



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 12:57 AM EDT

PDB ID : 5E4F / pdb_00005e4f
Title : The spring alpha-helix coordinates multiple modes of HCV NS3 helicase action
Authors : Gu, M.; Rice, C.M.
Deposited on : 2015-10-05
Resolution : 2.10 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

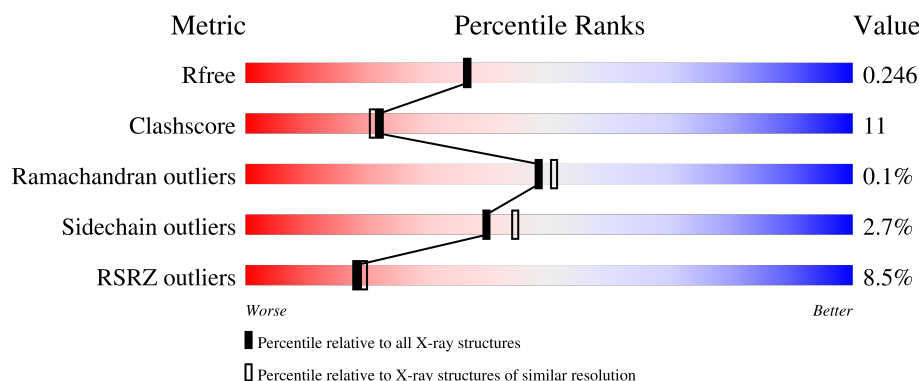
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	437	<div> <div>2%</div> <div>84%</div> <div>15%</div> </div>
1	B	437	<div> <div>15%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>

2 Entry composition [i](#)

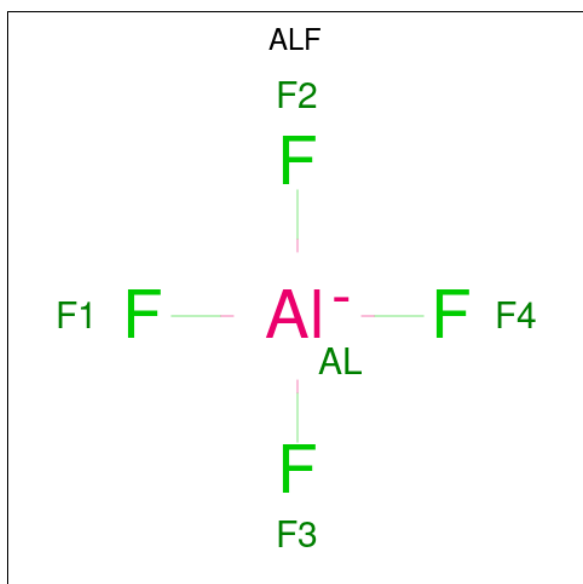
There are 5 unique types of molecules in this entry. The entry contains 7069 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine protease NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3280	2077	556	626	21			
1	B	429	Total	C	N	O	S	0	0	0
			3225	2042	547	615	21			

- Molecule 2 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Al	F	0	0
			5	1	4		
2	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

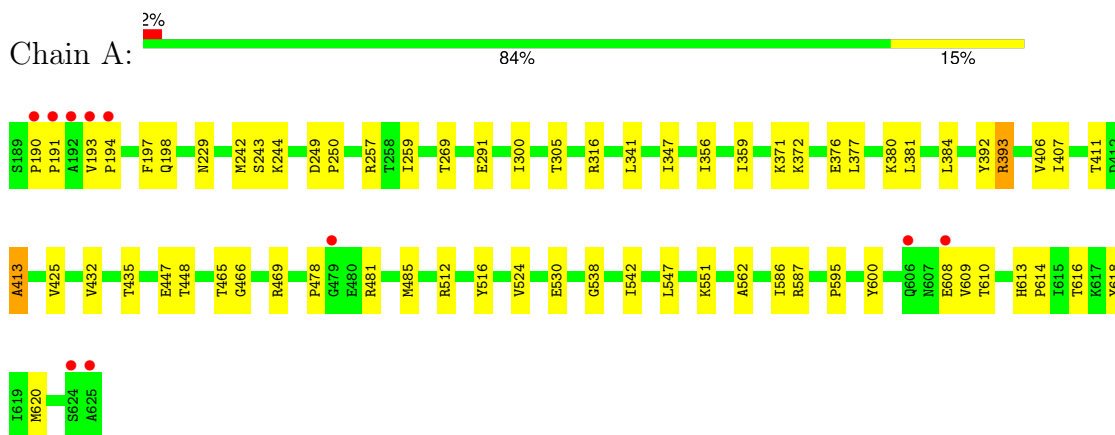
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	314	Total O 314 314	0	0
5	B	184	Total O 184 184	0	0

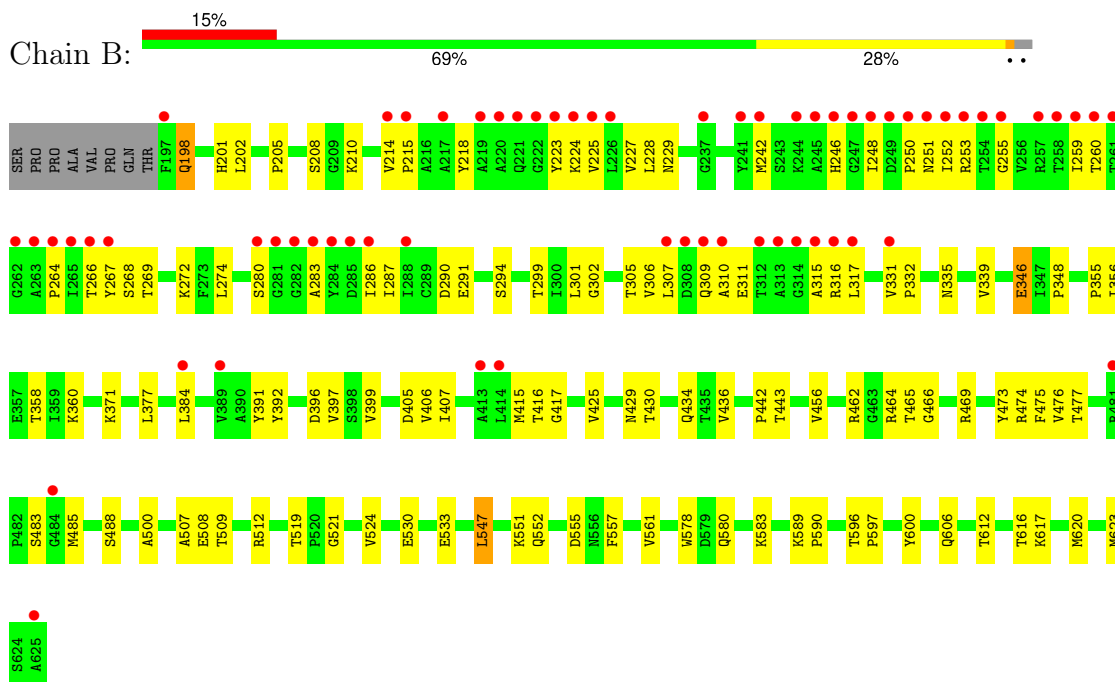
3 Residue-property plots

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: Serine protease NS3



• Molecule 1: Serine protease NS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.45Å 46.10Å 109.04Å 90.00° 104.05° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (50.00-2.10) 93.8 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.252 0.207 , 0.246	Depositor DCC
R_{free} test set	2536 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	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	0.92	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ALF, MG

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	0.34	0/3361	0.61	0/4592
1	B	0.31	0/3303	0.55	0/4509
All	All	0.33	0/6664	0.58	0/9101

There are no bond length outliers.

There are no bond angle outliers.

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	3280	0	3241	50	0
1	B	3225	0	3186	88	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	314	0	0	14	0
5	B	184	0	0	15	0
All	All	7069	0	6451	137	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 11.

All (137) 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:B:253:ARG:HH11	1:B:253:ARG:HB3	1.49	0.78
1:B:253:ARG:HB3	1:B:253:ARG:NH1	1.98	0.78
1:B:225:VAL:HG12	1:B:286:ILE:HB	1.64	0.78
1:A:250:PRO:HD2	5:A:801:HOH:O	1.85	0.76
1:A:435:THR:HG21	5:A:1078:HOH:O	1.87	0.74
1:A:191:PRO:HD2	5:A:815:HOH:O	1.90	0.72
1:A:485:MET:HG2	1:A:524:VAL:HG23	1.70	0.71
1:B:580:GLN:O	1:B:583:LYS:HG3	1.91	0.70
1:B:397:VAL:HG22	5:B:833:HOH:O	1.91	0.69
1:A:242:MET:HB2	5:A:801:HOH:O	1.93	0.69
1:A:249:ASP:HB3	5:A:997:HOH:O	1.95	0.66
1:B:202:LEU:HD21	1:B:214:VAL:HG21	1.77	0.66
1:A:257:ARG:NH1	1:A:259:ILE:HG12	2.12	0.65
1:B:391:TYR:OH	1:B:397:VAL:HG12	1.97	0.64
1:B:429:ASN:ND2	1:B:476:VAL:H	1.94	0.64
1:B:371:LYS:HG3	5:B:874:HOH:O	1.97	0.64
1:B:331:VAL:HG13	1:B:332:PRO:HD2	1.81	0.62
1:A:425:VAL:HG23	1:A:465:THR:HB	1.80	0.62
1:B:396:ASP:O	1:B:399:VAL:HG22	1.99	0.62
1:B:485:MET:HB2	1:B:524:VAL:O	1.99	0.61
1:B:355:PRO:HB2	1:B:358:THR:HG23	1.81	0.61
1:B:589:LYS:HB3	1:B:590:PRO:HD3	1.83	0.61
1:B:346:GLU:H	1:B:346:GLU:CD	2.04	0.60
1:B:255:GLY:HA2	1:B:272:LYS:HD3	1.84	0.60
1:B:251:ASN:HB2	1:B:266:THR:HG23	1.84	0.60
1:A:595:PRO:HA	1:A:608:GLU:HG3	1.84	0.60
1:B:612:THR:O	1:B:617:LYS:HE3	2.03	0.59
1:A:243:SER:N	5:A:801:HOH:O	2.34	0.59
1:A:305:THR:OG1	1:A:512:ARG:HD3	2.02	0.59
1:A:547:LEU:O	1:A:551:LYS:HG3	2.02	0.58
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.03	0.58
1:B:547:LEU:O	1:B:551:LYS:HG3	2.04	0.57
1:A:372:LYS:HE2	1:A:376:GLU:OE1	2.05	0.57
1:B:311:GLU:HB2	5:B:801:HOH:O	2.04	0.57
1:B:252:ILE:HD12	1:B:252:ILE:N	2.19	0.57
1:A:257:ARG:HH11	1:A:257:ARG:HG2	1.69	0.57
1:B:415:MET:O	1:B:464:ARG:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ASN:HD21	1:B:475:PHE:HB2	1.70	0.55
1:B:224:LYS:HA	1:B:264:PRO:O	2.07	0.54
1:A:616:THR:O	1:A:620:MET:HG3	2.07	0.54
1:B:530:GLU:HG3	5:B:898:HOH:O	2.07	0.53
1:B:346:GLU:OE2	1:B:356:ILE:HG13	2.08	0.53
1:B:229:ASN:O	1:B:269:THR:HA	2.09	0.53
1:A:542:ILE:HD11	1:A:562:ALA:HB3	1.91	0.53
1:B:242:MET:O	1:B:246:HIS:HB2	2.09	0.52
1:A:380:LYS:HD2	5:A:1081:HOH:O	2.10	0.52
1:B:339:VAL:O	1:B:474:ARG:HA	2.09	0.52
1:B:223:TYR:O	1:B:264:PRO:HB2	2.09	0.52
1:A:393:ARG:NE	1:A:393:ARG:H	2.08	0.52
1:B:508:GLU:O	1:B:512:ARG:HG3	2.10	0.51
1:B:507:ALA:HA	1:B:533:GLU:OE2	2.11	0.51
1:B:578:TRP:CZ2	1:B:589:LYS:HG3	2.46	0.51
1:A:194:PRO:HD2	5:A:1088:HOH:O	2.11	0.51
1:B:443:THR:O	1:B:623:MET:HE1	2.11	0.51
1:B:228:LEU:HD23	1:B:268:SER:HB3	1.93	0.50
1:B:294:SER:HB2	1:B:299:THR:HG21	1.92	0.50
1:A:538:GLY:HA3	1:A:618:TYR:CE2	2.46	0.50
1:A:193:VAL:HG23	5:A:952:HOH:O	2.12	0.50
1:B:214:VAL:N	1:B:215:PRO:HD2	2.27	0.49
1:B:429:ASN:HD21	1:B:476:VAL:H	1.61	0.49
1:A:229:ASN:O	1:A:269:THR:HA	2.13	0.49
1:A:250:PRO:CD	5:A:801:HOH:O	2.54	0.49
1:B:416:THR:HG23	5:B:942:HOH:O	2.13	0.49
1:B:466:GLY:HA2	1:B:469:ARG:O	2.13	0.49
1:B:309:GLN:N	5:B:804:HOH:O	2.46	0.48
1:B:225:VAL:HG12	1:B:286:ILE:CB	2.41	0.48
1:B:251:ASN:HA	1:B:259:ILE:O	2.14	0.48
1:B:485:MET:HA	5:B:841:HOH:O	2.13	0.48
1:A:393:ARG:HH21	1:A:413:ALA:HB3	1.79	0.47
1:A:371:LYS:HE3	1:A:392:TYR:CD2	2.49	0.46
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.29	0.46
1:A:356:ILE:HD11	1:A:384:LEU:HD13	1.97	0.46
1:B:198:GLN:HG3	5:B:814:HOH:O	2.15	0.46
1:B:227:VAL:HG13	1:B:267:TYR:HA	1.97	0.46
1:A:190:PRO:HA	1:A:191:PRO:HD2	1.88	0.45
1:A:432:VAL:HG12	1:A:448:THR:CG2	2.46	0.45
1:B:429:ASN:ND2	1:B:476:VAL:N	2.64	0.45
1:A:393:ARG:NH2	5:A:814:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLN:O	1:B:317:LEU:HD12	2.16	0.45
1:B:205:PRO:HG2	1:B:208:SER:HB3	1.98	0.45
1:B:360:LYS:HE3	5:B:966:HOH:O	2.16	0.45
1:B:456:VAL:HG23	1:B:483:SER:OG	2.17	0.45
1:A:393:ARG:NH2	1:A:411:THR:OG1	2.50	0.45
1:B:406:VAL:HG22	1:B:407:ILE:N	2.32	0.45
1:B:462:ARG:HG3	1:B:473:TYR:CG	2.52	0.45
1:A:341:LEU:HD23	5:A:961:HOH:O	2.16	0.44
1:B:436:VAL:HG11	1:B:488:SER:HB3	1.98	0.44
1:B:201:HIS:CE1	1:B:521:GLY:HA3	2.52	0.44
1:B:291:GLU:HG3	1:B:416:THR:HG22	1.98	0.44
1:B:253:ARG:HH11	1:B:253:ARG:CB	2.26	0.44
1:A:478:PRO:HD2	1:B:606:GLN:NE2	2.33	0.44
1:B:552:GLN:HG3	5:B:870:HOH:O	2.17	0.44
1:A:359:ILE:HD12	1:A:407:ILE:HD13	1.98	0.44
1:B:218:TYR:HB3	1:B:225:VAL:HG11	2.00	0.44
1:B:335:ASN:HB3	1:B:469:ARG:O	2.17	0.44
1:B:346:GLU:CD	1:B:346:GLU:N	2.69	0.44
1:B:301:LEU:HD21	1:B:509:THR:HG23	2.00	0.43
1:B:307:LEU:HD13	1:B:519:THR:OG1	2.18	0.43
1:A:406:VAL:HG22	1:A:407:ILE:N	2.34	0.43
1:B:429:ASN:ND2	1:B:477:THR:H	2.16	0.43
1:B:225:VAL:CG1	1:B:286:ILE:HD12	2.48	0.43
1:B:287:ILE:HG21	1:B:306:VAL:CG1	2.49	0.43
1:B:557:PHE:O	1:B:561:VAL:HG23	2.19	0.43
1:B:430:THR:HG21	5:B:930:HOH:O	2.19	0.42
1:B:250:PRO:O	1:B:252:ILE:HD12	2.19	0.42
1:B:612:THR:C	1:B:617:LYS:HE3	2.40	0.42
1:B:616:THR:O	1:B:620:MET:HG3	2.20	0.42
1:B:210:LYS:HE2	5:B:845:HOH:O	2.18	0.42
1:B:310:ALA:HB1	1:B:315:ALA:HB3	2.01	0.42
1:B:348:PRO:HB3	5:B:891:HOH:O	2.20	0.42
1:B:246:HIS:HB3	1:B:248:ILE:HG22	2.01	0.42
1:B:316:ARG:HB3	5:B:964:HOH:O	2.20	0.42
1:A:291:GLU:HA	1:A:291:GLU:OE2	2.19	0.42
1:A:193:VAL:HG22	1:A:316:ARG:CD	2.50	0.42
1:A:244:LYS:HD3	5:A:827:HOH:O	2.19	0.42
1:B:311:GLU:CB	5:B:801:HOH:O	2.66	0.42
1:A:586:ILE:HG23	1:A:587:ARG:N	2.35	0.41
1:A:609:VAL:HG12	1:A:610:THR:N	2.35	0.41
1:B:485:MET:CB	1:B:524:VAL:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:O	1:A:198:GLN:NE2	2.54	0.41
1:B:596:THR:HA	1:B:597:PRO:HD3	1.88	0.41
1:B:417:GLY:HA2	2:B:701:ALF:F1	2.11	0.41
1:A:466:GLY:HA2	1:A:469:ARG:O	2.21	0.41
1:B:228:LEU:HA	1:B:268:SER:O	2.21	0.41
1:B:500:ALA:HB1	1:B:551:LYS:HD3	2.03	0.41
1:A:193:VAL:CG2	1:A:316:ARG:HG3	2.50	0.41
1:A:193:VAL:O	1:A:193:VAL:HG13	2.20	0.41
1:A:244:LYS:HG2	1:A:244:LYS:O	2.21	0.41
1:A:542:ILE:HD11	1:A:562:ALA:CB	2.51	0.41
1:A:300:ILE:HD12	1:A:516:TYR:CZ	2.55	0.41
1:A:613:HIS:ND1	1:A:614:PRO:HD2	2.36	0.40
1:A:347:ILE:HD13	1:A:381:LEU:HD21	2.04	0.40
1:A:542:ILE:HG22	5:A:971:HOH:O	2.21	0.40
1:B:280:SER:HB2	1:B:283:ALA:HB3	2.02	0.40
1:B:201:HIS:HE1	1:B:521:GLY:HA3	1.87	0.40
1:B:274:LEU:HD21	1:B:302:GLY:HA2	2.04	0.40
1:B:425:VAL:HG23	1:B:465:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/437 (100%)	421 (97%)	13 (3%)	1 (0%)	44	45
1	B	427/437 (98%)	394 (92%)	33 (8%)	0	100	100
All	All	862/874 (99%)	815 (94%)	46 (5%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ALA

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	356/356 (100%)	350 (98%)	6 (2%)	56	63
1	B	349/356 (98%)	336 (96%)	13 (4%)	29	31
All	All	705/712 (99%)	686 (97%)	19 (3%)	40	44

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	LEU
1	A	393	ARG
1	A	447	GLU
1	A	481	ARG
1	A	530	GLU
1	A	600	TYR
1	B	198	GLN
1	B	260	THR
1	B	290	ASP
1	B	346	GLU
1	B	377	LEU
1	B	384	LEU
1	B	392	TYR
1	B	405	ASP
1	B	434	GLN
1	B	442	PRO
1	B	547	LEU
1	B	555	ASP
1	B	600	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	518	ASN
1	A	526	GLN
1	A	572	GLN
1	B	333	HIS
1	B	429	ASN
1	B	434	GLN
1	B	518	ASN
1	B	545	HIS
1	B	606	GLN

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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	ALF	B	701	-	4,4,4	0.07	0	-		
2	ALF	A	701	-	4,4,4	0.13	0	-		
3	ADP	A	702	4	24,29,29	1.36	3 (12%)	29,45,45	1.71	3 (10%)
3	ADP	B	702	4	24,29,29	1.28	3 (12%)	29,45,45	1.66	2 (6%)

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
3	ADP	B	702	4	-	3/12/32/32	0/3/3/3
3	ADP	A	702	4	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	ADP	O4'-C1'	3.90	1.46	1.40
3	B	702	ADP	O4'-C1'	3.07	1.44	1.40
3	B	702	ADP	C5-N7	-2.50	1.30	1.39
3	A	702	ADP	C2-N3	2.42	1.35	1.32
3	A	702	ADP	C5-N7	-2.38	1.31	1.39
3	B	702	ADP	PA-O3A	-2.30	1.57	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ADP	N3-C2-N1	-7.33	118.72	128.67
3	A	702	ADP	N3-C2-N1	-7.13	119.00	128.67
3	A	702	ADP	O4'-C1'-N9	4.00	114.05	108.75
3	B	702	ADP	O4'-C1'-N9	2.84	112.51	108.75
3	A	702	ADP	C4-C5-N7	-2.58	106.61	109.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

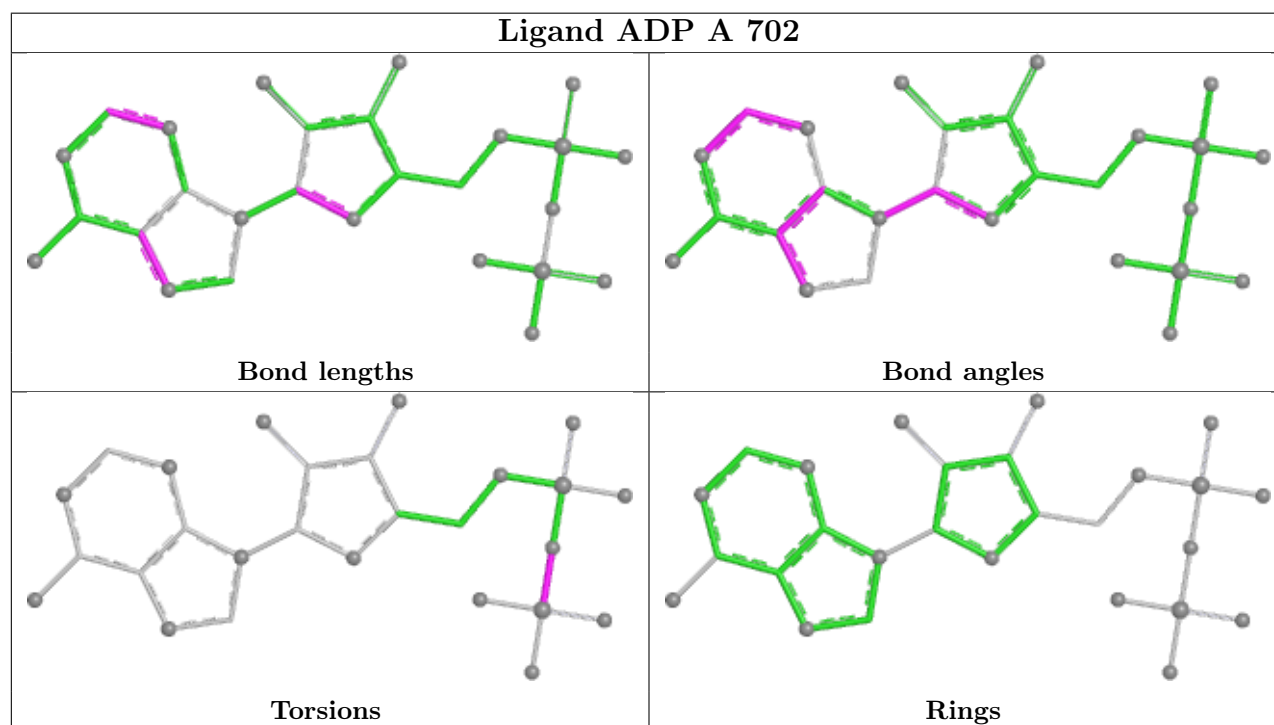
Mol	Chain	Res	Type	Atoms
3	B	702	ADP	PA-O3A-PB-O3B
3	A	702	ADP	PA-O3A-PB-O1B
3	B	702	ADP	PA-O3A-PB-O2B
3	B	702	ADP	PA-O3A-PB-O1B
3	A	702	ADP	PA-O3A-PB-O2B
3	A	702	ADP	PA-O3A-PB-O3B

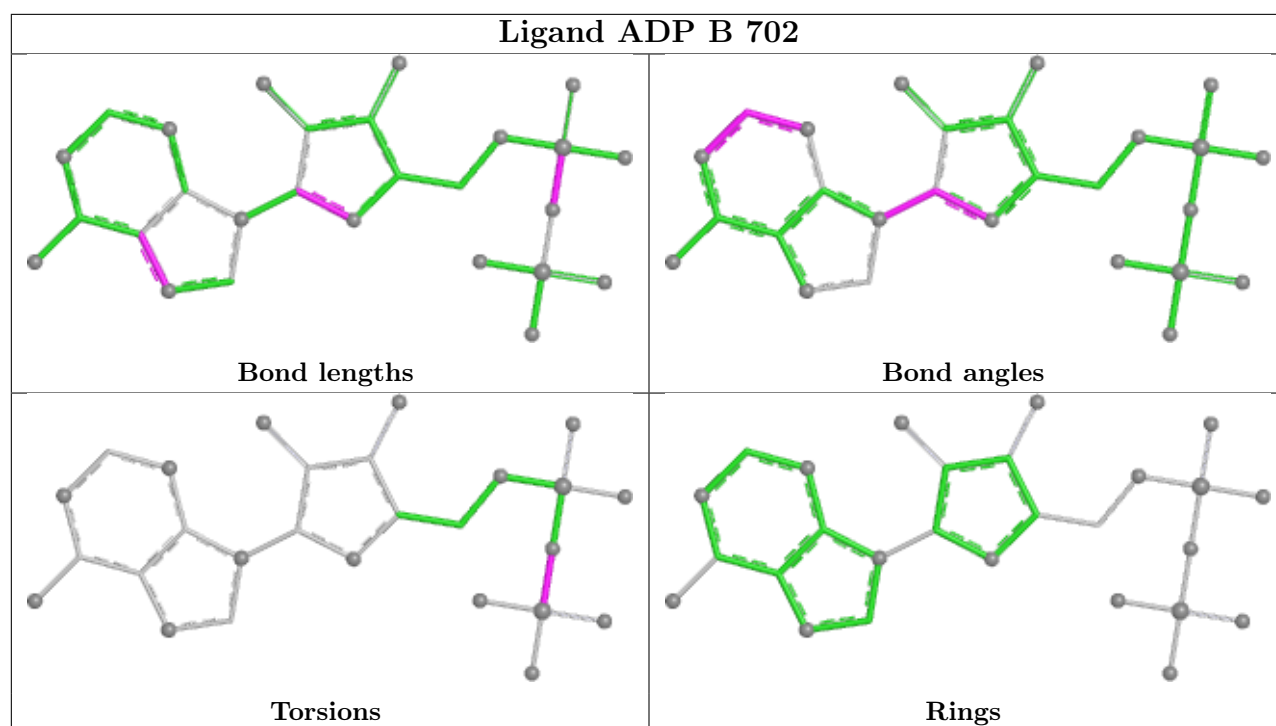
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ALF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	437/437 (100%)	-0.08	10 (2%) 61 63	6, 18, 35, 51	0
1	B	429/437 (98%)	0.84	64 (14%) 7 7	12, 29, 50, 56	0
All	All	866/874 (99%)	0.38	74 (8%) 18 19	6, 24, 47, 56	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	VAL	5.6
1	B	248	ILE	4.9
1	A	192	ALA	4.9
1	B	312	THR	4.6
1	B	250	PRO	4.5
1	A	479	GLY	4.5
1	B	260	THR	4.5
1	B	265	ILE	4.4
1	B	219	ALA	4.4
1	B	225	VAL	4.2
1	B	262	GLY	4.2
1	B	284	TYR	3.9
1	A	191	PRO	3.8
1	A	625	ALA	3.7
1	B	313	ALA	3.7
1	B	264	PRO	3.7
1	B	263	ALA	3.7
1	B	220	ALA	3.6
1	B	249	ASP	3.6
1	B	285	ASP	3.6
1	B	258	THR	3.5
1	B	261	THR	3.5
1	B	217	ALA	3.4
1	B	251	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	222	GLY	3.3
1	B	315	ALA	3.2
1	B	625	ALA	3.2
1	B	247	GLY	3.1
1	B	314	GLY	3.0
1	B	281	GLY	3.0
1	B	308	ASP	2.9
1	B	413	ALA	2.9
1	B	257	ARG	2.9
1	B	223	TYR	2.8
1	B	254	THR	2.8
1	A	190	PRO	2.8
1	B	310	ALA	2.7
1	B	252	ILE	2.7
1	B	237	GLY	2.7
1	B	226	LEU	2.7
1	B	280	SER	2.7
1	B	316	ARG	2.7
1	B	197	PHE	2.6
1	A	194	PRO	2.6
1	B	215	PRO	2.6
1	B	481	ARG	2.6
1	B	484	GLY	2.6
1	B	214	VAL	2.5
1	B	224	LYS	2.5
1	B	259	ILE	2.5
1	B	255	GLY	2.5
1	B	253	ARG	2.5
1	B	266	THR	2.5
1	B	241	TYR	2.4
1	B	283	ALA	2.4
1	B	245	ALA	2.4
1	B	286	ILE	2.4
1	B	307	LEU	2.3
1	A	608	GLU	2.3
1	B	244	LYS	2.3
1	B	267	TYR	2.2
1	B	282	GLY	2.2
1	B	221	GLN	2.2
1	B	384	LEU	2.2
1	B	414	LEU	2.2
1	A	624	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	288	ILE	2.2
1	B	246	HIS	2.1
1	B	242	MET	2.1
1	A	606	GLN	2.1
1	B	389	VAL	2.1
1	B	317	LEU	2.1
1	B	309	GLN	2.1
1	B	331	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

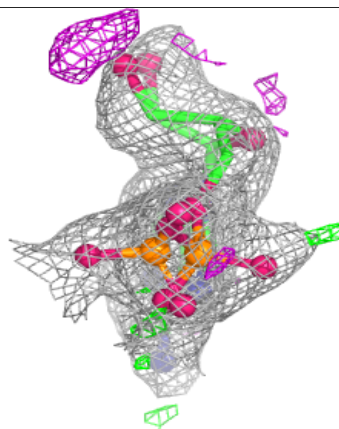
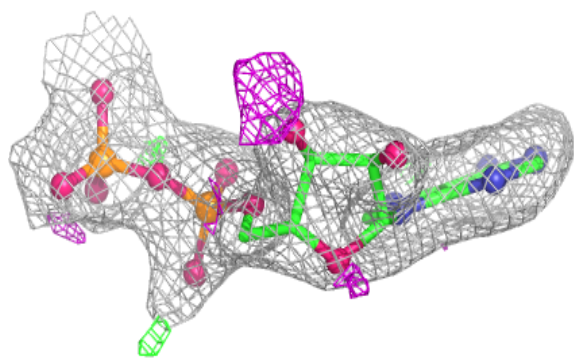
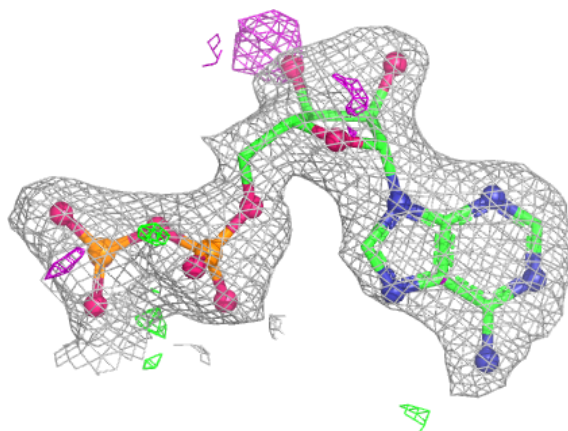
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	703	1/1	0.86	0.11	36,36,36,36	0
3	ADP	B	702	27/27	0.91	0.11	25,31,34,36	0
4	MG	A	703	1/1	0.95	0.07	12,12,12,12	0
2	ALF	B	701	5/5	0.96	0.06	21,22,22,22	0
3	ADP	A	702	27/27	0.98	0.06	6,15,19,21	0
2	ALF	A	701	5/5	0.98	0.05	10,12,15,15	0

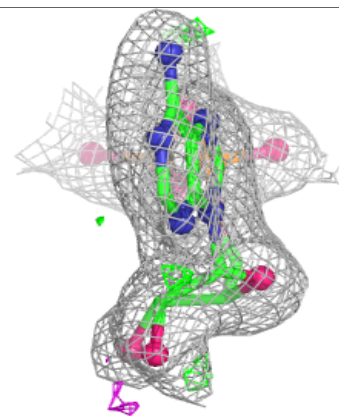
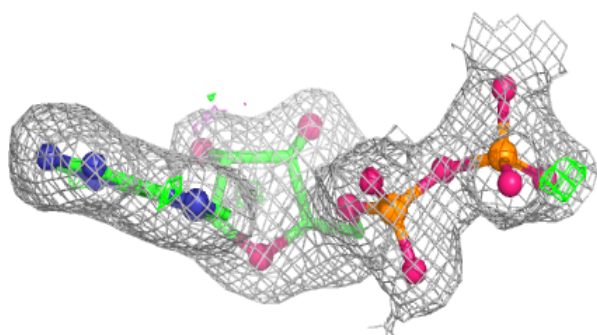
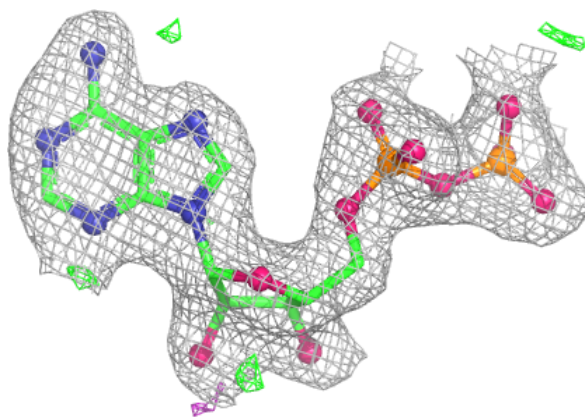
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.