



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:29 AM UTC

PDB ID : 4XVK / pdb_00004xvk
Title : Binary complex of human polymerase nu and DNA with the finger domain closed
Authors : Lee, Y.-S.; Yang, W.
Deposited on : 2015-01-27
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

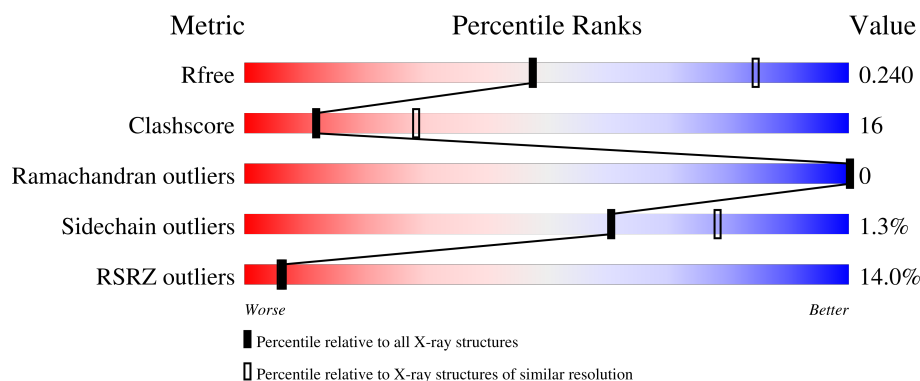
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	14% 69% 24% • 5%
2	P	15	7% 60% 40%
3	T	12	8% 58% 42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5558 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	630	Total	C	N	O	S	0	0	0
			4971	3167	874	905	25			

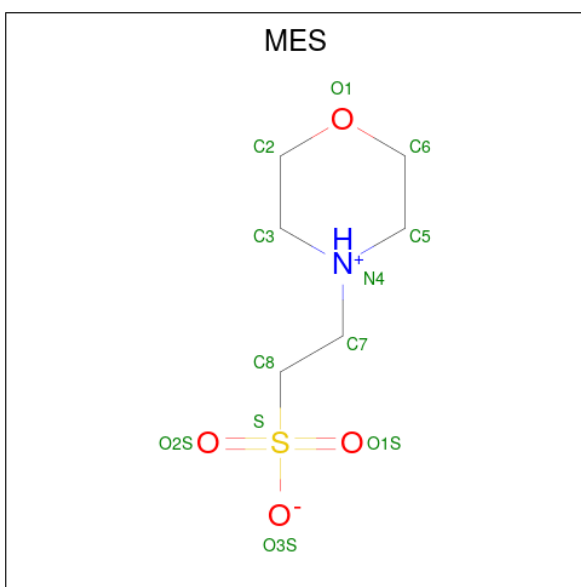
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*TP*CP*TP*GP*AP*CP*GP*CP*TP*AP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	15	Total	C	N	O	P	0	0	0
			306	146	58	88	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	12	Total	C	N	O	P	0	0	0
			244	116	43	73	12			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

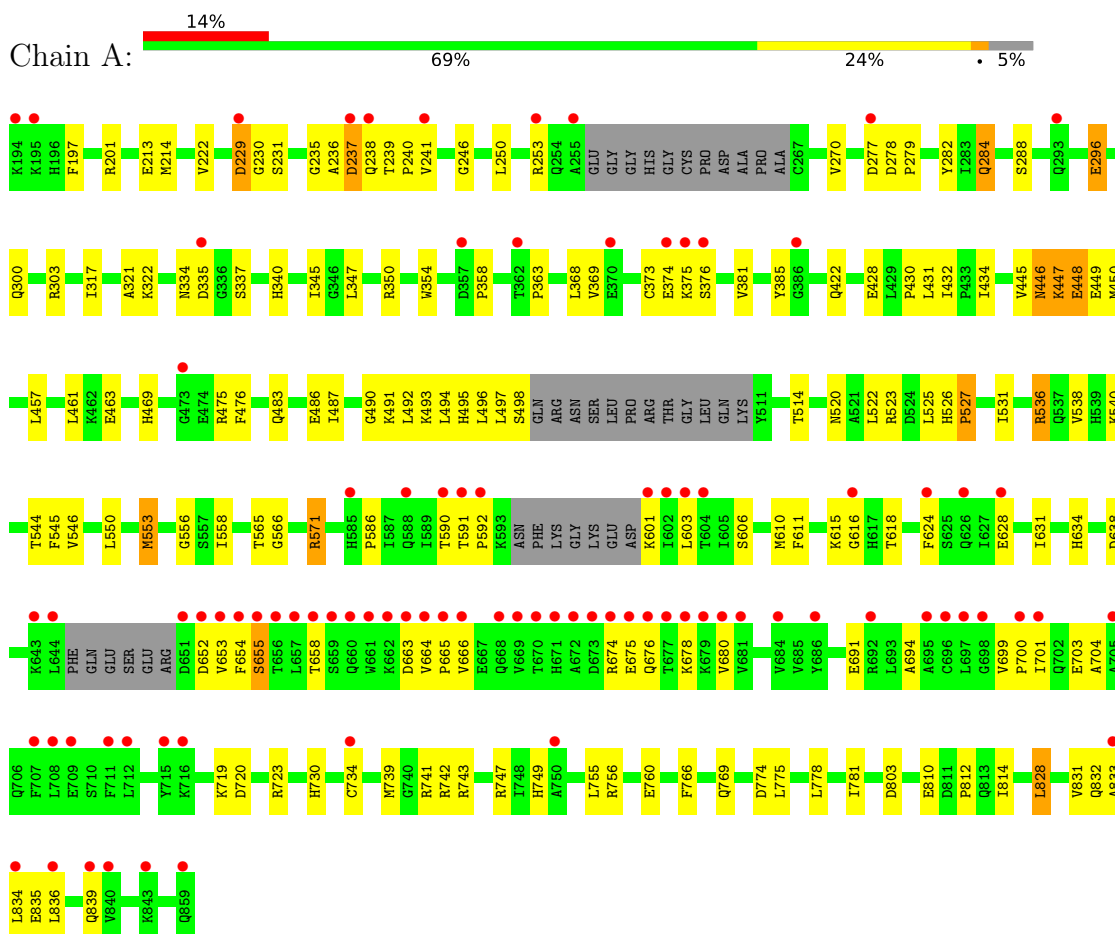
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	P	1	Total	O	0	0
			1	1		

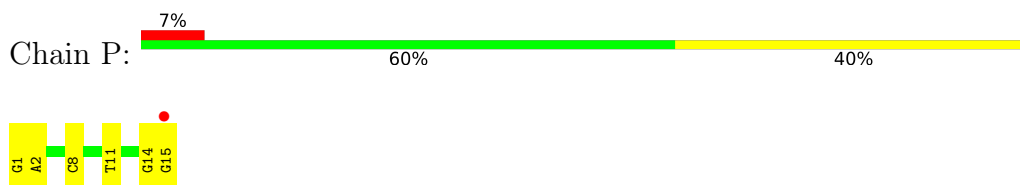
3 Residue-property plots [i](#)

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: DNA polymerase nu



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	290.88Å 290.88Å 110.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.64 – 2.95 29.64 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.64-2.95) 99.0 (29.64-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.241 0.223 , 0.240	Depositor DCC
R_{free} test set	1890 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5558	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, NA

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	0.56	1/5065 (0.0%)	0.88	13/6854 (0.2%)
2	P	0.15	0/343	0.65	0/528
3	T	0.15	0/272	0.69	0/417
All	All	0.53	1/5680 (0.0%)	0.86	13/7799 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	GLY	C-O	-7.11	1.16	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	N-CA-C	-9.29	94.11	108.42
1	A	334	ASN	N-CA-C	7.19	120.16	111.82
1	A	447	LYS	N-CA-C	-6.85	103.82	111.28
1	A	229	ASP	N-CA-C	6.04	117.87	111.28
1	A	527	PRO	CA-C-N	5.99	127.20	119.78
1	A	527	PRO	C-N-CA	5.99	127.20	119.78
1	A	238	GLN	N-CA-C	-5.65	106.06	113.12
1	A	638	ASP	CA-C-N	5.58	124.78	118.97
1	A	638	ASP	C-N-CA	5.58	124.78	118.97
1	A	446	ASN	N-CA-C	5.44	118.20	107.98
1	A	655	SER	N-CA-C	-5.16	105.73	112.23
1	A	448	GLU	N-CA-C	5.11	116.66	111.14
1	A	691	GLU	N-CA-C	5.08	116.50	110.97

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	4971	0	5071	166	0
2	P	306	0	170	8	0
3	T	244	0	136	5	0
4	A	12	0	12	1	0
5	A	1	0	0	0	0
6	A	23	0	0	7	0
6	P	1	0	0	0	0
All	All	5558	0	5389	172	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 16.

All (172) 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:526:HIS:ND1	1:A:527:PRO:HD2	1.51	1.23
1:A:486:GLU:O	1:A:490:GLY:HA3	1.57	1.04
1:A:655:SER:HB2	1:A:666:VAL:HG23	1.37	1.03
1:A:835:GLU:N	1:A:835:GLU:OE1	1.92	1.02
1:A:447:LYS:HB2	1:A:553:MET:HE1	1.39	1.02
1:A:448:GLU:N	1:A:448:GLU:OE1	2.00	0.95
1:A:526:HIS:ND1	1:A:527:PRO:CD	2.32	0.92
1:A:446:ASN:C	1:A:448:GLU:OE1	2.17	0.88
1:A:497:LEU:O	1:A:498:SER:OG	1.94	0.84
1:A:833:ALA:HB1	1:A:834:LEU:HA	1.58	0.83
1:A:449:GLU:HG3	1:A:610:MET:HE1	1.59	0.83
1:A:699:VAL:HG13	1:A:703:GLU:HB3	1.60	0.82
1:A:699:VAL:CG1	1:A:703:GLU:HB3	2.09	0.81
1:A:463:GLU:OE2	1:A:592:PRO:HB3	1.81	0.81
1:A:236:ALA:O	1:A:237:ASP:OD1	1.99	0.80
1:A:447:LYS:N	1:A:448:GLU:OE1	2.15	0.80
1:A:655:SER:HB2	1:A:666:VAL:CG2	2.09	0.80
1:A:526:HIS:CE1	1:A:527:PRO:HD2	2.16	0.80
1:A:213:GLU:HG2	6:A:1003:HOH:O	1.82	0.79
1:A:699:VAL:HG12	1:A:700:PRO:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:PHE:O	1:A:658:THR:HG23	1.86	0.76
1:A:486:GLU:O	1:A:490:GLY:CA	2.34	0.76
1:A:655:SER:CB	1:A:666:VAL:HG23	2.13	0.76
1:A:663:ASP:O	1:A:664:VAL:HG13	1.88	0.74
1:A:835:GLU:HG2	1:A:836:LEU:H	1.53	0.73
1:A:448:GLU:HG2	1:A:449:GLU:N	2.03	0.73
1:A:694:ALA:HB1	1:A:699:VAL:O	1.90	0.72
1:A:741:ARG:NH2	1:A:774:ASP:OD1	2.23	0.71
1:A:428:GLU:OE2	1:A:741:ARG:NH1	2.22	0.71
1:A:240:PRO:O	1:A:241:VAL:HG22	1.90	0.71
1:A:553:MET:HE2	1:A:556:GLY:HA2	1.72	0.71
1:A:832:GLN:OE1	1:A:833:ALA:HA	1.91	0.70
1:A:834:LEU:HB3	1:A:835:GLU:OE1	1.92	0.69
1:A:835:GLU:HG2	1:A:836:LEU:N	2.07	0.68
1:A:743:ARG:NH1	3:T:3:DG:OP1	2.27	0.66
1:A:492:LEU:HD13	1:A:526:HIS:CD2	2.31	0.66
1:A:540:LYS:NZ	2:P:11:DT:O2	2.29	0.66
1:A:527:PRO:O	1:A:531:ILE:HG12	1.96	0.66
1:A:810:GLU:HG2	1:A:812:PRO:HD2	1.78	0.65
1:A:288:SER:HB2	6:A:1005:HOH:O	1.96	0.65
1:A:663:ASP:C	1:A:664:VAL:HG13	2.22	0.65
1:A:719:LYS:HE3	1:A:723:ARG:HH11	1.62	0.65
1:A:526:HIS:CG	1:A:527:PRO:HD2	2.30	0.64
1:A:566:GLY:HA3	6:A:1008:HOH:O	1.96	0.64
1:A:448:GLU:H	1:A:448:GLU:CD	2.06	0.64
1:A:701:ILE:O	1:A:704:ALA:HB3	1.98	0.64
1:A:520:ASN:OD1	1:A:523:ARG:NH1	2.31	0.63
1:A:720:ASP:HA	1:A:723:ARG:NH2	2.12	0.63
1:A:449:GLU:CG	1:A:610:MET:HE1	2.29	0.62
1:A:694:ALA:HA	1:A:699:VAL:HB	1.82	0.62
1:A:495:HIS:CD2	1:A:496:LEU:CD2	2.82	0.62
1:A:836:LEU:O	1:A:836:LEU:HG	1.99	0.61
2:P:8:DC:H42	3:T:8:DG:H1	1.47	0.61
1:A:699:VAL:HG13	1:A:700:PRO:HD2	1.82	0.61
1:A:494:LEU:HD21	1:A:526:HIS:HB2	1.84	0.60
1:A:422:GLN:HG2	1:A:834:LEU:HD21	1.83	0.60
1:A:491:LYS:O	1:A:493:LYS:HG2	2.01	0.60
1:A:241:VAL:O	1:A:241:VAL:HG23	2.02	0.60
1:A:448:GLU:HG2	1:A:449:GLU:H	1.66	0.59
1:A:663:ASP:O	1:A:664:VAL:CG1	2.50	0.59
1:A:624:PHE:HB2	1:A:803:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HB2	1:A:494:LEU:HD12	1.85	0.59
1:A:497:LEU:C	1:A:498:SER:HG	2.03	0.59
1:A:491:LYS:O	1:A:493:LYS:CG	2.51	0.59
1:A:525:LEU:HD12	1:A:525:LEU:N	2.18	0.59
1:A:694:ALA:HB2	1:A:704:ALA:HB2	1.85	0.59
1:A:446:ASN:O	1:A:450:MET:HB2	2.04	0.58
1:A:457:LEU:HD22	1:A:538:VAL:HG13	1.86	0.57
1:A:631:ILE:HD11	1:A:775:LEU:HD12	1.86	0.57
1:A:495:HIS:NE2	1:A:496:LEU:HD21	2.20	0.56
1:A:655:SER:HB3	1:A:674:ARG:HH11	1.70	0.56
1:A:655:SER:CB	1:A:666:VAL:CG2	2.78	0.56
1:A:253:ARG:HD2	1:A:270:VAL:HG21	1.87	0.55
1:A:730:HIS:O	1:A:749:HIS:HE1	1.89	0.55
1:A:450:MET:HE2	1:A:610:MET:HB3	1.89	0.55
1:A:296:GLU:O	1:A:300:GLN:HG3	2.07	0.54
1:A:492:LEU:CB	1:A:494:LEU:HD12	2.39	0.53
1:A:445:VAL:HB	1:A:450:MET:HE1	1.89	0.53
1:A:495:HIS:CD2	1:A:496:LEU:HD23	2.43	0.53
1:A:369:VAL:O	1:A:373:CYS:HB2	2.09	0.52
1:A:446:ASN:CA	1:A:448:GLU:OE1	2.57	0.52
1:A:628:GLU:HB2	2:P:15:DG:H2"	1.92	0.52
1:A:525:LEU:N	1:A:525:LEU:CD1	2.73	0.52
1:A:664:VAL:HB	1:A:665:PRO:HD2	1.92	0.51
1:A:317:ILE:HG13	1:A:347:LEU:HB2	1.93	0.51
1:A:514:THR:O	1:A:536:ARG:NH1	2.44	0.51
1:A:586:PRO:HB3	1:A:606:SER:HB2	1.93	0.51
1:A:658:THR:HG21	1:A:674:ARG:HA	1.93	0.50
1:A:358:PRO:HG3	6:A:1022:HOH:O	2.11	0.50
1:A:719:LYS:HE3	1:A:723:ARG:NH1	2.25	0.50
1:A:457:LEU:O	1:A:461:LEU:HG	2.12	0.50
1:A:675:GLU:HA	1:A:678:LYS:HE3	1.93	0.50
1:A:448:GLU:CG	1:A:449:GLU:N	2.75	0.50
1:A:803:ASP:HB3	2:P:15:DG:OP1	2.11	0.50
1:A:445:VAL:HG23	1:A:553:MET:HE3	1.94	0.49
1:A:214:MET:HE1	1:A:279:PRO:HG3	1.94	0.49
1:A:494:LEU:HD23	1:A:525:LEU:CB	2.42	0.49
1:A:494:LEU:HD23	1:A:525:LEU:HB3	1.94	0.49
1:A:566:GLY:CA	6:A:1008:HOH:O	2.58	0.49
1:A:720:ASP:OD1	1:A:723:ARG:NH2	2.28	0.49
1:A:834:LEU:O	1:A:835:GLU:C	2.55	0.49
1:A:741:ARG:HG2	1:A:766:PHE:HZ	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD12	1:A:434:ILE:HD12	1.95	0.48
1:A:522:LEU:HD22	1:A:525:LEU:HD22	1.95	0.48
1:A:832:GLN:CD	1:A:833:ALA:HA	2.37	0.48
1:A:201:ARG:CZ	1:A:284:GLN:HG3	2.44	0.48
1:A:375:LYS:HG2	1:A:376:SER:H	1.79	0.48
1:A:739:MET:HE1	1:A:778:LEU:HD22	1.94	0.47
2:P:1:DG:H2'	2:P:2:DA:C8	2.49	0.47
1:A:676:GLN:O	1:A:680:VAL:HG23	2.14	0.47
1:A:345:ILE:H	4:A:901:MES:H21	1.79	0.47
1:A:778:LEU:HD23	1:A:828:LEU:HG	1.96	0.47
1:A:354:TRP:HB2	1:A:565:THR:HG23	1.98	0.46
1:A:618:THR:HG23	1:A:814:ILE:HD11	1.96	0.46
1:A:463:GLU:CD	1:A:592:PRO:HB3	2.40	0.46
1:A:628:GLU:CD	2:P:15:DG:H2''	2.41	0.46
1:A:491:LYS:O	1:A:493:LYS:HG3	2.16	0.46
1:A:450:MET:HB3	1:A:550:LEU:HD21	1.97	0.46
1:A:469:HIS:CD2	1:A:476:PHE:H	2.34	0.46
1:A:374:GLU:N	1:A:374:GLU:OE1	2.48	0.45
1:A:835:GLU:CG	1:A:836:LEU:H	2.25	0.45
1:A:831:VAL:HB	1:A:836:LEU:HD23	1.98	0.45
1:A:430:PRO:HG2	1:A:781:ILE:HD13	1.98	0.45
1:A:663:ASP:C	1:A:664:VAL:CG1	2.90	0.45
3:T:8:DG:H2''	3:T:9:DT:H5'	1.99	0.45
1:A:239:THR:HA	1:A:240:PRO:HD2	1.79	0.45
1:A:615:LYS:HD2	1:A:616:GLY:HA2	1.98	0.44
2:P:8:DC:N4	3:T:8:DG:H1	2.13	0.44
3:T:10:DC:H2''	3:T:11:DA:C8	2.52	0.44
1:A:229:ASP:HB2	1:A:231:SER:N	2.32	0.44
1:A:303:ARG:NH1	1:A:335:ASP:OD2	2.46	0.44
1:A:469:HIS:CD2	1:A:475:ARG:HA	2.52	0.44
1:A:699:VAL:CG1	1:A:700:PRO:HD2	2.48	0.44
1:A:222:VAL:HB	1:A:250:LEU:HB3	1.99	0.44
1:A:229:ASP:N	1:A:230:GLY:HA2	2.33	0.44
1:A:277:ASP:HA	1:A:278:ASP:HA	1.77	0.44
1:A:350:ARG:NH2	1:A:363:PRO:O	2.46	0.44
1:A:495:HIS:CD2	1:A:496:LEU:HD21	2.51	0.44
1:A:769:GLN:HG2	6:A:1013:HOH:O	2.18	0.43
1:A:236:ALA:O	1:A:237:ASP:CG	2.61	0.43
1:A:483:GLN:O	1:A:487:ILE:HG13	2.19	0.43
1:A:591:THR:HG22	1:A:601:LYS:O	2.18	0.43
1:A:321:ALA:HB3	1:A:432:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:CYS:SG	1:A:742:ARG:HB2	2.58	0.43
1:A:363:PRO:HG2	1:A:368:LEU:HD21	2.00	0.43
1:A:634:HIS:ND1	1:A:839:GLN:HG2	2.33	0.43
1:A:591:THR:HG21	1:A:601:LYS:HG2	2.00	0.43
1:A:553:MET:CE	1:A:556:GLY:HA2	2.46	0.43
1:A:654:PHE:O	1:A:658:THR:CG2	2.62	0.43
1:A:235:GLY:HA2	1:A:381:VAL:HB	2.01	0.42
1:A:374:GLU:HA	1:A:375:LYS:HA	1.72	0.42
1:A:558:ILE:HD11	1:A:611:PHE:HE2	1.83	0.42
1:A:495:HIS:NE2	1:A:496:LEU:CD2	2.82	0.42
1:A:544:THR:HG22	1:A:545:PHE:CD1	2.54	0.42
1:A:282:TYR:CE2	1:A:284:GLN:HG2	2.54	0.42
1:A:540:LYS:HA	1:A:540:LYS:HD2	1.83	0.42
1:A:590:THR:O	1:A:592:PRO:HD3	2.19	0.42
1:A:322:LYS:HE2	1:A:322:LYS:HB3	1.88	0.42
1:A:337:SER:H	1:A:340:HIS:CE1	2.38	0.41
1:A:652:ASP:OD1	1:A:653:VAL:N	2.44	0.41
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.94	0.41
1:A:571:ARG:CZ	1:A:769:GLN:HE21	2.33	0.41
1:A:747:ARG:HD3	1:A:755:LEU:HD13	2.02	0.41
1:A:832:GLN:HA	1:A:833:ALA:HA	1.86	0.41
1:A:450:MET:HG2	1:A:546:VAL:HG13	2.01	0.41
1:A:492:LEU:CB	1:A:494:LEU:CD1	2.99	0.41
1:A:603:LEU:HD12	1:A:603:LEU:HA	1.82	0.41
1:A:836:LEU:C	1:A:836:LEU:HD12	2.45	0.41
2:P:14:DG:H2'	2:P:15:DG:H5''	2.02	0.40
1:A:756:ARG:O	1:A:760:GLU:HG3	2.21	0.40
1:A:448:GLU:CG	1:A:449:GLU:H	2.34	0.40
1:A:385:TYR:OH	6:A:1001:HOH:O	2.11	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	620/666 (93%)	609 (98%)	11 (2%)	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	548/577 (95%)	541 (99%)	7 (1%)	61	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	PHE
1	A	284	GLN
1	A	296	GLU
1	A	536	ARG
1	A	553	MET
1	A	571	ARG
1	A	828	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	A	382	ASN
1	A	588	GLN
1	A	749	HIS
1	A	765	ASN
1	A	769	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	MES	A	901	-	12,12,12	2.34	1 (8%)	15,16,16	1.85	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	901	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	MES	C8-S	-7.85	1.66	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	MES	C5-N4-C3	4.62	118.79	108.84
4	A	901	MES	C6-C5-N4	-2.80	105.86	110.12
4	A	901	MES	O1S-S-C8	2.12	109.93	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	MES	1	0

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	630/666 (94%)	0.82	90 (14%) 6 6	29, 69, 139, 173	0
2	P	15/15 (100%)	0.87	1 (6%) 24 20	71, 85, 100, 105	0
3	T	12/12 (100%)	0.71	1 (8%) 17 15	50, 71, 96, 119	0
All	All	657/693 (94%)	0.82	92 (14%) 6 6	29, 70, 139, 173	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	657	LEU	6.3
1	A	696	CYS	6.1
1	A	695	ALA	6.0
1	A	661	TRP	5.9
1	A	679	LYS	5.8
1	A	697	LEU	5.7
1	A	678	LYS	5.3
1	A	662	LYS	4.6
1	A	194	LYS	4.6
1	A	656	THR	4.5
1	A	628	GLU	4.5
1	A	707	PHE	4.4
1	A	644	LEU	4.4
1	A	675	GLU	4.3
1	A	654	PHE	4.3
1	A	665	PRO	4.3
1	A	660	GLN	4.2
1	A	676	GLN	4.1
1	A	658	THR	4.0
1	A	655	SER	3.9
1	A	692	ARG	3.8
1	A	237	ASP	3.7
1	A	673	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	681	VAL	3.6
1	A	677	THR	3.6
1	A	716	LYS	3.6
1	A	653	VAL	3.6
1	A	370	GLU	3.6
1	A	238	GLN	3.5
1	A	833	ALA	3.5
1	A	701	ILE	3.5
1	A	674	ARG	3.5
1	A	834	LEU	3.5
1	A	684	VAL	3.5
1	A	374	GLU	3.3
1	A	712	LEU	3.2
1	A	666	VAL	3.2
1	A	659	SER	3.2
1	A	335	ASP	3.2
1	A	711	PHE	3.2
2	P	15	DG	3.1
1	A	686	TYR	3.1
1	A	473	GLY	3.1
1	A	603	LEU	3.1
1	A	602	ILE	3.0
1	A	670	THR	3.0
1	A	626	GLN	2.9
1	A	362	THR	2.8
1	A	229	ASP	2.8
1	A	375	LYS	2.7
1	A	715	TYR	2.7
1	A	705	ALA	2.7
1	A	386	GLY	2.6
1	A	672	ALA	2.6
1	A	601	LYS	2.6
1	A	651	ASP	2.6
1	A	253	ARG	2.6
1	A	652	ASP	2.5
1	A	664	VAL	2.5
1	A	277	ASP	2.5
1	A	255	ALA	2.5
1	A	843	LYS	2.5
3	T	0	DT	2.4
1	A	668	GLN	2.4
1	A	859	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	708	LEU	2.4
1	A	590	THR	2.4
1	A	734	CYS	2.3
1	A	680	VAL	2.3
1	A	616	GLY	2.3
1	A	293	GLN	2.3
1	A	840	VAL	2.3
1	A	671	HIS	2.2
1	A	592	PRO	2.2
1	A	588	GLN	2.2
1	A	669	VAL	2.2
1	A	195	LYS	2.2
1	A	643	LYS	2.2
1	A	709	GLU	2.2
1	A	839	GLN	2.1
1	A	357	ASP	2.1
1	A	376	SER	2.1
1	A	836	LEU	2.1
1	A	591	THR	2.1
1	A	585	HIS	2.1
1	A	241	VAL	2.1
1	A	700	PRO	2.1
1	A	750	ALA	2.1
1	A	698	GLY	2.0
1	A	604	THR	2.0
1	A	663	ASP	2.0
1	A	624	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	A	902	1/1	0.90	0.42	48,48,48,48	1
4	MES	A	901	12/12	0.92	0.10	49,67,86,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.