



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:35 am BST

PDB ID : 3ZGZ
Title : Ternary complex of E. coli leucyl-tRNA synthetase, tRNA(leu) and toxic moiety from agrocin 84 (TM84) in aminoacylation-like conformation
Authors : Chopra, S.; Palencia, A.; Virus, C.; Tripathy, A.; Temple, B.R.; Velazquez-Campoy, A.; Cusack, S.; Reader, J.S.
Deposited on : 2012-12-19
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

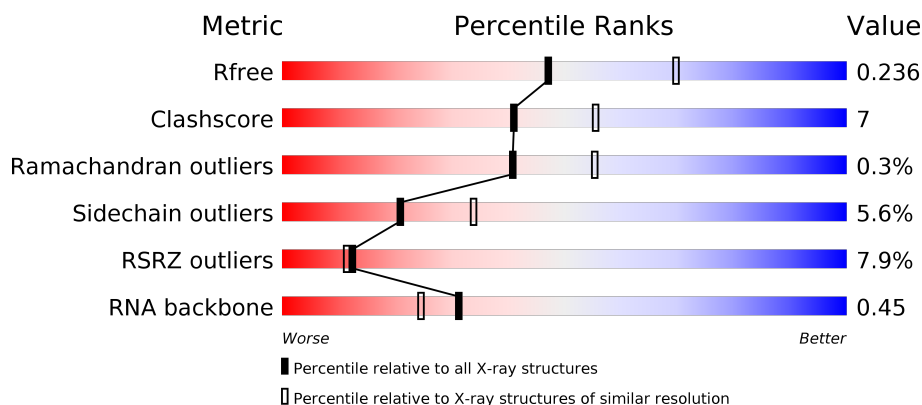
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	880	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	D	880	<div> <div>14%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	B	88	<div> <div>3%</div> <div>57%</div> <div>30%</div> <div>7%</div> <div>7%</div> </div>
2	E	88	<div> <div>8%</div> <div>70%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17522 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 LEUCINE-TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	0	0
			6834	4339	1159	1291	45			
1	D	867	Total	C	N	O	S	0	0	0
			6881	4369	1168	1299	45			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07813
A	-18	GLY	-	expression tag	UNP P07813
A	-17	SER	-	expression tag	UNP P07813
A	-16	SER	-	expression tag	UNP P07813
A	-15	HIS	-	expression tag	UNP P07813
A	-14	HIS	-	expression tag	UNP P07813
A	-13	HIS	-	expression tag	UNP P07813
A	-12	HIS	-	expression tag	UNP P07813
A	-11	HIS	-	expression tag	UNP P07813
A	-10	HIS	-	expression tag	UNP P07813
A	-9	SER	-	expression tag	UNP P07813
A	-8	SER	-	expression tag	UNP P07813
A	-7	GLY	-	expression tag	UNP P07813
A	-6	LEU	-	expression tag	UNP P07813
A	-5	VAL	-	expression tag	UNP P07813
A	-4	PRO	-	expression tag	UNP P07813
A	-3	ARG	-	expression tag	UNP P07813
A	-2	GLY	-	expression tag	UNP P07813
A	-1	SER	-	expression tag	UNP P07813
A	0	HIS	-	expression tag	UNP P07813
D	-19	MET	-	expression tag	UNP P07813
D	-18	GLY	-	expression tag	UNP P07813
D	-17	SER	-	expression tag	UNP P07813
D	-16	SER	-	expression tag	UNP P07813
D	-15	HIS	-	expression tag	UNP P07813

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P07813
D	-13	HIS	-	expression tag	UNP P07813
D	-12	HIS	-	expression tag	UNP P07813
D	-11	HIS	-	expression tag	UNP P07813
D	-10	HIS	-	expression tag	UNP P07813
D	-9	SER	-	expression tag	UNP P07813
D	-8	SER	-	expression tag	UNP P07813
D	-7	GLY	-	expression tag	UNP P07813
D	-6	LEU	-	expression tag	UNP P07813
D	-5	VAL	-	expression tag	UNP P07813
D	-4	PRO	-	expression tag	UNP P07813
D	-3	ARG	-	expression tag	UNP P07813
D	-2	GLY	-	expression tag	UNP P07813
D	-1	SER	-	expression tag	UNP P07813
D	0	HIS	-	expression tag	UNP P07813

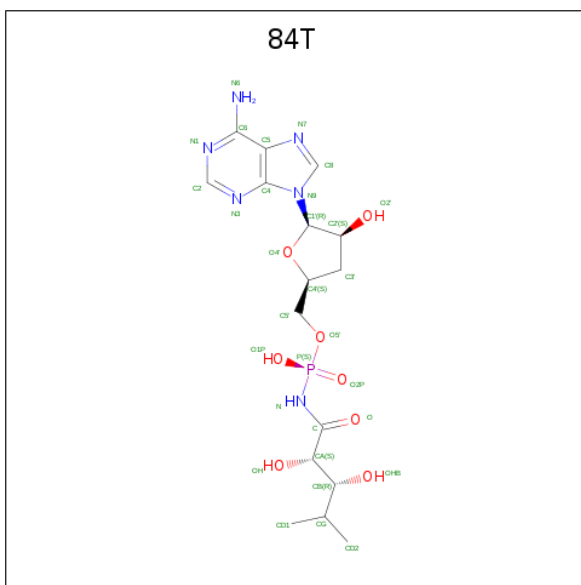
- Molecule 2 is a RNA chain called TRNA-LEU UAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	P	0	0	1
			1692	749	304	558	81			
2	E	80	Total	C	N	O	P	0	0	1
			1675	743	304	549	79			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is [(2S,4S,5R)-5-(6-aminopurin-9-yl)-4-oxidanyl-oxolan-2-yl]methoxy-N-[(2S,3R)-4-methyl-2,3-bis(oxidanyl)pentanoyl]phosphonamidic acid (three-letter code: 84T) (formula: C₁₆H₂₅N₆O₈P).



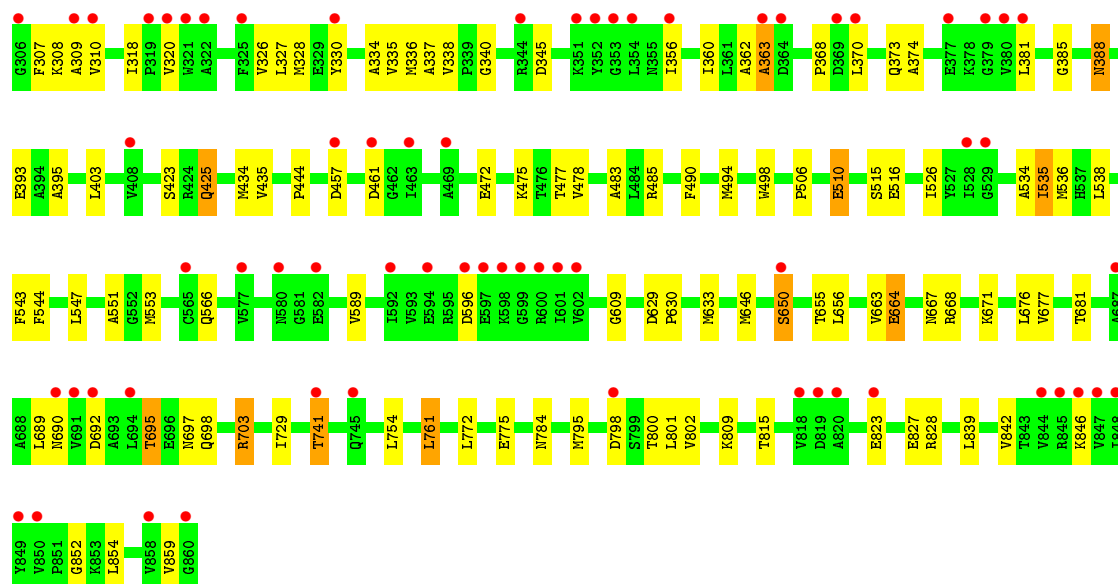
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	16	6	8	1		
4	D	1	Total	C	N	O	P	0	0
			31	16	6	8	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	Mg	0	0
			5	5		
5	E	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

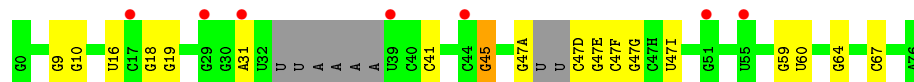
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		
6	B	75	Total	O	0	0
			75	75		
6	D	42	Total	O	0	0
			42	42		
6	E	5	Total	O	0	0
			5	5		



• Molecule 2: TRNA-LEU UAA ISOACCEPTOR



• Molecule 2: TRNA-LEU UAA ISOACCEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.58Å 68.19Å 226.22Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	43.59 – 2.40 43.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (43.59-2.40) 93.3 (43.59-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.187 , 0.238 0.187 , 0.236	Depositor DCC
R_{free} test set	4280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	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	0.95	EDS
Total number of atoms	17522	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: ZN, 84T, 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	0.74	1/6995 (0.0%)	0.85	12/9497 (0.1%)
1	D	0.56	1/7043 (0.0%)	0.65	0/9562
2	B	0.54	1/1887 (0.1%)	0.99	9/2939 (0.3%)
2	E	0.31	0/1869	0.76	0/2911
All	All	0.62	3/17794 (0.0%)	0.78	21/24909 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	C	O3'-P	-5.64	1.54	1.61
1	A	585	TRP	CD2-CE2	5.47	1.48	1.41
1	D	498	TRP	CD2-CE2	5.02	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASP	N-CA-CB	-12.27	88.52	110.60
1	A	179	CYS	N-CA-C	-10.79	81.86	111.00
1	A	180	ASP	N-CA-C	7.79	132.02	111.00
1	A	668	ARG	NE-CZ-NH1	7.65	124.13	120.30
2	B	0	G	O3'-P-O5'	-7.56	89.64	104.00
1	A	668	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	B	11	U	O5'-P-OP2	-7.28	99.15	105.70
1	A	426	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	B	23	C	O3'-P-O5'	-6.37	91.90	104.00
2	B	26	A	O5'-P-OP2	-6.09	100.22	105.70
2	B	47(E)	G	O3'-P-O5'	-6.01	92.59	104.00
2	B	47(C)	U	P-O3'-C3'	5.76	126.61	119.70
1	A	703	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	663	VAL	CB-CA-C	-5.62	100.72	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	B	39	U	P-O3'-C3'	-5.56	113.03	119.70
2	B	69	G	O5'-P-OP2	-5.47	100.77	105.70
1	A	67	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	47	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	364	ASP	CB-CG-OD1	5.16	122.94	118.30
2	B	61	C	OP2-P-O3'	5.11	116.44	105.20

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	6834	0	6687	107	0
1	D	6881	0	6733	114	0
2	B	1692	0	853	11	0
2	E	1675	0	848	3	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	24	2	0
4	D	31	0	24	0	0
5	B	5	0	0	0	0
5	E	2	0	0	0	0
6	A	247	0	0	8	0
6	B	75	0	0	0	0
6	D	42	0	0	2	0
6	E	5	0	0	1	0
All	All	17522	0	15169	228	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 7.

All (228) 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:D:262:ALA:HB3	1:D:328:MET:HE2	1.27	1.11
1:A:434:MET:HE2	1:A:444:PRO:HA	1.41	1.02
1:D:262:ALA:HB3	1:D:328:MET:CE	1.93	0.98
1:A:729:ILE:HD13	1:A:761:LEU:HD13	1.43	0.97
1:A:161:ASN:ND2	1:A:181:THR:HG21	1.81	0.95
1:D:381:LEU:HD11	1:D:395:ALA:HB1	1.49	0.94
1:A:262:ALA:HB3	1:A:328:MET:HE2	1.53	0.90
1:D:551:ALA:HB3	1:D:553:MET:HE3	1.52	0.90
1:A:288:THR:HG22	1:A:295:MET:HE3	1.54	0.88
1:D:156:VAL:HG13	1:D:165:VAL:HG13	1.56	0.85
1:A:156:VAL:HG13	1:A:165:VAL:HG13	1.59	0.84
1:D:262:ALA:CB	1:D:328:MET:HE2	2.07	0.84
1:A:262:ALA:HB3	1:A:328:MET:CE	2.08	0.83
1:D:633:MET:CE	1:D:663:VAL:HG11	2.09	0.83
2:E:45:G:N7	6:E:2004:HOH:O	2.11	0.83
1:D:633:MET:HE3	1:D:663:VAL:HG11	1.58	0.83
1:D:243:LEU:HD11	1:D:334:ALA:HB2	1.60	0.82
1:A:288:THR:HG22	1:A:295:MET:CE	2.11	0.80
1:A:305:THR:HG23	1:A:307:PHE:H	1.46	0.80
1:D:695:THR:HG22	1:D:698:GLN:H	1.50	0.77
1:A:636:ARG:HD3	1:D:609:GLY:O	1.89	0.72
1:A:161:ASN:HD22	1:A:181:THR:HG21	1.52	0.72
1:D:90:ALA:O	1:D:93:ASN:O	2.07	0.71
1:D:156:VAL:CG1	1:D:165:VAL:HG13	2.21	0.71
1:D:54:ARG:HD3	1:D:566:GLN:OE1	1.91	0.70
1:A:155:ALA:HB2	1:A:329:GLU:OE2	1.91	0.70
1:D:551:ALA:HB3	1:D:553:MET:CE	2.20	0.70
2:B:5:G:H5"	2:B:5:G:H8	1.56	0.69
1:A:434:MET:CE	1:A:444:PRO:HA	2.23	0.67
1:A:164:THR:HG22	1:A:165:VAL:O	1.95	0.67
1:D:472:GLU:OE2	1:D:475:LYS:NZ	2.28	0.66
1:A:608:ALA:HB2	1:D:93:ASN:CB	2.26	0.66
1:D:633:MET:HE3	1:D:663:VAL:CG1	2.26	0.66
1:A:156:VAL:CG1	1:A:165:VAL:HG13	2.27	0.65
1:D:243:LEU:HD13	1:D:265:HIS:CE1	2.32	0.65
1:D:809:LYS:NZ	2:E:47(I):U:OP2	2.25	0.65
1:D:288:THR:HB	1:D:298:MET:HE1	1.78	0.65
1:D:381:LEU:CD1	1:D:395:ALA:HB1	2.26	0.64
1:A:608:ALA:HB2	1:D:93:ASN:CG	2.17	0.64
1:A:323:ALA:HB1	1:A:325:PHE:CE2	2.33	0.63
2:B:5:G:C8	2:B:5:G:H5"	2.33	0.63
1:A:288:THR:CG2	1:A:295:MET:CE	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:O	1:A:434:MET:HE2	1.98	0.62
1:A:161:ASN:ND2	1:A:181:THR:CG2	2.60	0.62
1:A:305:THR:CG2	1:A:307:PHE:H	2.13	0.61
1:D:435:VAL:CG1	1:D:483:ALA:HB1	2.31	0.61
1:D:44:PRO:HA	1:D:108:MET:SD	2.40	0.61
1:A:729:ILE:CD1	1:A:761:LEU:HD13	2.27	0.61
1:D:677:VAL:HG11	1:D:772:LEU:HD22	1.84	0.60
1:D:236:VAL:HG12	6:D:2020:HOH:O	2.00	0.60
1:D:435:VAL:HG11	1:D:478:VAL:HG21	1.83	0.60
1:A:265:HIS:HB2	1:A:328:MET:HE1	1.82	0.60
1:D:434:MET:HE2	1:D:444:PRO:HA	1.84	0.60
1:D:95:THR:HG22	1:D:96:ALA:H	1.67	0.59
1:A:1:MET:CE	1:A:678:TYR:HA	2.32	0.59
1:A:711:LYS:NZ	1:A:715:ASP:OD2	2.26	0.59
1:A:262:ALA:CB	1:A:328:MET:HE2	2.32	0.58
1:D:247:THR:HG21	1:D:336:MET:HE1	1.85	0.58
1:A:773:TRP:HB2	1:A:782:ILE:HD12	1.86	0.58
1:D:156:VAL:HG11	1:D:165:VAL:HG22	1.85	0.58
2:E:47(D):C:O4'	2:E:47(D):C:O2	2.20	0.58
1:D:543:PHE:CZ	1:D:547:LEU:HD11	2.39	0.58
1:A:161:ASN:HD21	1:A:181:THR:HG21	1.67	0.58
1:A:433:PRO:O	1:A:434:MET:CE	2.53	0.57
1:A:443:MET:HE2	6:A:2157:HOH:O	2.04	0.57
1:A:401:ASP:OD1	1:A:411:ARG:NH2	2.37	0.57
1:A:660:GLU:O	1:A:663:VAL:HG22	2.04	0.57
1:D:223:TRP:CD2	1:D:535:ILE:HG21	2.40	0.57
1:A:193:ILE:HD12	1:A:422:VAL:HG11	1.87	0.57
1:D:305:THR:HG21	1:D:320:VAL:HB	1.88	0.56
1:A:846:LYS:HE3	1:A:848:ILE:HD11	1.86	0.56
1:D:741:THR:HG22	6:D:2038:HOH:O	2.05	0.56
1:A:1:MET:HE3	1:A:678:TYR:HA	1.87	0.56
1:D:95:THR:HG22	1:D:96:ALA:N	2.20	0.56
1:A:327:LEU:HD22	1:A:330:TYR:CE2	2.40	0.55
1:A:368:PRO:HB3	1:A:375:LEU:HD22	1.87	0.55
1:D:360:ILE:HD13	1:D:381:LEU:HD22	1.89	0.55
1:D:91:VAL:HG11	1:D:178:ARG:NH2	2.22	0.54
1:A:272:ALA:HB2	1:A:282:ILE:HD12	1.87	0.54
1:D:81:ALA:HB1	1:D:101:THR:HG21	1.90	0.54
1:A:695:THR:HG22	1:A:696:GLU:N	2.23	0.54
1:A:402:LYS:HD2	6:A:2142:HOH:O	2.06	0.54
2:B:47(D):C:O2	2:B:47(D):C:O4'	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:GLY:HA2	1:D:370:LEU:HD13	1.90	0.53
1:A:695:THR:HG22	1:A:696:GLU:H	1.74	0.53
1:D:81:ALA:HB3	1:D:128:CYS:HB3	1.90	0.53
1:A:5:TYR:CE1	1:A:768:ILE:HD12	2.44	0.52
1:A:153:THR:HG23	1:A:187:GLU:HB3	1.91	0.52
1:A:792:GLU:HG2	6:A:2234:HOH:O	2.08	0.52
1:D:667:ASN:OD1	1:D:671:LYS:NZ	2.42	0.52
1:A:624:LYS:HD2	6:A:2187:HOH:O	2.09	0.52
1:D:664:GLU:O	1:D:668:ARG:HG3	2.10	0.52
1:A:161:ASN:HD22	1:A:181:THR:CG2	2.18	0.52
1:D:265:HIS:HB2	1:D:328:MET:HE1	1.91	0.52
1:D:435:VAL:HG13	1:D:483:ALA:HB1	1.92	0.52
1:A:176:CYS:SG	1:A:177:TRP:N	2.84	0.51
1:A:360:ILE:HD13	1:A:381:LEU:HD23	1.92	0.51
1:A:265:HIS:CB	1:A:328:MET:HE1	2.41	0.51
1:A:155:ALA:CB	1:A:329:GLU:OE2	2.59	0.51
1:D:247:THR:HG21	1:D:336:MET:CE	2.41	0.51
1:D:232:ILE:HD13	1:D:253:PHE:CE1	2.46	0.51
1:A:98:ALA:HB3	1:A:99:PRO:CD	2.42	0.50
1:A:633:MET:HE2	1:A:663:VAL:HG11	1.93	0.50
1:A:743:GLY:O	1:A:747:ARG:HG3	2.12	0.50
1:D:676:LEU:HD23	1:D:754:LEU:HD21	1.94	0.50
2:B:43:U:H2'	2:B:44:C:O4'	2.13	0.49
1:D:490:PHE:CD1	1:D:494:MET:HE2	2.47	0.49
1:D:305:THR:HG23	1:D:307:PHE:H	1.77	0.49
1:A:42:PRO:HD2	1:A:78:GLY:O	2.13	0.49
1:A:576:TYR:OH	1:D:94:ASN:HB3	2.13	0.49
1:D:258:TYR:CE1	1:D:337:ALA:CB	2.96	0.49
1:A:182:LYS:HB3	1:A:287:ASN:ND2	2.28	0.49
1:D:801:LEU:HD23	1:D:802:VAL:N	2.28	0.49
1:D:98:ALA:HB3	1:D:99:PRO:CD	2.43	0.49
1:A:272:ALA:HB2	1:A:282:ILE:CD1	2.43	0.48
1:A:608:ALA:HB2	1:D:93:ASN:HB3	1.94	0.48
1:A:633:MET:CE	1:A:663:VAL:HG11	2.43	0.48
1:A:838:TYR:OH	2:B:47(G):G:H5''	2.13	0.48
1:D:187:GLU:C	1:D:188:ILE:HD12	2.34	0.48
1:A:227:SER:OG	1:A:248:THR:HG21	2.13	0.48
1:D:305:THR:CG2	1:D:320:VAL:HB	2.43	0.48
1:D:125:LEU:HD21	1:D:506:PRO:CB	2.44	0.48
1:D:137:GLN:O	1:D:141:THR:HG23	2.14	0.47
1:A:82:PHE:CE2	1:A:128:CYS:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ALA:HB3	1:D:99:PRO:HD3	1.94	0.47
1:D:263:ALA:HB1	1:D:282:ILE:HG12	1.97	0.47
1:A:54:ARG:HD3	1:A:566:GLN:OE1	2.15	0.47
1:D:385:GLY:O	1:D:388:ASN:ND2	2.45	0.47
1:D:650:SER:HB2	1:D:656:LEU:HD13	1.97	0.47
1:A:703:ARG:HG3	1:A:795:MET:HA	1.97	0.47
1:A:844:VAL:HA	1:A:859:VAL:HG23	1.96	0.47
1:A:470:ASP:OD1	1:A:471:PRO:HD2	2.13	0.47
1:D:236:VAL:HB	1:D:239:TYR:HB3	1.97	0.46
1:A:402:LYS:CD	6:A:2142:HOH:O	2.63	0.46
1:A:695:THR:HG21	1:A:697:ASN:HD22	1.81	0.46
1:A:848:ILE:HG13	2:B:56:C:C2	2.51	0.46
1:D:262:ALA:HB3	1:D:328:MET:HE1	1.91	0.46
1:A:57:THR:HG22	1:A:647:MET:SD	2.56	0.46
1:D:153:THR:HG23	1:D:187:GLU:HB3	1.97	0.46
1:D:23:THR:O	1:D:67:ARG:NH2	2.47	0.46
1:D:243:LEU:HD11	1:D:334:ALA:CB	2.40	0.46
1:A:109:LYS:HG3	1:A:121:TRP:CZ3	2.51	0.46
4:A:1862:84T:O5'	4:A:1862:84T:H8	2.15	0.46
1:A:289:LYS:O	1:A:295:MET:CE	2.64	0.46
1:A:195:ILE:HG22	1:A:419:ASP:HA	1.98	0.46
1:D:162:ASP:HB2	1:D:164:THR:HG22	1.98	0.46
1:A:289:LYS:O	1:A:295:MET:HE3	2.16	0.46
1:A:256:CYS:HA	1:A:337:ALA:O	2.16	0.46
2:B:9:G:H2'	2:B:9:G:N3	2.30	0.46
1:A:49:HIS:HA	1:A:628:ILE:O	2.16	0.45
1:D:327:LEU:HB3	1:D:330:TYR:CD1	2.50	0.45
1:D:232:ILE:HG12	1:D:403:LEU:HD13	1.99	0.45
1:D:633:MET:CE	1:D:663:VAL:CG1	2.89	0.45
1:D:84:LEU:HD21	1:D:170:GLN:NE2	2.30	0.45
1:D:695:THR:CG2	1:D:697:ASN:H	2.30	0.45
1:A:175:CYS:SG	1:A:181:THR:N	2.90	0.45
1:A:695:THR:HG21	1:A:697:ASN:ND2	2.32	0.45
1:D:155:ALA:HB2	1:D:185:ARG:NH2	2.32	0.45
1:D:26:VAL:HG11	1:D:73:VAL:O	2.17	0.45
1:A:265:HIS:CA	1:A:328:MET:HE1	2.47	0.44
1:D:543:PHE:CE2	1:D:547:LEU:HD11	2.52	0.44
1:A:255:GLY:O	1:A:257:THR:HG23	2.16	0.44
1:A:299:GLU:OE2	1:A:351:LYS:NZ	2.44	0.44
1:A:305:THR:CG2	1:A:307:PHE:HB2	2.48	0.44
1:A:773:TRP:CE2	1:A:778:GLY:HA3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ALA:HB3	1:D:318:ILE:HG13	1.99	0.44
1:D:534:ALA:HA	1:D:538:LEU:HD12	2.00	0.44
1:D:84:LEU:HD21	1:D:170:GLN:HE22	1.83	0.44
1:D:236:VAL:HG13	1:D:308:LYS:O	2.17	0.44
1:D:589:VAL:HG12	1:D:589:VAL:O	2.18	0.44
1:D:729:ILE:HG21	1:D:761:LEU:CD2	2.48	0.44
1:D:703:ARG:HB2	1:D:795:MET:HA	2.00	0.44
1:D:839:LEU:HD22	1:D:859:VAL:HG21	2.00	0.44
1:A:131:GLU:CD	1:A:131:GLU:H	2.20	0.44
1:A:360:ILE:HD13	1:A:381:LEU:CD2	2.48	0.44
1:D:262:ALA:HB2	1:D:326:VAL:O	2.18	0.44
1:A:252:THR:HB	1:A:338:VAL:HG11	1.98	0.43
2:B:48:U:O2'	2:B:59:G:H4'	2.18	0.43
1:A:305:THR:HB	1:A:320:VAL:O	2.18	0.43
1:D:336:MET:HE3	1:D:338:VAL:HG21	2.00	0.43
1:D:165:VAL:HG21	1:D:425:GLN:HG3	1.99	0.43
1:A:186:LYS:HG2	1:A:188:ILE:HG13	2.00	0.43
1:D:362:ALA:O	1:D:363:ALA:C	2.57	0.43
1:D:123:ARG:HA	1:D:506:PRO:HG3	2.01	0.43
1:A:529:GLY:O	1:A:565:CYS:HA	2.18	0.43
1:D:535:ILE:HG22	1:D:536:MET:N	2.34	0.43
2:B:31:A:O2'	2:B:32:U:O5'	2.23	0.43
1:D:551:ALA:CB	1:D:553:MET:CE	2.95	0.43
1:A:443:MET:CE	6:A:2157:HOH:O	2.65	0.43
1:D:800:THR:HG21	1:D:852:GLY:HA2	2.01	0.42
1:A:44:PRO:HA	1:A:108:MET:SD	2.58	0.42
1:D:689:LEU:HD12	1:D:690:ASN:N	2.34	0.42
1:D:729:ILE:HG21	1:D:761:LEU:HD21	2.02	0.42
1:D:681:THR:HG21	1:D:775:GLU:O	2.20	0.42
2:B:8:U:H2'	2:B:21:G:N2	2.35	0.42
1:D:203:LEU:HD12	1:D:221:ARG:HG2	2.00	0.42
1:D:633:MET:HE2	1:D:663:VAL:HG11	1.95	0.42
1:D:84:LEU:N	1:D:85:PRO:CD	2.83	0.42
1:A:109:LYS:HG3	1:A:121:TRP:CH2	2.55	0.42
1:D:153:THR:HG22	1:D:153:THR:O	2.19	0.42
1:D:362:ALA:HB2	1:D:368:PRO:HB3	2.02	0.42
1:D:223:TRP:CE3	1:D:535:ILE:HG21	2.54	0.42
1:A:476:THR:OG1	1:A:477:THR:N	2.53	0.41
1:A:227:SER:HB2	6:A:2097:HOH:O	2.19	0.41
1:A:422:VAL:HG11	1:A:494:MET:HE1	2.02	0.41
1:A:566:GLN:NE2	4:A:1862:84T:N3	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:SER:O	1:A:619:LYS:C	2.58	0.41
1:D:510:GLU:CD	1:D:510:GLU:N	2.73	0.41
1:D:695:THR:HG22	1:D:698:GLN:N	2.25	0.41
1:D:43:TYR:HE2	1:D:82:PHE:O	2.03	0.41
1:A:485:ARG:HB3	6:A:2155:HOH:O	2.20	0.41
1:A:311:HIS:HA	1:A:312:PRO:HD3	1.95	0.41
1:A:367:GLU:HG2	1:A:382:PHE:CE2	2.55	0.41
1:D:67:ARG:NH1	1:D:784:ASN:OD1	2.54	0.41
1:A:193:ILE:CD1	1:A:422:VAL:HG11	2.50	0.41
1:D:125:LEU:HD21	1:D:506:PRO:HB3	2.03	0.41
1:D:62:ILE:HD13	1:D:526:ILE:HD13	2.03	0.40
1:D:729:ILE:HD13	1:D:761:LEU:HD13	2.02	0.40
2:B:19:G:H4'	2:B:20:U:OP1	2.21	0.40
1:D:842:VAL:HG21	1:D:859:VAL:HG11	2.03	0.40
1:A:171:VAL:HG11	1:A:289:LYS:HD2	2.03	0.40
1:A:435:VAL:HG13	1:A:437:LEU:HD23	2.04	0.40
1:A:826:ARG:HH22	1:A:844:VAL:HG21	1.86	0.40
1:D:370:LEU:HD22	1:D:374:ALA:HA	2.03	0.40
1:D:629:ASP:OD1	1:D:630:PRO:HD2	2.20	0.40
1:A:224:ILE:HA	1:A:417:LEU:HB2	2.03	0.40
1:A:825:VAL:HG12	1:A:855:LEU:HD22	2.03	0.40
1:D:337:ALA:HB1	1:D:345:ASP:HB3	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	858/880 (98%)	834 (97%)	23 (3%)	1 (0%)	51 68
1	D	863/880 (98%)	816 (95%)	42 (5%)	5 (1%)	25 36
All	All	1721/1760 (98%)	1650 (96%)	65 (4%)	6 (0%)	41 55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	363	ALA
1	A	439	ASP
1	D	284	GLU
1	D	393	GLU
1	D	535	ILE
1	D	388	ASN

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	724/741 (98%)	688 (95%)	36 (5%)	24	40
1	D	729/741 (98%)	683 (94%)	46 (6%)	18	28
All	All	1453/1482 (98%)	1371 (94%)	82 (6%)	21	34

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	34	LYS
1	A	36	TYR
1	A	84	LEU
1	A	95	THR
1	A	143	LEU
1	A	153	THR
1	A	156	VAL
1	A	177	TRP
1	A	181	THR
1	A	261	VAL
1	A	274	ASN
1	A	290	VAL
1	A	298	MET
1	A	305	THR
1	A	372	GLN
1	A	376	THR

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Mol	Chain	Res	Type
1	A	412	LYS
1	A	425	GLN
1	A	435	VAL
1	A	464	THR
1	A	465	SER
1	A	477	THR
1	A	485	ARG
1	A	596	ASP
1	A	602	VAL
1	A	622	LYS
1	A	655	THR
1	A	661	SER
1	A	663	VAL
1	A	664	GLU
1	A	761	LEU
1	A	818	VAL
1	A	827	GLU
1	A	840	ASP
1	A	859	VAL
1	D	34	LYS
1	D	36	TYR
1	D	84	LEU
1	D	143	LEU
1	D	152	LYS
1	D	153	THR
1	D	156	VAL
1	D	175	CYS
1	D	177	TRP
1	D	181	THR
1	D	210	ASP
1	D	227	SER
1	D	269	GLN
1	D	298	MET
1	D	305	THR
1	D	310	VAL
1	D	335	VAL
1	D	356	ILE
1	D	373	GLN
1	D	423	SER
1	D	425	GLN
1	D	457	ASP
1	D	461	ASP

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Mol	Chain	Res	Type
1	D	477	THR
1	D	485	ARG
1	D	510	GLU
1	D	515	SER
1	D	516	GLU
1	D	544	PHE
1	D	596	ASP
1	D	646	MET
1	D	650	SER
1	D	655	THR
1	D	664	GLU
1	D	692	ASP
1	D	695	THR
1	D	703	ARG
1	D	741	THR
1	D	761	LEU
1	D	798	ASP
1	D	815	THR
1	D	823	GLU
1	D	827	GLU
1	D	828	ARG
1	D	846	LYS
1	D	854	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	ASN
1	A	555	ASN
1	A	580	ASN
1	A	659	GLN
1	A	697	ASN
1	D	392	HIS
1	D	690	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/88 (86%)	12 (15%)	1 (1%)
2	E	75/88 (85%)	15 (20%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	151/176 (85%)	27 (17%)	2 (1%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	G
2	B	16	U
2	B	19	G
2	B	41	C
2	B	43	U
2	B	45	G
2	B	47(A)	G
2	B	47(D)	C
2	B	47(F)	C
2	B	55	U
2	B	69	G
2	E	9	G
2	E	10	G
2	E	16	U
2	E	18	G
2	E	19	G
2	E	31	A
2	E	41	C
2	E	45	G
2	E	47(A)	G
2	E	47(E)	G
2	E	47(F)	C
2	E	47(G)	G
2	E	59	G
2	E	64	G
2	E	67	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	47(G)	G
2	E	60	U

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	84T	A	1862	-	29,33,33	1.33	3 (10%)	31,49,49	2.14	11 (35%)
4	84T	D	1862	-	29,33,33	1.34	3 (10%)	31,49,49	1.74	4 (12%)

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	84T	A	1862	-	-	1/21/39/39	0/3/3/3
4	84T	D	1862	-	-	1/21/39/39	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1862	84T	C2'-C1'	-3.93	1.50	1.54
4	D	1862	84T	P-O2P	3.43	1.51	1.46
4	A	1862	84T	C2'-C1'	-3.24	1.51	1.54
4	A	1862	84T	P-O2P	2.68	1.50	1.46
4	A	1862	84T	P-O1P	-2.62	1.49	1.56
4	D	1862	84T	O4'-C1'	2.23	1.44	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1862	84T	O1P-P-O2P	6.13	122.77	109.92
4	D	1862	84T	N3-C2-N1	-4.77	121.23	128.68
4	A	1862	84T	N3-C2-N1	-4.64	121.42	128.68
4	A	1862	84T	O1P-P-O2P	3.77	117.83	109.92
4	A	1862	84T	C4-C5-N7	-3.68	105.56	109.40
4	A	1862	84T	OH-CA-CB	-3.56	102.92	110.45
4	A	1862	84T	CA-C-N	3.49	118.61	115.47
4	A	1862	84T	O5'-P-O2P	-3.13	102.19	114.24
4	A	1862	84T	CD1-CG-CB	-3.13	106.11	111.20
4	A	1862	84T	CD1-CG-CD2	3.03	119.07	110.59
4	A	1862	84T	CD2-CG-CB	-2.75	106.72	111.20
4	D	1862	84T	C1'-N9-C4	-2.57	122.13	126.64
4	A	1862	84T	C1'-N9-C4	-2.50	122.25	126.64
4	A	1862	84T	O4'-C4'-C3'	2.13	107.82	105.07
4	D	1862	84T	OHB-CB-CA	-2.03	105.50	109.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

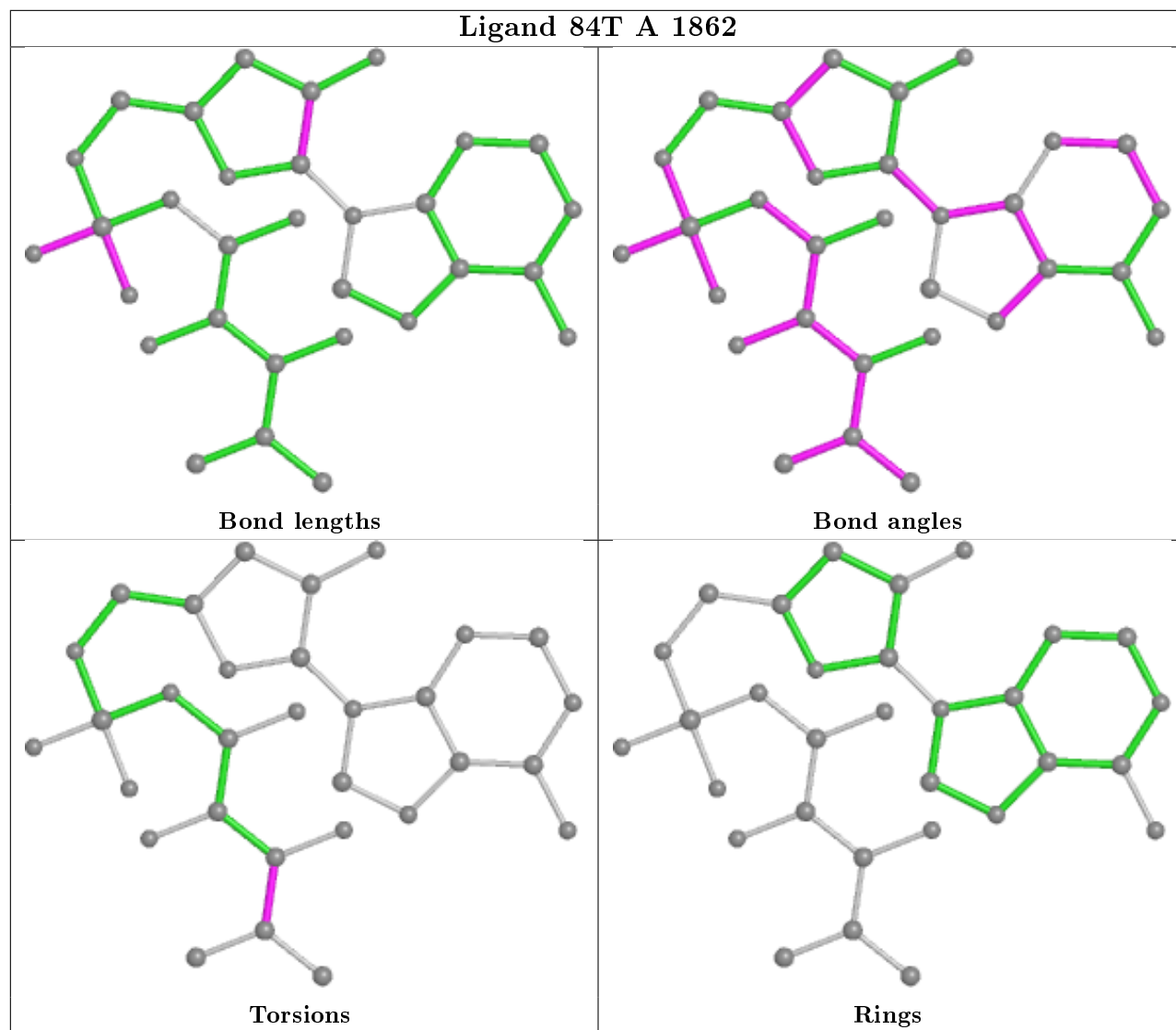
Mol	Chain	Res	Type	Atoms
4	A	1862	84T	OHB-CB-CG-CD1
4	D	1862	84T	C-N-P-O2P

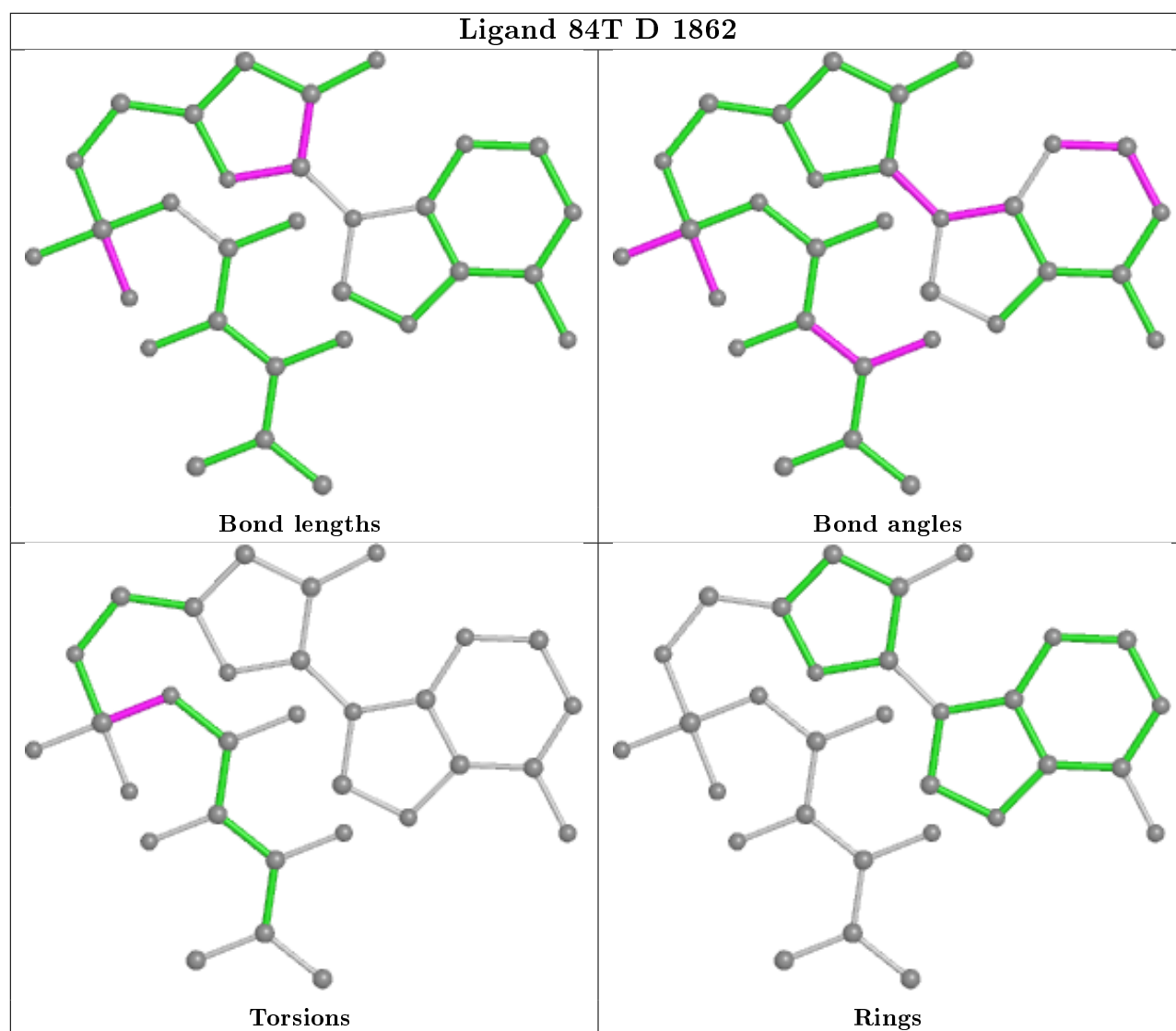
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1862	84T	2	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	860/880 (97%)	0.04	13 (1%) 73 72	19, 35, 67, 122	0
1	D	867/880 (98%)	0.78	126 (14%) 2 2	39, 66, 116, 153	0
2	B	82/88 (93%)	-0.30	3 (3%) 41 41	24, 39, 92, 120	0
2	E	80/88 (90%)	0.45	7 (8%) 10 9	48, 78, 105, 118	0
All	All	1889/1936 (97%)	0.38	149 (7%) 12 11	19, 51, 108, 153	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	303	VAL	8.4
1	D	596	ASP	7.2
1	D	860	GLY	6.2
1	D	177	TRP	5.7
1	D	463	ILE	5.7
1	D	597	GLU	5.7
1	D	819	ASP	5.6
1	D	602	VAL	5.5
1	D	847	VAL	5.4
1	D	172	ILE	5.4
1	D	174	GLY	5.2
1	A	161	ASN	5.2
1	D	305	THR	5.1
1	D	180	ASP	5.1
1	D	237	ASN	5.0
1	D	299	GLU	4.9
1	D	321	TRP	4.7
1	D	302	GLY	4.7
1	D	272	ALA	4.6
1	D	274	ASN	4.6
1	D	281	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	279	ALA	4.4
1	D	275	ASN	4.2
1	D	858	VAL	4.2
1	D	178	ARG	4.1
1	D	845	ARG	4.1
1	D	304	ASP	4.1
1	D	269	GLN	4.0
1	D	276	PRO	3.9
1	D	283	ASP	3.9
1	D	600	ARG	3.9
1	D	370	LEU	3.8
1	D	469	ALA	3.8
1	D	352	TYR	3.7
1	D	598	LYS	3.7
1	D	166	LEU	3.7
1	D	280	ALA	3.7
1	D	320	VAL	3.7
1	D	325	PHE	3.7
1	D	297	THR	3.6
1	D	181	THR	3.6
1	D	582	GLU	3.6
1	A	179	CYS	3.6
1	D	379	GLY	3.6
1	D	601	ILE	3.6
1	D	160	PRO	3.5
1	D	175	CYS	3.5
1	D	351	LYS	3.5
1	D	161	ASN	3.5
1	D	238	ASP	3.5
1	D	271	ALA	3.5
1	D	263	ALA	3.4
1	D	173	ASP	3.4
1	D	694	LEU	3.4
1	D	163	GLN	3.4
1	D	310	VAL	3.3
1	A	580	ASN	3.3
1	D	363	ALA	3.2
1	D	844	VAL	3.2
1	A	178	ARG	3.2
1	D	306	GLY	3.2
1	D	179	CYS	3.2
1	D	184	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	818	VAL	3.1
2	E	55	U	3.1
1	A	274	ASN	3.1
1	D	165	VAL	3.1
1	D	846	LYS	3.0
1	D	691	VAL	2.9
1	A	177	TRP	2.9
1	D	319	PRO	2.9
1	D	182	LYS	2.9
1	D	344	ARG	2.9
1	D	849	TYR	2.9
1	D	322	ALA	2.9
1	D	289	LYS	2.9
1	D	234	PHE	2.8
1	D	286	ARG	2.8
2	B	47(B)	U	2.8
1	D	273	GLU	2.8
2	B	30	G	2.8
1	D	330	TYR	2.8
1	D	356	ILE	2.8
1	D	820	ALA	2.8
1	D	381	LEU	2.8
2	E	44	C	2.8
1	A	173	ASP	2.8
1	D	296	ALA	2.7
1	D	592	ILE	2.7
2	E	17	C	2.7
1	A	597	GLU	2.7
1	A	175	CYS	2.6
1	D	580	ASN	2.6
2	E	31	A	2.6
1	D	309	ALA	2.6
1	D	353	GLY	2.6
1	D	848	ILE	2.6
2	B	31	A	2.6
2	E	39	U	2.5
1	D	301	LYS	2.5
1	D	288	THR	2.5
1	D	741	THR	2.5
1	D	687	ALA	2.5
1	D	408	VAL	2.5
1	D	298	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	598	LYS	2.5
1	D	270	LYS	2.4
1	D	380	VAL	2.4
1	D	162	ASP	2.4
1	D	377	GLU	2.4
1	D	230	VAL	2.4
1	D	300	LYS	2.4
1	A	692	ASP	2.4
1	D	183	VAL	2.4
1	D	158	TRP	2.3
1	A	330	TYR	2.3
1	D	264	GLY	2.3
1	D	457	ASP	2.3
1	D	164	THR	2.3
1	D	294	GLU	2.3
1	D	285	CYS	2.3
1	D	228	GLU	2.3
1	D	823	GLU	2.3
1	D	850	VAL	2.3
1	D	599	GLY	2.3
1	D	159	CYS	2.2
1	D	565	CYS	2.2
1	D	354	LEU	2.2
2	E	29	G	2.2
1	D	369	ASP	2.2
1	D	577	VAL	2.2
1	D	364	ASP	2.2
1	A	180	ASP	2.1
1	D	268	ALA	2.1
2	E	51	G	2.1
1	D	6	ARG	2.1
1	D	278	LEU	2.1
1	D	157	ASN	2.1
1	D	529	GLY	2.1
1	D	528	ILE	2.1
1	D	690	ASN	2.1
1	D	594	GLU	2.1
1	D	650	SER	2.0
1	D	461	ASP	2.0
1	D	798	ASP	2.0
1	D	233	THR	2.0
1	D	58	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	692	ASP	2.0
1	D	745	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

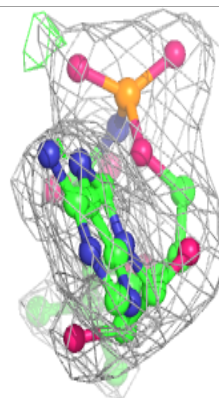
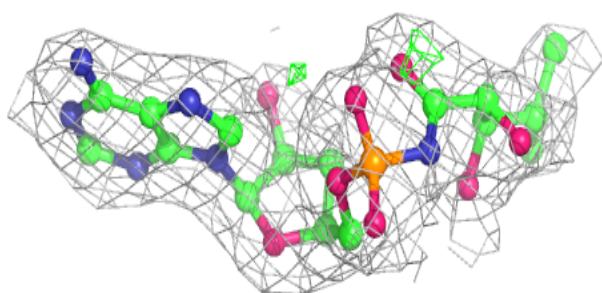
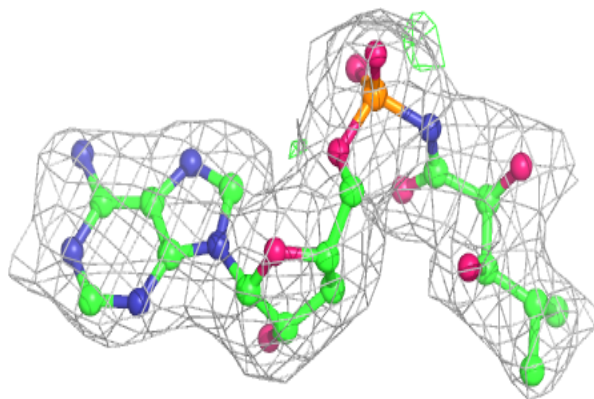
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	E	1078	1/1	0.70	0.32	59,59,59,59	0
5	MG	B	1078	1/1	0.76	0.12	62,62,62,62	0
3	ZN	D	1861	1/1	0.83	0.14	125,125,125,125	0
3	ZN	A	1861	1/1	0.85	0.09	118,118,118,118	0
5	MG	B	1081	1/1	0.88	0.09	55,55,55,55	0
5	MG	B	1079	1/1	0.89	0.07	43,43,43,43	0
5	MG	E	1077	1/1	0.90	0.15	60,60,60,60	0
5	MG	B	1077	1/1	0.95	0.09	32,32,32,32	0
5	MG	B	1080	1/1	0.98	0.05	41,41,41,41	0
4	84T	D	1862	31/31	0.98	0.20	38,39,41,43	0
4	84T	A	1862	31/31	0.98	0.20	18,19,22,23	0

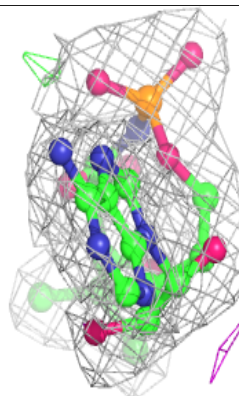
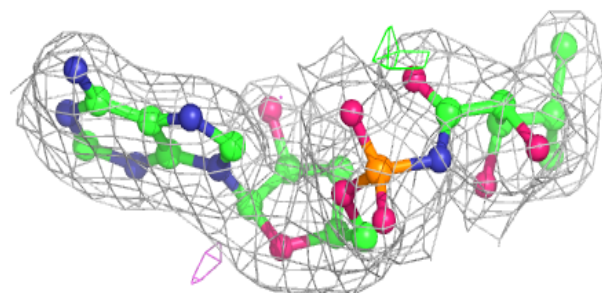
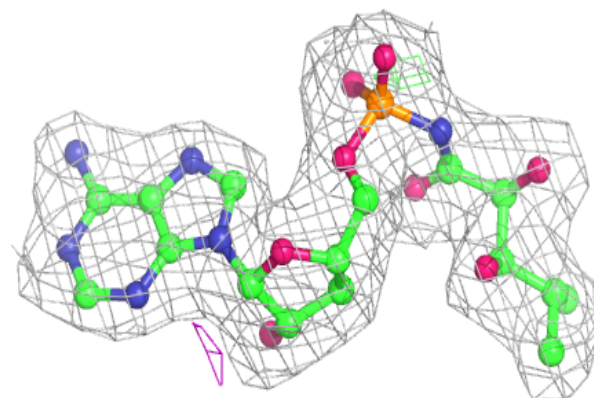
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 84T D 1862:

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

**Electron density around 84T A 1862:**

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



6.5 Other polymers

There are no such residues in this entry.