



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:44 AM UTC

PDB ID : 3ZGZ / pdb_00003zgz
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 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

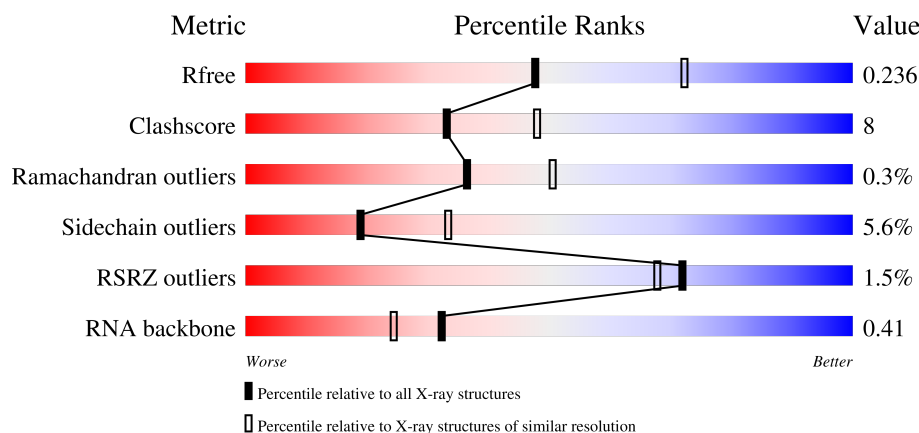
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	880	
1	D	880	
2	B	88	

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Mol	Chain	Length	Quality of chain
2	E	88	70% 19% • 9%

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

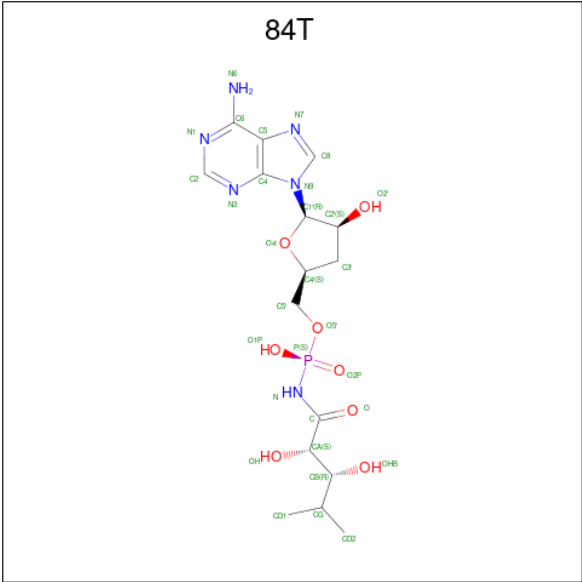
- Molecule 2 is a RNA chain called TRNA-LEU UAA ISOACCEPTOR.

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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.

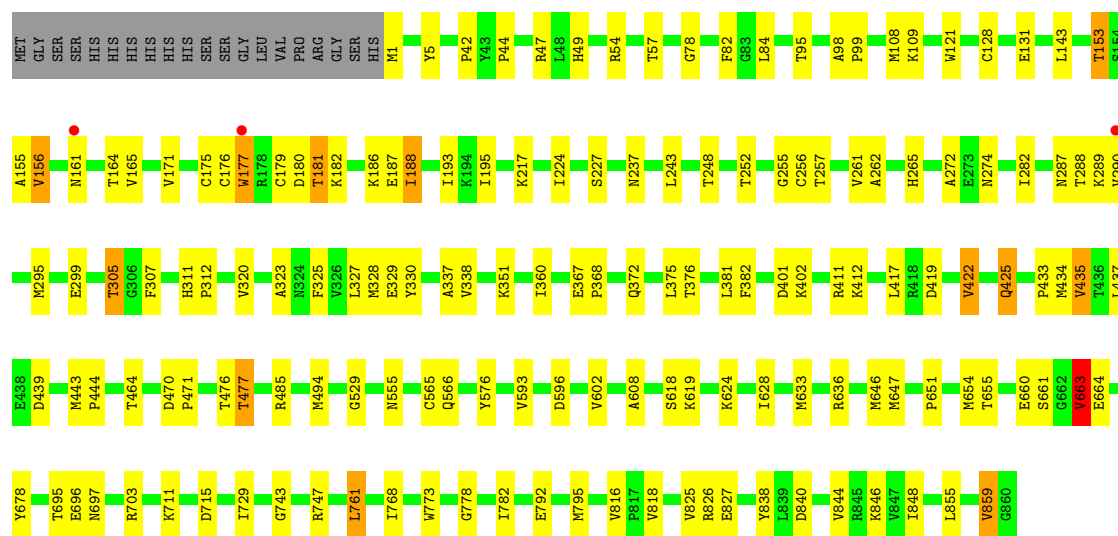
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		
6	B	75	Total	O	0	0
			75	75		
6	D	42	Total	O	0	0
			42	42		
6	E	5	Total	O	0	0
			5	5		

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.

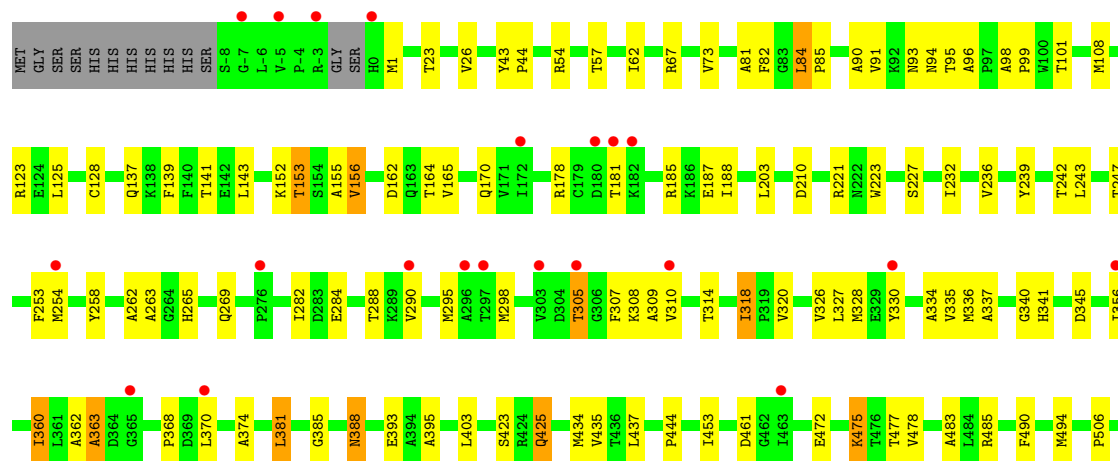
• Molecule 1: LEUCINE-TRNA LIGASE

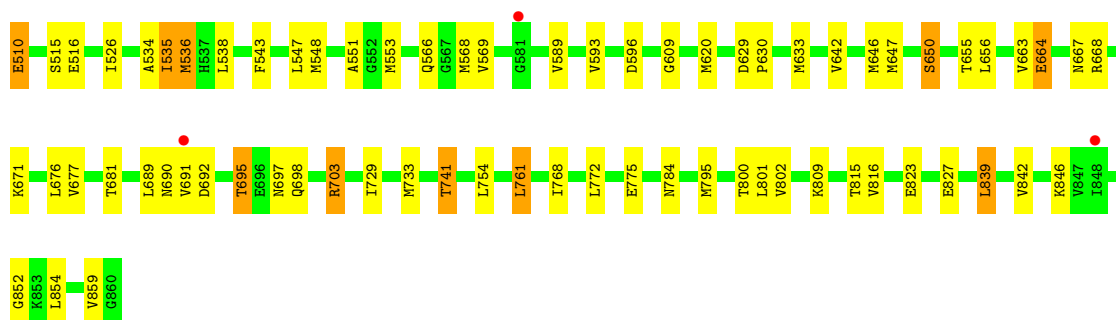
Chain A: 



• Molecule 1: LEUCINE-TRNA LIGASE

Chain D: 

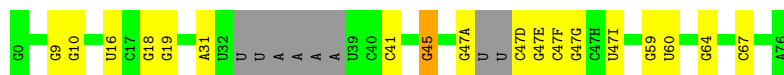




• Molecule 2: TRNA-LEU UAA ISOACCEPTOR



• 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 , 44.8	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: MG, ZN, 84T

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	0.97	0/6995	1.01	9/9497 (0.1%)
1	D	0.72	0/7043	0.82	1/9562 (0.0%)
2	B	0.52	0/1887	1.07	13/2939 (0.4%)
2	E	0.40	0/1869	0.87	0/2911
All	All	0.79	0/17794	0.93	23/24909 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	CYS	N-CA-C	-19.32	81.86	110.46
1	A	180	ASP	N-CA-CB	-14.65	88.52	110.35
1	A	180	ASP	N-CA-C	13.65	132.02	107.99
2	B	0	G	O3'-P-O5'	-9.57	89.64	104.00
1	A	555	ASN	N-CA-C	8.38	120.50	111.36
2	B	23	C	O3'-P-O5'	-8.07	91.90	104.00
1	A	663	VAL	CB-CA-C	-7.38	100.72	112.16
1	A	237	ASN	N-CA-C	6.62	118.29	111.14
1	A	179	CYS	CA-C-N	6.37	131.77	122.41
1	A	179	CYS	C-N-CA	6.37	131.77	122.41
1	D	536	MET	N-CA-C	6.23	117.77	110.97
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
2	B	15	A	C2'-C3'-O3'	-5.71	105.13	113.70
2	B	58	A	O3'-P-O5'	-5.71	95.44	104.00
2	B	19	G	O3'-P-O5'	-5.68	95.49	104.00
2	B	24	A	C4'-C3'-O3'	-5.65	104.53	113.00
1	A	422	VAL	N-CA-C	5.63	117.58	112.29
2	B	69	G	O3'-P-O5'	-5.54	95.69	104.00
2	B	21	G	C4'-C3'-O3'	-5.37	104.95	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	U	C3'-C2'-O2'	5.27	118.61	110.70
2	B	45	G	O3'-P-O5'	-5.16	96.27	104.00
2	B	64	G	O3'-P-O5'	5.03	111.54	104.00

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	115	0
1	D	6881	0	6733	130	0
2	B	1692	0	853	12	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	1	0
5	B	5	0	0	0	0
5	E	2	0	0	0	0
6	A	247	0	0	10	0
6	B	75	0	0	1	0
6	D	42	0	0	2	0
6	E	5	0	0	1	0
All	All	17522	0	15169	253	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 8.

All (253) 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:288:THR:HG22	1:A:295:MET:HE1	1.19	1.12
1:D:262:ALA:HB3	1:D:328:MET:HE2	1.34	1.10
1:A:288:THR:CG2	1:A:295:MET:HE1	1.90	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:MET:HE3	1:D:663:VAL:HG11	1.43	0.98
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:433:PRO:O	1:A:434:MET:HE2	1.67	0.93
1:D:247:THR:HG21	1:D:336:MET:HE2	1.56	0.87
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: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:243:LEU:HD11	1:D:334:ALA:HB2	1.60	0.82
1:A:305:THR:HG23	1:A:307:PHE:H	1.46	0.80
1:D:262:ALA:CB	1:D:328:MET:HE2	2.12	0.80
1:A:262:ALA:HB3	1:A:328:MET:HE2	1.65	0.78
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
1:A:608:ALA:HB2	1:D:93:ASN:CG	2.17	0.70
2:B:5:G:H5"	2:B:5:G:H8	1.56	0.69
1:A:1:MET:HE3	1:A:678:TYR:HA	1.73	0.68
1:D:676:LEU:HD22	1:D:733:MET:HE1	1.76	0.68
1:A:434:MET:CE	1:A:444:PRO:HA	2.23	0.68
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:A:288:THR:HG22	1:A:295:MET:CE	2.11	0.65
1:A:156:VAL:CG1	1:A:165:VAL:HG13	2.27	0.65
1:A:651:PRO:CG	1:A:654:MET:HE3	2.26	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:381:LEU:CD1	1:D:395:ALA:HB1	2.26	0.64
1:D:551:ALA:HB3	1:D:553:MET:HE2	1.80	0.63
1:A:323:ALA:HB1	1:A:325:PHE:CE2	2.33	0.63
2:B:5:G:H5"	2:B:5:G:C8	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PHE:HE1	1:D:553:MET:HE1	1.62	0.63
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:A:633:MET:HE3	1:A:663:VAL:HG11	1.82	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:434:MET:HE2	1:A:444:PRO:HA	1.81	0.60
1:D:95:THR:HG22	1:D:96:ALA:H	1.67	0.59
1:D:254:MET:HE1	1:D:314:THR:HG23	1.84	0.59
1:A:1:MET:CE	1:A:678:TYR:HA	2.32	0.59
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:D:551:ALA:CB	1:D:553:MET:HE2	2.34	0.58
1:A:289:LYS:O	1:A:295:MET:HE3	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:265:HIS:HB2	1:A:328:MET:HE1	1.88	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:551:ALA:HB3	1:D:553:MET:HE3	1.87	0.55
1:A:651:PRO:HG3	1:A:654:MET:HE3	1.88	0.55
1:D:360:ILE:HD13	1:D:381:LEU:HD22	1.89	0.55
1:D:288:THR:HG22	1:D:298:MET:HE1	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:D:288:THR:CG2	1:D:298:MET:HE1	2.37	0.54
1:D:290:VAL:O	1:D:295:MET:HE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:247:THR:CG2	1:D:336:MET:HE2	2.36	0.53
1:A:422:VAL:HG11	1:A:494:MET:HE1	1.89	0.53
2:B:47(D):C:O2	2:B:47(D):C:O4'	2.23	0.53
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:187:GLU:C	1:D:188:ILE:HD12	2.34	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:288:THR:CG2	1:A:295:MET:CE	2.76	0.52
1:D:548:MET:HA	1:D:553:MET:HE3	1.91	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:262:ALA:HB3	1:D:328:MET:HE1	1.84	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:434:MET:HE1	1:D:444:PRO:HB3	1.92	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:435:VAL:HG13	1:D:483:ALA:HB1	1.92	0.52
1:A:262:ALA:HB3	1:A:328:MET:HE1	1.89	0.51
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:D:490:PHE:CD1	1:D:494:MET:HE3	2.45	0.51
1:A:155:ALA:CB	1:A:329:GLU:OE2	2.59	0.51
1:D:232:ILE:HD13	1:D:253:PHE:CE1	2.46	0.51
1:D:676:LEU:CD2	1:D:733:MET:HE1	2.40	0.50
1:D:633:MET:HE2	1:D:642:VAL:HG22	1.94	0.50
1:A:98:ALA:HB3	1:A:99:PRO:CD	2.42	0.50
1:D:265:HIS:HB2	1:D:328:MET:HE1	1.94	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
1:A:131:GLU:CD	1:A:131:GLU:H	2.20	0.49
2:B:43:U:H2'	2:B:44:C:O4'	2.13	0.49
1:D:305:THR:HG23	1:D:307:PHE:H	1.77	0.49
1:D:490:PHE:CE1	1:D:494:MET:HE3	2.48	0.49
1:D:1:MET:HE2	1:D:775:GLU:HB3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HB3	1:A:287:ASN:ND2	2.28	0.49
1:D:98:ALA:HB3	1:D:99:PRO:CD	2.43	0.49
1:D:801:LEU:HD23	1:D:802:VAL:N	2.28	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:838:TYR:OH	2:B:47(G):G:H5''	2.13	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:362:ALA:O	1:D:363:ALA:C	2.57	0.48
1:A:633:MET:CE	1:A:663:VAL:HG11	2.43	0.47
1:D:137:GLN:O	1:D:141:THR:HG23	2.14	0.47
1:A:711:LYS:NZ	1:A:715:ASP:OD2	2.26	0.47
1:A:82:PHE:CE2	1:A:128:CYS:HA	2.49	0.47
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:A:262:ALA:CB	1:A:328:MET:HE2	2.40	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:618:SER:O	1:A:619:LYS:C	2.58	0.46
1:A:695:THR:HG21	1:A:697:ASN:HD22	1.81	0.46
1:A:217:LYS:NZ	6:A:2084:HOH:O	2.38	0.46
1:A:848:ILE:HG13	2:B:56:C:C2	2.51	0.46
1:D:510:GLU:N	1:D:510:GLU:CD	2.73	0.46
1:A:57:THR:HG22	1:A:647:MET:SD	2.56	0.46
1:D:23:THR:O	1:D:67:ARG:NH2	2.47	0.46
1:D:153:THR:HG23	1:D:187:GLU:HB3	1.97	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
1:A:195:ILE:HG22	1:A:419:ASP:HA	1.98	0.46
1:A:289:LYS:O	1:A:295:MET:CE	2.64	0.46
4:A:1862:84T:O5'	4:A:1862:84T:H8	2.15	0.46
1:D:162:ASP:HB2	1:D:164:THR:HG22	1.98	0.46
1:A:256:CYS:HA	1:A:337:ALA:O	2.16	0.46
2:B:9:G:N3	2:B:9:G:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:HIS:HA	1:A:628:ILE:O	2.16	0.45
1:A:654:MET:HE1	6:A:2198:HOH: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:425:GLN:N	1:A:425:GLN:CD	2.75	0.45
1:A:695:THR:HG21	1:A:697:ASN:ND2	2.32	0.45
1:D:26:VAL:HG11	1:D:73:VAL:O	2.17	0.45
1:D:155:ALA:HB2	1:D:185:ARG:NH2	2.32	0.45
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:443:MET:CE	6:A:2157:HOH:O	2.65	0.44
1:A:773:TRP:CE2	1:A:778:GLY:HA3	2.52	0.44
1:D:309:ALA:HB3	1:D:318:ILE:HG13	1.99	0.44
1:D:84:LEU:HD21	1:D:170:GLN:HE22	1.83	0.44
1:D:534:ALA:HA	1:D:538:LEU:HD12	2.00	0.44
1:D:236:VAL:HG13	1:D:308:LYS:O	2.17	0.44
1:D:589:VAL:O	1:D:589:VAL:HG12	2.18	0.44
1:D:729:ILE:HG21	1:D:761:LEU:CD2	2.48	0.44
1:D:801:LEU:HD23	1:D:801:LEU:C	2.42	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: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:433:PRO:O	1:A:434:MET:CE	2.53	0.43
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: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: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:288:THR:HB	1:D:298:MET:HE1	2.01	0.43
1:D:800:THR:HG21	1:D:852:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:681:THR:HG21	1:D:775:GLU:O	2.20	0.42
1:D:729:ILE:HG21	1:D:761:LEU:HD21	2.02	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:568:MET:HE3	4:D:1862:84T:C6	2.49	0.42
1:A:711:LYS:HZ2	1:A:715:ASP:CG	2.17	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:O	1:D:153:THR:HG22	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:566:GLN:NE2	4:A:1862:84T:N3	2.68	0.41
1:D:57:THR:HB	1:D:647:MET:HE3	2.02	0.41
1:D:434:MET:HE2	1:D:444:PRO:HA	2.02	0.41
1:D:695:THR:HG22	1:D:698:GLN:N	2.25	0.41
1:A:54:ARG:HB2	1:A:646:MET:HE2	2.02	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:D:265:HIS:N	1:D:328:MET:HE3	2.35	0.41
1:A:443:MET:HE2	6:A:2157:HOH:O	2.20	0.41
1:A:193:ILE:CD1	1:A:422:VAL:HG11	2.50	0.41
2:B:18:G:O2'	6:B:2027:HOH:O	2.20	0.41
1:D:125:LEU:HD21	1:D:506:PRO:HB3	2.03	0.41
1:D:340:GLY:C	1:D:341:HIS:CG	2.98	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:A:494:MET:HB2	1:A:494:MET:HE2	1.79	0.40
1:D:629:ASP:OD1	1:D:630:PRO:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:569:VAL:HG12	1:D:620:MET:HE3	2.04	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%)	48	64
1	D	863/880 (98%)	816 (95%)	42 (5%)	5 (1%)	21	32
All	All	1721/1760 (98%)	1650 (96%)	65 (4%)	6 (0%)	36	50

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 [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	724/741 (98%)	690 (95%)	34 (5%)	23	41
1	D	729/741 (98%)	681 (93%)	48 (7%)	15	26
All	All	1453/1482 (98%)	1371 (94%)	82 (6%)	19	33

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

Mol	Chain	Res	Type
1	A	47	ARG
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	188	ILE
1	A	243	LEU
1	A	261	VAL
1	A	274	ASN
1	A	290	VAL
1	A	305	THR
1	A	372	GLN
1	A	376	THR
1	A	412	LYS
1	A	425	GLN
1	A	435	VAL
1	A	464	THR
1	A	477	THR
1	A	593	VAL
1	A	596	ASP
1	A	602	VAL
1	A	655	THR
1	A	661	SER
1	A	663	VAL
1	A	664	GLU
1	A	761	LEU
1	A	816	VAL
1	A	818	VAL
1	A	827	GLU
1	A	840	ASP
1	A	859	VAL

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Mol	Chain	Res	Type
1	D	84	LEU
1	D	143	LEU
1	D	152	LYS
1	D	153	THR
1	D	156	VAL
1	D	181	THR
1	D	210	ASP
1	D	227	SER
1	D	242	THR
1	D	269	GLN
1	D	305	THR
1	D	310	VAL
1	D	318	ILE
1	D	335	VAL
1	D	356	ILE
1	D	360	ILE
1	D	381	LEU
1	D	423	SER
1	D	425	GLN
1	D	437	LEU
1	D	453	ILE
1	D	461	ASP
1	D	475	LYS
1	D	477	THR
1	D	485	ARG
1	D	510	GLU
1	D	515	SER
1	D	516	GLU
1	D	593	VAL
1	D	596	ASP
1	D	646	MET
1	D	650	SER
1	D	655	THR
1	D	664	GLU
1	D	691	VAL
1	D	692	ASP
1	D	695	THR
1	D	703	ARG
1	D	741	THR
1	D	761	LEU
1	D	768	ILE
1	D	815	THR

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Mol	Chain	Res	Type
1	D	816	VAL
1	D	823	GLU
1	D	827	GLU
1	D	839	LEU
1	D	846	LYS
1	D	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	161	ASN
1	A	211	HIS
1	A	235	ASN
1	A	555	ASN
1	A	659	GLN
1	A	697	ASN
1	D	190	GLN
1	D	383	ASN
1	D	392	HIS
1	D	479	ASN
1	D	659	GLN
1	D	690	ASN
1	D	807	ASN
1	D	824	GLN

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%)
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

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Mol	Chain	Res	Type
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	31,33,33	1.45	6 (19%)	41,49,49	2.41	16 (39%)
4	84T	D	1862	-	31,33,33	1.23	5 (16%)	41,49,49	2.04	12 (29%)

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	-	-	2/25/39/39	0/3/3/3
4	84T	D	1862	-	-	1/25/39/39	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1862	84T	P-O2P	3.57	1.51	1.46
4	A	1862	84T	C5-N7	-3.19	1.33	1.39
4	A	1862	84T	C8-N9	-3.15	1.32	1.37
4	A	1862	84T	P-O2P	2.79	1.50	1.46
4	A	1862	84T	P-O1P	-2.67	1.49	1.56
4	A	1862	84T	C4-N9	-2.57	1.32	1.37
4	D	1862	84T	P-N	2.33	1.67	1.63
4	D	1862	84T	C8-N7	2.31	1.36	1.31
4	D	1862	84T	C5-N7	-2.26	1.35	1.39
4	D	1862	84T	C4-N9	-2.09	1.33	1.37
4	A	1862	84T	P-N	2.03	1.66	1.63

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1862	84T	O1P-P-O2P	6.01	122.77	109.87
4	A	1862	84T	C5-C4-N3	-5.35	119.35	126.72
4	D	1862	84T	N1-C2-N3	-4.86	121.23	128.58
4	A	1862	84T	N1-C2-N3	-4.73	121.42	128.58
4	A	1862	84T	C4-C5-N7	-4.39	105.56	110.58
4	D	1862	84T	C5-C4-N3	-4.35	120.72	126.72
4	A	1862	84T	O5'-P-O2P	-4.07	102.19	114.27
4	A	1862	84T	O1P-P-O2P	3.71	117.83	109.87
4	D	1862	84T	N9-C8-N7	-3.68	108.72	113.94
4	A	1862	84T	C5-C4-N9	3.60	109.73	105.81
4	A	1862	84T	CA-C-N	3.52	118.61	115.49
4	A	1862	84T	OH-CA-CB	-3.44	102.92	110.38
4	A	1862	84T	N9-C8-N7	-3.43	109.08	113.94
4	A	1862	84T	C2-N3-C4	3.42	120.19	111.83
4	A	1862	84T	C5-N7-C8	3.16	108.41	103.45
4	D	1862	84T	C2-N3-C4	3.15	119.51	111.83
4	A	1862	84T	CD1-CG-CB	-3.14	106.11	111.23
4	A	1862	84T	CD1-CG-CD2	3.09	119.07	110.58
4	A	1862	84T	CD2-CG-CB	-2.76	106.72	111.23
4	D	1862	84T	C5-N7-C8	2.66	107.63	103.45
4	D	1862	84T	C4-C5-N7	-2.65	107.55	110.58
4	D	1862	84T	N3-C4-N9	2.51	131.43	127.17
4	D	1862	84T	O5'-P-O2P	-2.47	106.94	114.27
4	D	1862	84T	C4-N9-C8	2.38	108.24	105.74
4	A	1862	84T	N3-C4-N9	2.20	130.91	127.17
4	D	1862	84T	O2P-P-N	-2.18	107.55	111.03
4	A	1862	84T	O4'-C4'-C3'	2.17	107.82	105.07
4	D	1862	84T	OHB-CB-CA	-2.11	105.50	109.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1862	84T	OHB-CB-CG-CD1
4	A	1862	84T	C5'-O5'-P-O2P
4	D	1862	84T	C-N-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

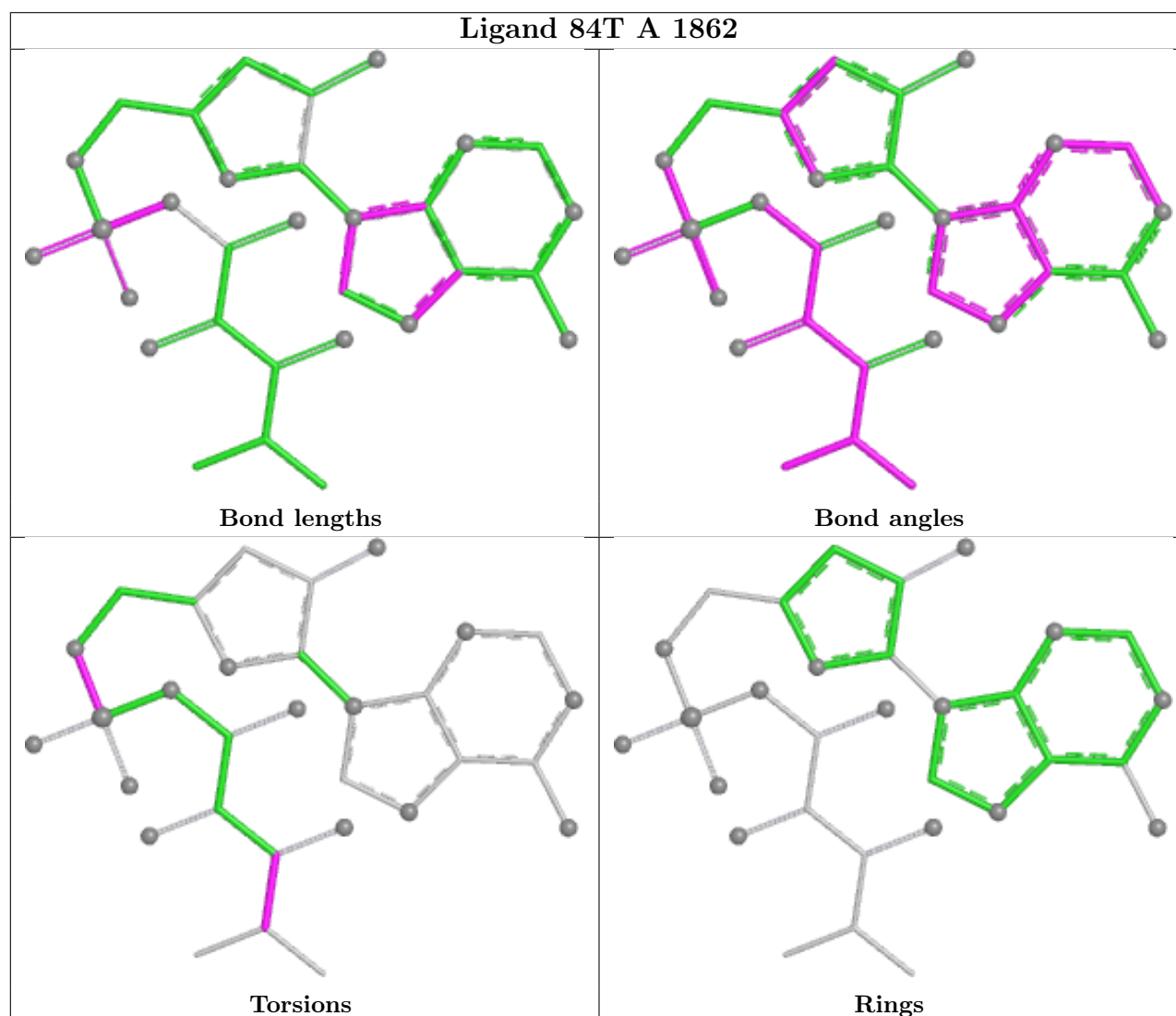
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1862	84T	2	0

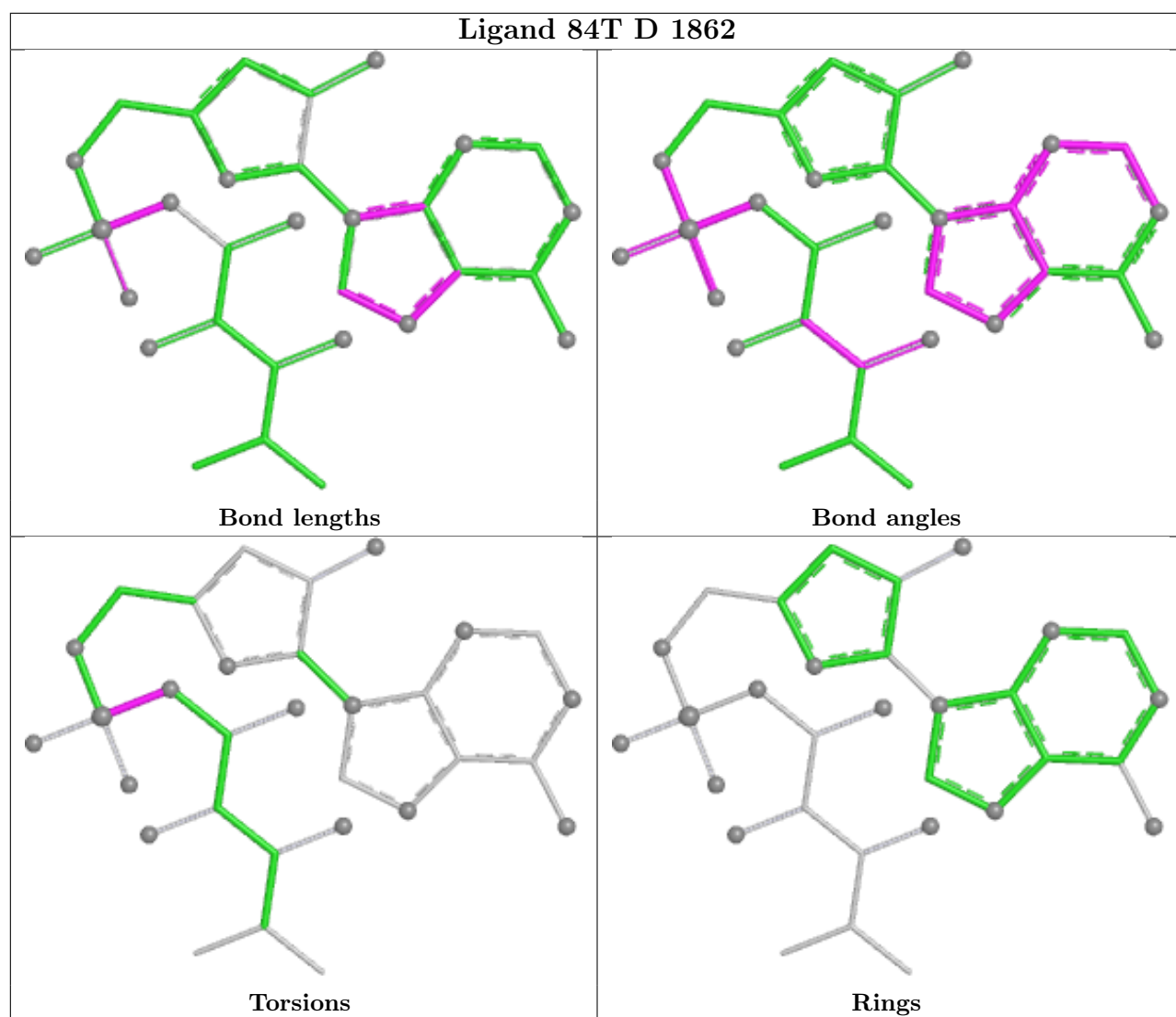
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1862	84T	1	0

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	860/880 (97%)	-0.37	3 (0%) 90 88	19, 35, 67, 122	0
1	D	867/880 (98%)	0.23	24 (2%) 55 51	39, 66, 116, 153	0
2	B	82/88 (93%)	-0.67	1 (1%) 76 73	24, 38, 92, 120	0
2	E	80/88 (90%)	-0.09	0 100 100	48, 78, 105, 118	0
All	All	1889/1936 (97%)	-0.09	28 (1%) 72 68	19, 51, 108, 153	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ASN	3.7
1	D	276	PRO	3.6
1	A	177	TRP	3.1
1	D	-5	VAL	2.9
1	D	330	TYR	2.7
1	D	290	VAL	2.7
1	D	303	VAL	2.6
1	D	297	THR	2.5
1	D	-7	GLY	2.4
1	D	180	ASP	2.3
1	D	172	ILE	2.3
1	D	356	ILE	2.3
1	D	305	THR	2.3
1	D	370	LEU	2.3
1	D	-3	ARG	2.3
1	A	290	VAL	2.2
1	D	463	ILE	2.2
1	D	182	LYS	2.2
1	D	365	GLY	2.2
2	B	47(B)	U	2.2
1	D	254	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	181	THR	2.1
1	D	310	VAL	2.1
1	D	581	GLY	2.1
1	D	0	HIS	2.1
1	D	691	VAL	2.0
1	D	296	ALA	2.0
1	D	848	ILE	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](#)

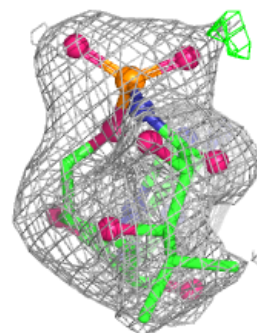
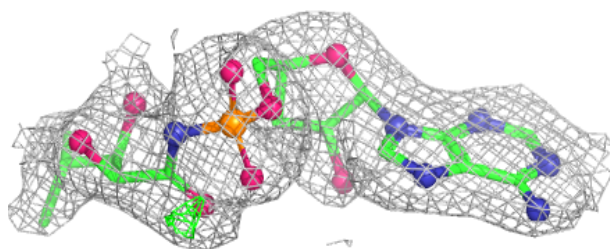
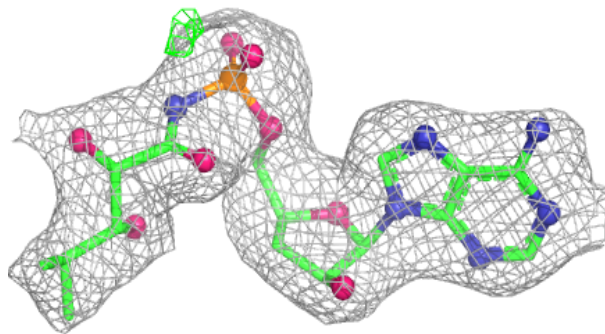
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	B	1081	1/1	0.84	0.10	55,55,55,55	0
5	MG	E	1078	1/1	0.84	0.29	59,59,59,59	0
5	MG	E	1077	1/1	0.85	0.28	60,60,60,60	0
5	MG	B	1078	1/1	0.90	0.15	62,62,62,62	0
3	ZN	D	1861	1/1	0.92	0.08	125,125,125,125	0
3	ZN	A	1861	1/1	0.94	0.07	118,118,118,118	0
5	MG	B	1079	1/1	0.96	0.07	43,43,43,43	0
4	84T	D	1862	31/31	0.97	0.06	38,39,41,43	0
5	MG	B	1077	1/1	0.98	0.08	32,32,32,32	0
4	84T	A	1862	31/31	0.98	0.05	18,19,22,23	0
5	MG	B	1080	1/1	0.99	0.03	41,41,41,41	0

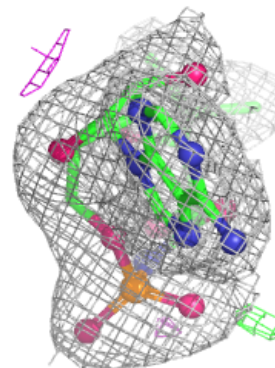
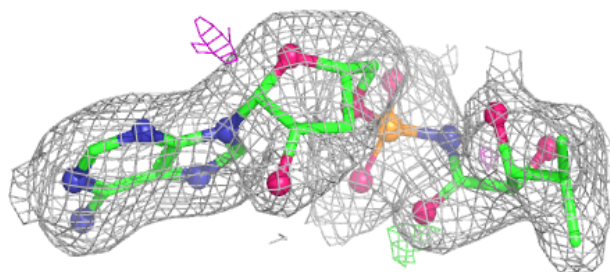
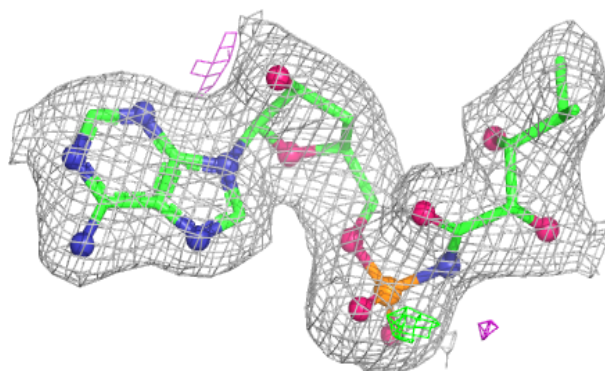
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.