:664:VAL:CG2	2.01	0.90
1:A:832:GLN:HG2	1:A:835:GLU:CB	2.01	0.90
3:P:2:DA:H2''	3:P:3:DT:H5'	1.53	0.90
1:A:450:MET:CG	1:A:550:LEU:HD21	2.03	0.90
1:A:832:GLN:N	1:A:833:ALA:CA	2.36	0.89
1:A:704:ALA:O	1:A:707:PHE:N	2.05	0.88
1:A:590:THR:O	1:A:592:PRO:HD3	1.74	0.88
1:A:664:VAL:CG1	1:A:665:PRO:CD	2.52	0.87
1:A:450:MET:HG2	1:A:550:LEU:HD21	1.56	0.87
1:A:488:LEU:CD2	1:A:528:LEU:HD23	2.05	0.87
1:A:700:PRO:HG2	1:A:703:GLU:CB	2.04	0.86
1:A:580:GLN:OE1	1:A:802:HIS:NE2	2.10	0.85
1:A:366:GLU:N	1:A:366:GLU:OE1	2.08	0.85
1:A:662:LYS:HB3	1:A:664:VAL:HG21	1.56	0.85
1:A:384:THR:HG22	1:A:385:TYR:N	1.90	0.84
1:A:662:LYS:C	1:A:664:VAL:HG23	2.02	0.83
1:A:453:THR:HG23	1:A:605:ILE:HD11	1.59	0.83
1:A:224:THR:HG22	1:A:401:LEU:HD21	1.60	0.83
1:A:526:HIS:CE1	1:A:528:LEU:HB2	2.14	0.83
1:A:651:ASP:O	1:A:652:ASP:OD1	1.99	0.81
1:A:492:LEU:HB2	1:A:494:LEU:CD2	2.11	0.81
1:A:562:TRP:HZ3	1:A:580:GLN:HE21	1.25	0.80
1:A:719:LYS:HZ1	1:A:723:ARG:HD2	1.48	0.79
1:A:378:THR:CG2	1:A:379:VAL:N	2.16	0.79
1:A:661:TRP:HZ3	1:A:707:PHE:CD1	1.99	0.79
1:A:364:SER:CB	1:A:366:GLU:OE1	2.30	0.79
1:A:229:ASP:OD1	1:A:240:PRO:O	1.99	0.78
1:A:453:THR:HG21	1:A:605:ILE:CD1	2.11	0.78
1:A:526:HIS:CG	1:A:527:PRO:HD2	2.20	0.77
1:A:586:PRO:HB3	1:A:606:SER:HB2	1.65	0.77
1:A:424:PHE:CE2	1:A:429:LEU:HD11	2.19	0.76
1:A:858:LEU:O	1:A:858:LEU:CD1	2.26	0.76
1:A:428:GLU:OE2	1:A:741:ARG:NH1	2.18	0.76
1:A:582:ILE:HD13	1:A:611:PHE:CE1	2.20	0.76
1:A:662:LYS:O	1:A:664:VAL:HG23	1.85	0.76
1:A:832:GLN:CG	1:A:835:GLU:HB3	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:GLU:CB	1:A:830:GLN:OE1	2.33	0.76
1:A:654:PHE:CE1	1:A:678:LYS:HA	2.21	0.76
1:A:832:GLN:HB3	1:A:835:GLU:H	1.51	0.76
1:A:319:PHE:O	1:A:348:ASP:OD2	2.04	0.75
1:A:664:VAL:HG12	1:A:665:PRO:N	2.00	0.75
1:A:364:SER:HB3	1:A:366:GLU:OE1	1.87	0.75
1:A:661:TRP:HZ3	1:A:707:PHE:HD1	1.34	0.75
1:A:421:TRP:CH2	1:A:425:ARG:HD3	2.21	0.74
1:A:456:LEU:HD11	1:A:591:THR:HG22	1.68	0.74
1:A:828:LEU:O	1:A:830:GLN:N	2.20	0.74
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.22	0.74
1:A:659:SER:HA	1:A:662:LYS:HB2	1.70	0.74
2:T:5:DC:H42	3:P:9:DG:H1	1.36	0.73
1:A:384:THR:HG22	1:A:385:TYR:H	1.52	0.73
1:A:393:VAL:O	1:A:397:VAL:HG23	1.89	0.73
1:A:381:VAL:HG22	1:A:381:VAL:O	1.87	0.73
1:A:580:GLN:OE1	1:A:802:HIS:CD2	2.41	0.72
1:A:803:ASP:OD2	3:P:13:DG:H4'	1.89	0.72
1:A:652:ASP:HB3	1:A:674:ARG:HH12	1.53	0.72
1:A:664:VAL:HG12	1:A:665:PRO:CD	2.18	0.72
3:P:6:DG:H1'	3:P:7:DA:C8	2.25	0.71
1:A:834:LEU:HD23	1:A:837:GLN:OE1	1.90	0.71
1:A:829:GLU:C	1:A:830:GLN:OE1	2.34	0.71
1:A:454:SER:HB2	1:A:546:VAL:HG11	1.72	0.71
1:A:546:VAL:O	1:A:550:LEU:HG	1.89	0.71
1:A:453:THR:HG21	1:A:605:ILE:HD13	1.69	0.71
1:A:734:CYS:SG	1:A:742:ARG:HD2	2.30	0.70
1:A:832:GLN:N	1:A:833:ALA:C	2.49	0.70
1:A:704:ALA:O	1:A:705:ALA:C	2.35	0.70
1:A:704:ALA:C	1:A:706:GLN:N	2.46	0.69
1:A:303:ARG:HH11	1:A:335:ASP:CG	2.01	0.69
1:A:719:LYS:HZ1	1:A:723:ARG:HH21	1.41	0.68
1:A:540:LYS:O	1:A:544:THR:HG23	1.94	0.68
1:A:783:VAL:CG2	1:A:825:MET:HG3	2.24	0.68
1:A:366:GLU:CD	1:A:366:GLU:H	1.95	0.67
1:A:317:ILE:HD11	1:A:409:MET:HE3	1.76	0.67
1:A:832:GLN:CG	1:A:835:GLU:CB	2.70	0.67
1:A:453:THR:CG2	1:A:605:ILE:HD12	2.24	0.67
1:A:739:MET:HE2	1:A:836:LEU:HD12	1.73	0.67
3:P:5:DT:H2''	3:P:6:DG:C8	2.30	0.67
1:A:319:PHE:O	1:A:348:ASP:OD1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LEU:HD23	1:A:604:THR:N	2.11	0.66
1:A:364:SER:HB2	1:A:366:GLU:OE1	1.96	0.66
1:A:658:THR:O	1:A:662:LYS:HG2	1.95	0.66
1:A:378:THR:HG23	1:A:379:VAL:H	1.51	0.66
1:A:618:THR:HG23	1:A:814:ILE:CD1	2.25	0.66
1:A:628:GLU:HG2	1:A:768:VAL:HG12	1.77	0.65
1:A:421:TRP:CZ2	1:A:425:ARG:HD3	2.31	0.65
1:A:418:TYR:HD2	1:A:742:ARG:NH2	1.95	0.65
1:A:234:LEU:N	1:A:235:GLY:HA2	2.12	0.65
1:A:429:LEU:N	1:A:430:PRO:HD2	2.12	0.65
1:A:492:LEU:HB2	1:A:494:LEU:HD23	1.78	0.65
1:A:450:MET:HG3	1:A:550:LEU:HD21	1.77	0.64
1:A:384:THR:CG2	1:A:385:TYR:N	2.58	0.63
1:A:229:ASP:O	1:A:385:TYR:HB2	1.98	0.63
1:A:526:HIS:ND1	1:A:528:LEU:HB2	2.12	0.63
1:A:694:ALA:CB	1:A:701:ILE:HA	2.28	0.63
1:A:229:ASP:HB2	1:A:231:SER:N	2.14	0.63
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.80	0.63
1:A:618:THR:CG2	1:A:814:ILE:HG13	2.29	0.63
1:A:741:ARG:HG2	1:A:766:PHE:HZ	1.64	0.63
1:A:844:VAL:HG12	1:A:845:SER:N	2.14	0.63
1:A:544:THR:HG22	2:T:7:DT:H4'	1.80	0.62
1:A:450:MET:HG2	1:A:550:LEU:CD2	2.26	0.62
1:A:661:TRP:CZ3	1:A:707:PHE:CD1	2.86	0.62
1:A:587:ILE:HG13	1:A:588:GLN:H	1.64	0.62
1:A:618:THR:CG2	1:A:814:ILE:CG1	2.77	0.62
1:A:229:ASP:HB3	1:A:384:THR:HG23	1.80	0.62
1:A:741:ARG:NH2	1:A:774:ASP:OD1	2.32	0.61
1:A:829:GLU:O	1:A:836:LEU:O	2.18	0.61
1:A:664:VAL:CG1	1:A:665:PRO:N	2.64	0.61
1:A:664:VAL:HG12	1:A:665:PRO:O	2.00	0.61
1:A:201:ARG:NH1	1:A:284:GLN:HG2	2.16	0.61
1:A:384:THR:CG2	1:A:385:TYR:H	2.12	0.61
1:A:618:THR:HG21	1:A:814:ILE:HG13	1.82	0.61
1:A:418:TYR:HD2	1:A:742:ARG:HH22	1.47	0.60
1:A:460:ARG:NH2	1:A:534:GLU:OE2	2.34	0.60
1:A:701:ILE:HG23	1:A:702:GLN:N	2.16	0.60
1:A:828:LEU:O	1:A:829:GLU:C	2.43	0.60
1:A:441:HIS:HB2	1:A:796:ARG:CZ	2.32	0.60
2:T:6:DG:H1	3:P:8:DC:H42	1.48	0.60
1:A:719:LYS:NZ	1:A:723:ARG:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:O	1:A:278:ASP:HB3	2.02	0.59
1:A:587:ILE:HG13	1:A:588:GLN:N	2.17	0.59
1:A:492:LEU:CB	1:A:494:LEU:CD2	2.80	0.59
1:A:445:VAL:HG21	1:A:553:MET:SD	2.42	0.59
1:A:633:THR:HG21	1:A:840:VAL:HG21	1.85	0.59
1:A:236:ALA:O	1:A:237:ASP:HB2	2.03	0.59
1:A:662:LYS:HB3	1:A:664:VAL:HG23	1.81	0.58
1:A:228:THR:HA	1:A:245:ARG:HD2	1.86	0.58
1:A:238:GLN:CG	1:A:350:ARG:HH22	2.16	0.58
1:A:831:VAL:N	1:A:833:ALA:O	2.36	0.58
1:A:587:ILE:CG1	1:A:588:GLN:N	2.67	0.57
1:A:618:THR:CG2	1:A:814:ILE:HD11	2.32	0.57
3:P:4:DT:H2''	3:P:5:DT:H72	1.87	0.57
1:A:212:ILE:HG23	1:A:308:GLN:HG3	1.86	0.57
1:A:783:VAL:HG11	1:A:807:PHE:HZ	1.69	0.57
3:P:6:DG:OP2	3:P:6:DG:H2'	2.05	0.57
1:A:234:LEU:O	1:A:234:LEU:HG	2.05	0.57
1:A:586:PRO:HB3	1:A:606:SER:CB	2.33	0.56
1:A:701:ILE:HG23	1:A:702:GLN:H	1.71	0.56
1:A:832:GLN:N	1:A:833:ALA:O	2.38	0.56
1:A:699:VAL:N	1:A:700:PRO:HD2	2.20	0.56
1:A:385:TYR:CD1	1:A:393:VAL:HG21	2.41	0.56
1:A:739:MET:HE3	1:A:836:LEU:CD1	2.31	0.56
1:A:659:SER:O	1:A:663:ASP:CA	2.53	0.56
1:A:317:ILE:CD1	1:A:409:MET:HE3	2.36	0.55
1:A:707:PHE:CE2	1:A:711:PHE:HD1	2.23	0.55
1:A:230:GLY:N	1:A:385:TYR:CD2	2.72	0.55
1:A:783:VAL:HG21	1:A:825:MET:CG	2.36	0.55
1:A:320:ASN:O	1:A:323:ASP:HB2	2.07	0.55
1:A:832:GLN:OE1	1:A:832:GLN:HA	2.06	0.55
1:A:254:GLN:HE21	1:A:267:CYS:N	2.05	0.55
1:A:443:ILE:HG12	1:A:798:VAL:CG1	2.37	0.55
1:A:644:LEU:HD11	1:A:653:VAL:HG13	1.89	0.54
1:A:707:PHE:C	1:A:707:PHE:CD2	2.85	0.54
1:A:488:LEU:CD2	1:A:528:LEU:CD2	2.84	0.54
1:A:694:ALA:HB1	1:A:701:ILE:HA	1.89	0.54
1:A:783:VAL:CG2	1:A:825:MET:CG	2.85	0.54
1:A:719:LYS:HZ1	1:A:723:ARG:CD	2.20	0.53
1:A:310:MET:HE2	1:A:328:VAL:HG11	1.91	0.53
1:A:582:ILE:HD13	1:A:611:PHE:CZ	2.43	0.53
1:A:238:GLN:CD	1:A:350:ARG:HH22	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:DA:H5"	2:T:3:DA:H8	1.72	0.53
1:A:434:ILE:HG12	1:A:784:PHE:CD2	2.43	0.53
1:A:836:LEU:HD21	1:A:838:LEU:HD11	1.89	0.53
1:A:526:HIS:CD2	1:A:527:PRO:HD2	2.44	0.53
1:A:203:LEU:HD22	1:A:207:ALA:HB3	1.90	0.53
1:A:234:LEU:N	1:A:235:GLY:CA	2.72	0.52
1:A:241:VAL:O	1:A:242:SER:HB2	2.09	0.52
1:A:654:PHE:HE1	1:A:678:LYS:HA	1.69	0.52
1:A:858:LEU:O	1:A:859:GLN:HG2	2.09	0.52
1:A:707:PHE:CZ	1:A:711:PHE:HD1	2.27	0.52
1:A:232:THR:OG1	1:A:234:LEU:HB3	2.08	0.52
1:A:319:PHE:HA	1:A:349:PRO:HD2	1.91	0.52
1:A:655:SER:O	1:A:659:SER:N	2.35	0.52
1:A:699:VAL:N	1:A:700:PRO:CD	2.73	0.52
1:A:783:VAL:HG21	1:A:825:MET:HG3	1.92	0.52
1:A:583:SER:HA	3:P:11:DT:H5"	1.91	0.52
1:A:460:ARG:O	1:A:460:ARG:HG3	2.10	0.52
1:A:381:VAL:O	1:A:381:VAL:CG2	2.57	0.52
1:A:418:TYR:CD2	1:A:742:ARG:NH2	2.73	0.52
1:A:633:THR:CG2	1:A:840:VAL:HG21	2.40	0.52
1:A:738:ILE:HG22	1:A:739:MET:HG3	1.91	0.52
1:A:829:GLU:CA	1:A:830:GLN:OE1	2.59	0.52
1:A:321:ALA:O	1:A:322:LYS:C	2.53	0.51
1:A:454:SER:HB2	1:A:546:VAL:CG1	2.40	0.51
1:A:544:THR:HG22	2:T:7:DT:C5'	2.40	0.51
1:A:704:ALA:O	1:A:706:GLN:N	2.42	0.51
2:T:5:DC:N3	3:P:9:DG:N2	2.48	0.51
1:A:229:ASP:HB2	1:A:231:SER:H	1.75	0.51
1:A:237:ASP:O	1:A:238:GLN:HB2	2.09	0.51
1:A:213:GLU:O	1:A:217:GLN:HG2	2.11	0.51
1:A:782:HIS:NE2	1:A:831:VAL:HG21	2.26	0.51
1:A:801:ILE:CD1	1:A:801:ILE:N	2.73	0.51
1:A:836:LEU:HD23	1:A:838:LEU:HD13	1.92	0.51
1:A:274:PHE:CD2	1:A:275:VAL:HG13	2.46	0.50
1:A:488:LEU:HD21	1:A:528:LEU:HG	1.93	0.50
1:A:658:THR:O	1:A:662:LYS:CG	2.60	0.50
1:A:709:GLU:O	1:A:710:SER:C	2.55	0.50
1:A:830:GLN:C	1:A:833:ALA:O	2.54	0.50
1:A:704:ALA:C	1:A:707:PHE:H	2.19	0.50
1:A:317:ILE:HG23	1:A:408:THR:HG21	1.94	0.50
1:A:424:PHE:CZ	1:A:429:LEU:HD21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:DT:C2'	3:P:4:DT:H72	2.42	0.50
1:A:429:LEU:N	1:A:430:PRO:CD	2.75	0.49
1:A:707:PHE:CE2	1:A:711:PHE:CD1	3.00	0.49
1:A:385:TYR:CE1	1:A:393:VAL:HG21	2.46	0.49
1:A:272:GLU:HB3	1:A:274:PHE:CZ	2.48	0.49
1:A:307:PHE:CE2	1:A:311:LYS:HD3	2.48	0.49
1:A:603:LEU:HD23	1:A:604:THR:O	2.13	0.49
1:A:800:GLN:HG2	1:A:801:ILE:O	2.13	0.49
1:A:832:GLN:CG	1:A:835:GLU:HB2	2.43	0.49
1:A:628:GLU:HB2	3:P:13:DG:O3'	2.13	0.48
1:A:617:HIS:CD2	1:A:810:GLU:HA	2.48	0.48
1:A:700:PRO:CG	1:A:703:GLU:CB	2.86	0.48
1:A:828:LEU:C	1:A:830:GLN:N	2.66	0.48
1:A:569:THR:O	1:A:770:GLY:HA2	2.13	0.48
1:A:275:VAL:HB	1:A:279:PRO:HB3	1.95	0.48
1:A:513:SER:OG	1:A:514:THR:N	2.45	0.48
1:A:801:ILE:N	1:A:801:ILE:HD12	2.28	0.48
3:P:8:DC:H2''	3:P:9:DG:C8	2.49	0.48
1:A:582:ILE:CD1	1:A:611:PHE:CZ	2.97	0.48
1:A:662:LYS:CB	1:A:664:VAL:HG23	2.43	0.48
1:A:719:LYS:NZ	1:A:723:ARG:HH21	2.07	0.47
1:A:844:VAL:CG1	1:A:845:SER:N	2.76	0.47
1:A:603:LEU:HD23	1:A:604:THR:H	1.78	0.47
1:A:526:HIS:CG	1:A:527:PRO:CD	2.94	0.47
1:A:654:PHE:CE1	1:A:678:LYS:CB	2.98	0.47
1:A:453:THR:HG21	1:A:605:ILE:HD12	1.87	0.47
1:A:674:ARG:O	1:A:678:LYS:HG2	2.14	0.47
1:A:796:ARG:O	1:A:798:VAL:HG23	2.15	0.47
1:A:231:SER:OG	1:A:240:PRO:CB	2.62	0.47
3:P:3:DT:H2''	3:P:4:DT:C7	2.45	0.47
1:A:362:THR:HA	1:A:363:PRO:HD3	1.58	0.47
1:A:244:VAL:HG12	1:A:245:ARG:N	2.28	0.47
1:A:681:VAL:HG12	1:A:711:PHE:CZ	2.51	0.46
1:A:366:GLU:O	1:A:367:ASP:C	2.57	0.46
1:A:618:THR:CG2	1:A:814:ILE:CD1	2.93	0.46
1:A:510:LYS:HB3	1:A:511:TYR:H	1.47	0.46
2:T:6:DG:H1	3:P:8:DC:N4	2.14	0.46
1:A:274:PHE:HD2	1:A:275:VAL:HG13	1.80	0.46
1:A:528:LEU:N	1:A:529:PRO:CD	2.78	0.46
1:A:276:SER:O	1:A:279:PRO:HD3	2.16	0.46
1:A:562:TRP:HZ3	1:A:580:GLN:NE2	2.05	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ALA:HA	1:A:210:GLN:HB2	1.97	0.45
1:A:777:LYS:O	1:A:781:ILE:HG13	2.16	0.45
1:A:825:MET:HB2	1:A:844:VAL:HG21	1.98	0.45
1:A:662:LYS:CB	1:A:664:VAL:CG2	2.85	0.45
1:A:224:THR:HG21	1:A:234:LEU:HD22	1.99	0.45
1:A:587:ILE:HG23	1:A:605:ILE:HB	1.98	0.45
1:A:798:VAL:HG21	1:A:808:GLU:HB2	1.98	0.45
1:A:818:ALA:HB1	1:A:846:LEU:HD13	1.98	0.45
2:T:7:DT:H2''	2:T:8:DC:O5'	2.17	0.45
1:A:228:THR:O	1:A:228:THR:HG22	2.16	0.44
1:A:227:TYR:O	1:A:230:GLY:HA2	2.17	0.44
1:A:486:GLU:O	1:A:490:GLY:N	2.50	0.44
1:A:542:LYS:NZ	1:A:547:ASP:OD2	2.41	0.44
1:A:233:GLN:C	1:A:235:GLY:HA2	2.42	0.44
1:A:418:TYR:HD2	1:A:742:ARG:CZ	2.31	0.44
1:A:654:PHE:HE1	1:A:681:VAL:HG21	1.82	0.44
1:A:602:ILE:O	1:A:602:ILE:CG1	2.66	0.43
1:A:775:LEU:HD21	1:A:836:LEU:HD11	1.99	0.43
1:A:232:THR:OG1	1:A:234:LEU:CB	2.66	0.43
1:A:238:GLN:OE1	1:A:350:ARG:NH2	2.51	0.43
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.80	0.43
1:A:231:SER:OG	1:A:240:PRO:HB3	2.19	0.43
1:A:317:ILE:HD11	1:A:409:MET:CE	2.47	0.43
1:A:583:SER:HA	3:P:11:DT:C5'	2.47	0.43
1:A:494:LEU:CD1	1:A:525:LEU:HB3	2.48	0.43
1:A:532:ILE:HA	1:A:532:ILE:HD13	1.75	0.43
1:A:486:GLU:O	1:A:490:GLY:CA	2.66	0.43
1:A:783:VAL:HG11	1:A:807:PHE:CZ	2.51	0.43
1:A:836:LEU:CD2	1:A:838:LEU:CD1	2.97	0.43
1:A:424:PHE:CZ	1:A:429:LEU:HD11	2.54	0.43
1:A:456:LEU:HG	1:A:589:ILE:HD11	2.00	0.43
1:A:418:TYR:CD2	1:A:742:ARG:NH1	2.87	0.42
1:A:450:MET:HE2	1:A:610:MET:HB3	2.00	0.42
1:A:678:LYS:O	1:A:681:VAL:HG22	2.18	0.42
1:A:445:VAL:CG2	1:A:553:MET:SD	3.07	0.42
1:A:617:HIS:CD2	1:A:810:GLU:HG3	2.53	0.42
1:A:726:ILE:HG13	1:A:764:VAL:HG23	2.00	0.42
2:T:3:DA:H5''	2:T:3:DA:C8	2.53	0.42
3:P:4:DT:C2'	3:P:5:DT:H72	2.48	0.42
1:A:421:TRP:CZ2	1:A:425:ARG:CD	3.01	0.42
1:A:428:GLU:C	1:A:430:PRO:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:O	1:A:366:GLU:C	2.60	0.42
3:P:7:DA:H2'	3:P:8:DC:C6	2.53	0.42
3:P:13:DG:H5''	3:P:13:DG:H8	1.85	0.42
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.92	0.42
1:A:486:GLU:O	1:A:490:GLY:HA3	2.19	0.42
1:A:606:SER:HA	1:A:607:PRO:HD3	1.72	0.41
3:P:3:DT:C6	3:P:4:DT:H72	2.55	0.41
1:A:277:ASP:HA	1:A:278:ASP:HA	1.80	0.41
1:A:463:GLU:OE2	1:A:592:PRO:CB	2.68	0.41
1:A:846:LEU:O	1:A:858:LEU:HG	2.20	0.41
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.67	0.41
1:A:694:ALA:HB2	1:A:701:ILE:HA	1.99	0.41
1:A:850:ARG:HE	1:A:850:ARG:HB2	1.75	0.41
3:P:5:DT:H2''	3:P:6:DG:N7	2.35	0.41
1:A:378:THR:HG23	1:A:379:VAL:HG22	2.03	0.41
1:A:318:CYS:O	1:A:348:ASP:HA	2.21	0.41
1:A:617:HIS:NE2	1:A:810:GLU:HG3	2.36	0.41
1:A:678:LYS:HA	1:A:681:VAL:HG22	2.02	0.41
1:A:488:LEU:HD21	1:A:528:LEU:CG	2.50	0.41
1:A:644:LEU:CD1	1:A:653:VAL:HG13	2.51	0.41
1:A:704:ALA:O	1:A:708:LEU:N	2.43	0.41
1:A:234:LEU:HD11	1:A:404:LEU:HD22	2.03	0.41
1:A:828:LEU:C	1:A:830:GLN:H	2.29	0.41
1:A:357:ASP:HA	1:A:358:PRO:HD2	1.72	0.40
1:A:532:ILE:HD12	1:A:532:ILE:HG23	1.91	0.40
1:A:665:PRO:O	1:A:666:VAL:C	2.64	0.40
1:A:738:ILE:HD13	1:A:738:ILE:HG21	1.80	0.40
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.92	0.40
1:A:457:LEU:CD2	1:A:589:ILE:HG21	2.51	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	615/666 (92%)	608 (99%)	7 (1%)	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	545/577 (94%)	522 (96%)	23 (4%)	26	60

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

Mol	Chain	Res	Type
1	A	223	ILE
1	A	241	VAL
1	A	247	ILE
1	A	309	THR
1	A	317	ILE
1	A	332	PHE
1	A	351	ILE
1	A	369	VAL
1	A	495	HIS
1	A	518	VAL
1	A	525	LEU
1	A	571	ARG
1	A	575	LYS
1	A	590	THR
1	A	602	ILE
1	A	605	ILE
1	A	728	GLN
1	A	738	ILE
1	A	801	ILE
1	A	834	LEU
1	A	838	LEU
1	A	847	SER
1	A	859	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	287	HIS
1	A	295	GLN
1	A	340	HIS
1	A	391	ASN
1	A	469	HIS
1	A	576	HIS
1	A	578	ASN
1	A	585	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	627/666 (94%)	0.58	70 (11%) 10 7	36, 72, 143, 165	0
2	T	9/9 (100%)	0.49	0 100 100	61, 72, 82, 99	0
3	P	13/13 (100%)	0.92	0 100 100	82, 102, 108, 109	0
All	All	649/688 (94%)	0.58	70 (10%) 11 7	36, 72, 143, 165	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	VAL	7.2
1	A	378	THR	5.6
1	A	373	CYS	4.9
1	A	271	LEU	4.6
1	A	696	CYS	4.5
1	A	289	ALA	4.4
1	A	699	VAL	4.3
1	A	661	TRP	4.1
1	A	272	GLU	4.0
1	A	237	ASP	4.0
1	A	602	ILE	4.0
1	A	204	ASP	3.8
1	A	657	LEU	3.8
1	A	255	ALA	3.8
1	A	591	THR	3.8
1	A	254	GLN	3.7
1	A	545	PHE	3.7
1	A	381	VAL	3.6
1	A	290	ILE	3.6
1	A	835	GLU	3.6
1	A	335	ASP	3.5
1	A	690	LYS	3.4
1	A	660	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	3.3
1	A	288	SER	3.2
1	A	662	LYS	3.2
1	A	669	VAL	3.2
1	A	239	THR	3.2
1	A	859	GLN	3.1
1	A	236	ALA	3.0
1	A	357	ASP	2.9
1	A	811	ASP	2.9
1	A	382	ASN	2.9
1	A	858	LEU	2.9
1	A	516	GLU	2.8
1	A	834	LEU	2.8
1	A	274	PHE	2.8
1	A	270	VAL	2.8
1	A	374	GLU	2.7
1	A	269	PRO	2.7
1	A	282	TYR	2.7
1	A	360	ASP	2.7
1	A	369	VAL	2.6
1	A	593	LYS	2.6
1	A	363	PRO	2.5
1	A	238	GLN	2.5
1	A	666	VAL	2.5
1	A	361	ALA	2.4
1	A	362	THR	2.4
1	A	291	TRP	2.4
1	A	546	VAL	2.4
1	A	496	LEU	2.4
1	A	391	ASN	2.3
1	A	802	HIS	2.3
1	A	287	HIS	2.3
1	A	385	TYR	2.3
1	A	380	LYS	2.3
1	A	659	SER	2.3
1	A	833	ALA	2.3
1	A	712	LEU	2.3
1	A	747	ARG	2.2
1	A	656	THR	2.1
1	A	196	HIS	2.1
1	A	293	GLN	2.1
1	A	528	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	2.1
1	A	671	HIS	2.1
1	A	695	ALA	2.1
1	A	675	GLU	2.1
1	A	644	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.