



Full wwPDB EM Validation Report (i)

Nov 6, 2023 – 05:03 pm GMT

PDB ID : 8QHC
EMDB ID : EMD-18407
Title : Cryo-EM structure of SidH from Legionella pneumophila in complex with LubX
Authors : Sharma, R.; Adams, M.; Bhogaraju, S.
Deposited on : 2023-09-07
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the (i) 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 \(1\)](#)) were used in the production of this report:

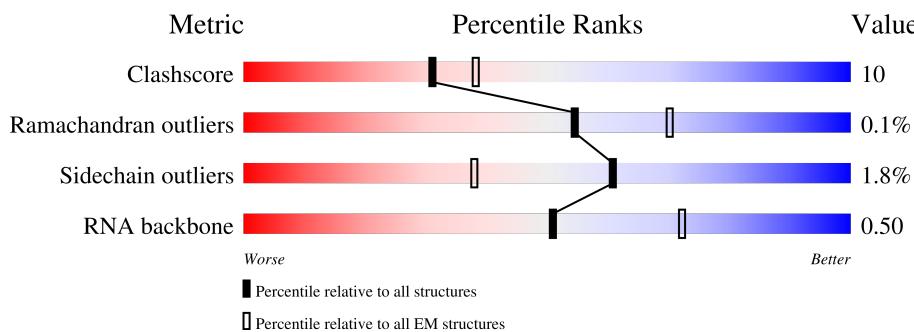
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : FAILED
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

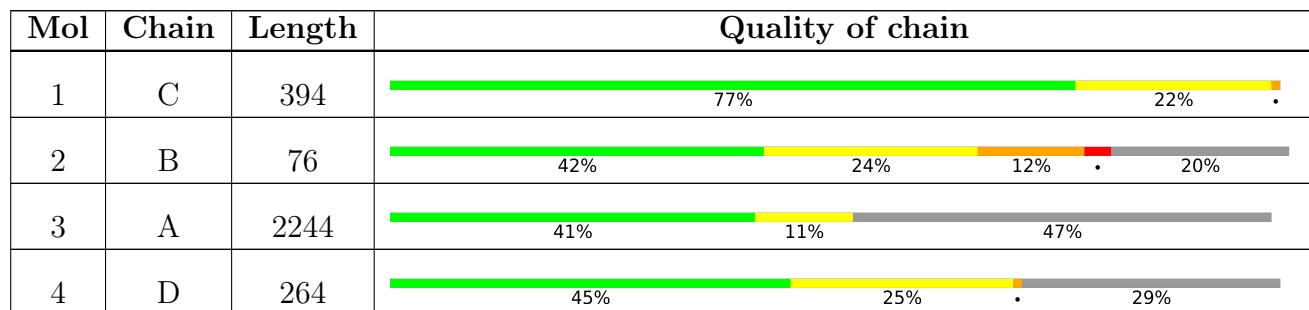
The reported resolution of this entry is 3.10 Å.

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14829 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	393	2937	1864	513	547	13	0	0

- Molecule 2 is a RNA chain called t-RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	B	61	1309	584	231	432	61	1	0	0

- Molecule 3 is a protein called Protein SidH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1183	9015	5746	1516	1730	23	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q6RCQ4
A	-17	GLY	-	expression tag	UNP Q6RCQ4
A	-16	SER	-	expression tag	UNP Q6RCQ4
A	-15	SER	-	expression tag	UNP Q6RCQ4
A	-14	HIS	-	expression tag	UNP Q6RCQ4
A	-13	HIS	-	expression tag	UNP Q6RCQ4
A	-12	HIS	-	expression tag	UNP Q6RCQ4
A	-11	HIS	-	expression tag	UNP Q6RCQ4
A	-10	HIS	-	expression tag	UNP Q6RCQ4
A	-9	HIS	-	expression tag	UNP Q6RCQ4
A	-8	SER	-	expression tag	UNP Q6RCQ4
A	-7	SER	-	expression tag	UNP Q6RCQ4
A	-6	GLY	-	expression tag	UNP Q6RCQ4
A	-5	LEU	-	expression tag	UNP Q6RCQ4
A	-4	VAL	-	expression tag	UNP Q6RCQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	expression tag	UNP Q6RCQ4
A	-2	ARG	-	expression tag	UNP Q6RCQ4
A	-1	GLY	-	expression tag	UNP Q6RCQ4
A	0	SER	-	expression tag	UNP Q6RCQ4

- Molecule 4 is a protein called E3 ubiquitin–protein ligase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	188	Total	C 1535	N 986	O 258	S 288	1 3

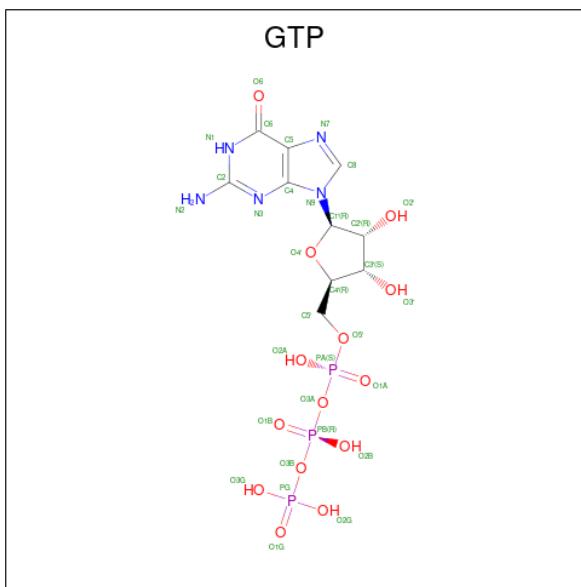
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	MET	-	initiating methionine	UNP A0A2S6F0E3
D	-16	HIS	-	expression tag	UNP A0A2S6F0E3
D	-15	HIS	-	expression tag	UNP A0A2S6F0E3
D	-14	HIS	-	expression tag	UNP A0A2S6F0E3
D	-13	HIS	-	expression tag	UNP A0A2S6F0E3
D	-12	HIS	-	expression tag	UNP A0A2S6F0E3
D	-11	HIS	-	expression tag	UNP A0A2S6F0E3
D	-10	SER	-	expression tag	UNP A0A2S6F0E3
D	-9	ALA	-	expression tag	UNP A0A2S6F0E3
D	-8	GLY	-	expression tag	UNP A0A2S6F0E3
D	-7	LEU	-	expression tag	UNP A0A2S6F0E3
D	-6	GLU	-	expression tag	UNP A0A2S6F0E3
D	-5	VAL	-	expression tag	UNP A0A2S6F0E3
D	-4	LEU	-	expression tag	UNP A0A2S6F0E3
D	-3	PHE	-	expression tag	UNP A0A2S6F0E3
D	-2	GLN	-	expression tag	UNP A0A2S6F0E3
D	-1	GLY	-	expression tag	UNP A0A2S6F0E3
D	0	PRO	-	expression tag	UNP A0A2S6F0E3

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

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total 1	Mg 1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

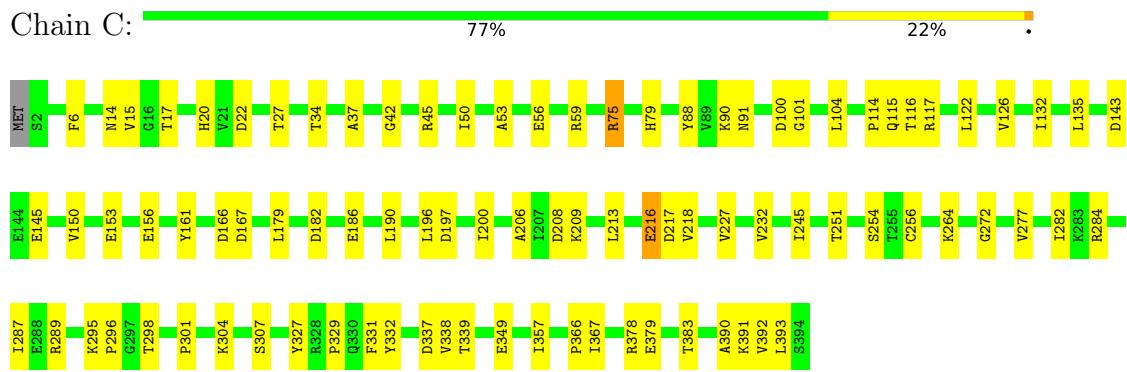


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total 32	C 10	N 5	O 14	P 3	0

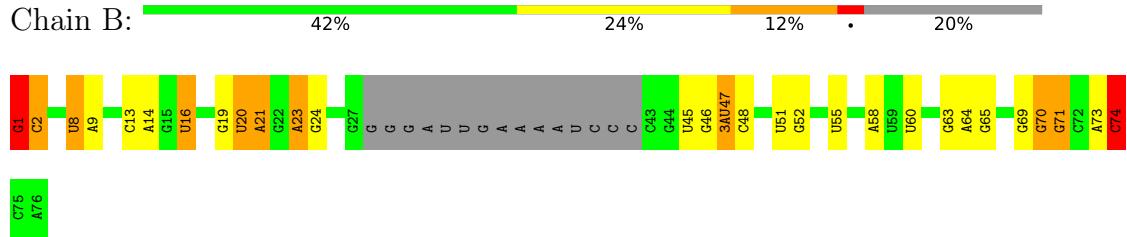
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

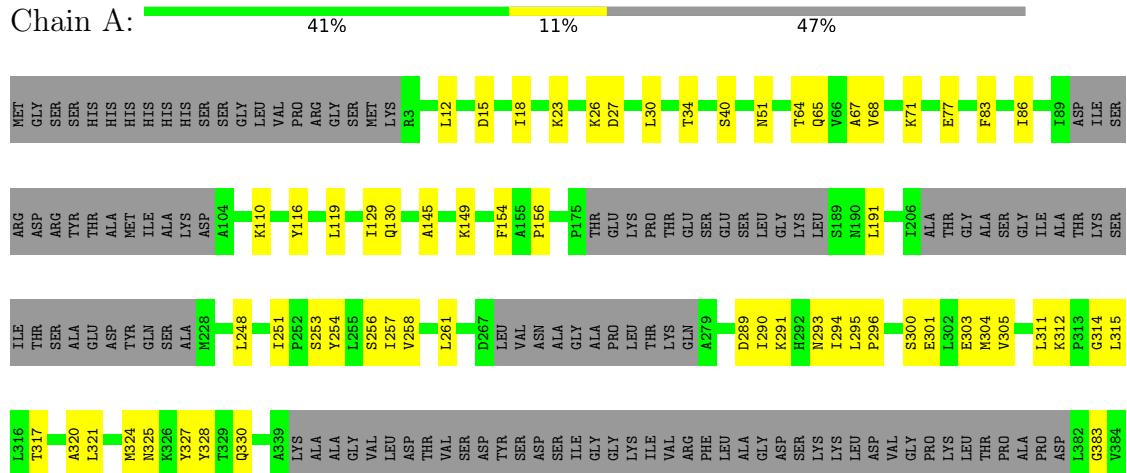
- Molecule 1: Elongation factor Tu

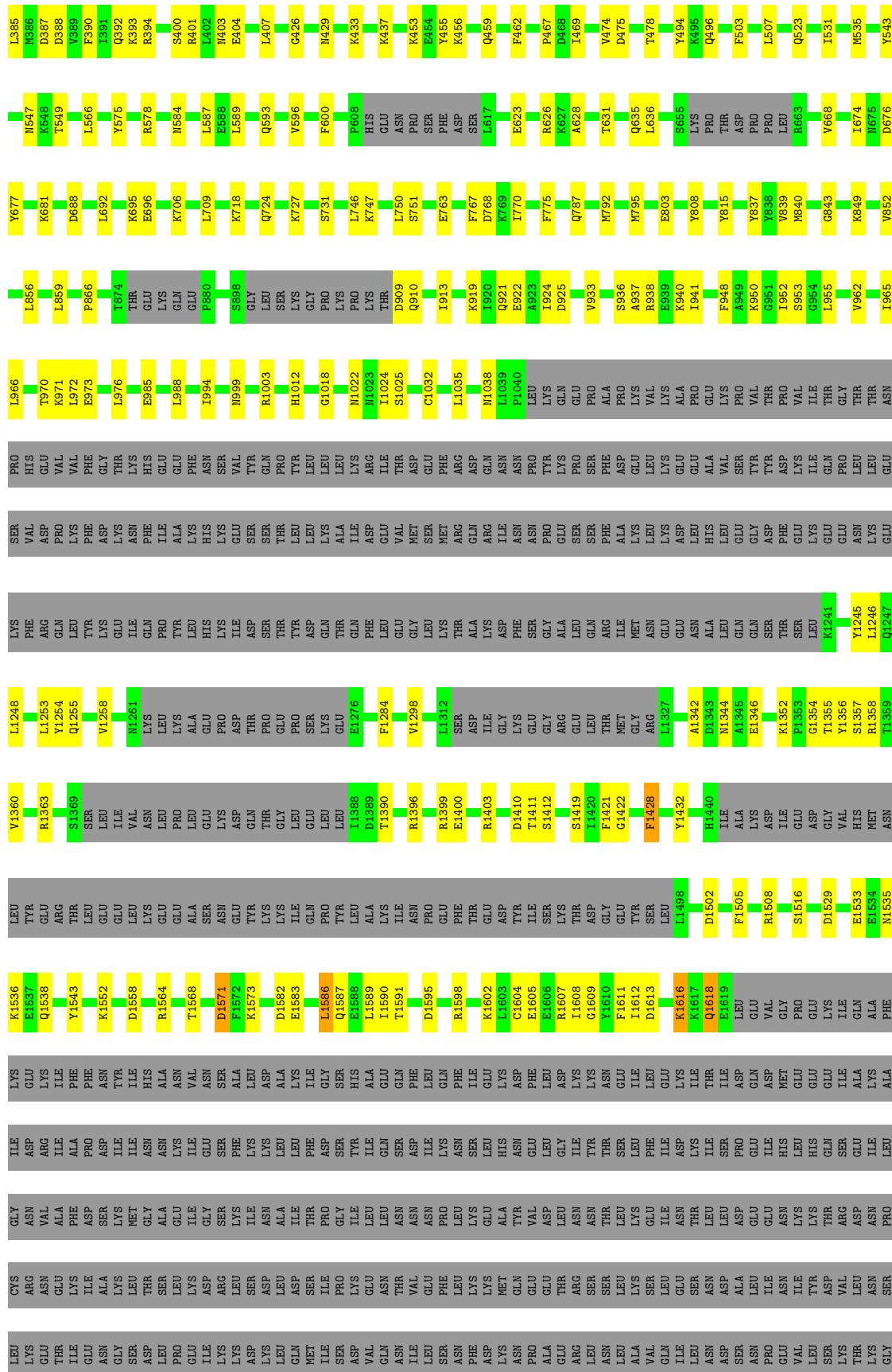


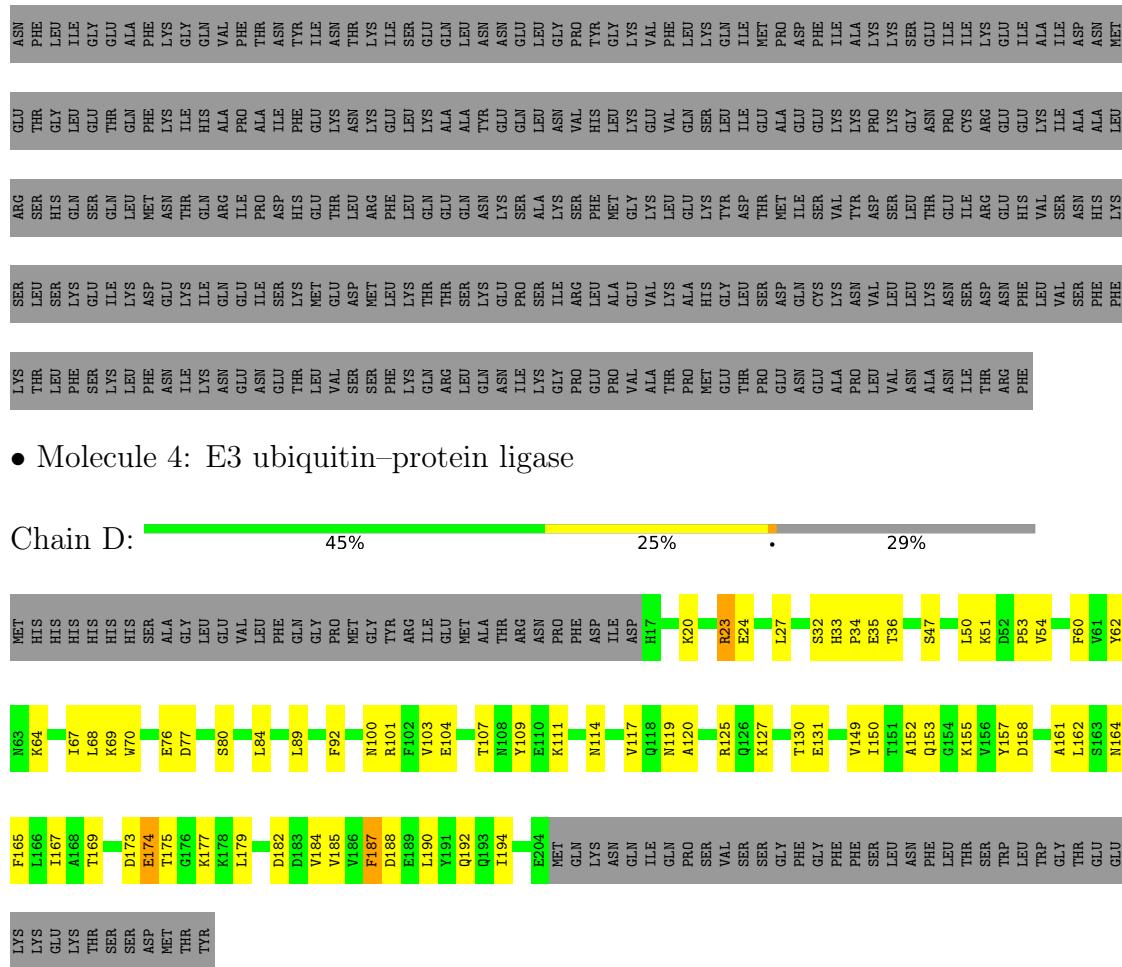
- Molecule 2: t-RNA



- Molecule 3: Protein SidH







- Molecule 4: E3 ubiquitin–protein ligase

Chain D: 45% MET, 25% LYS, 29% GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255829	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.37	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: MG, 4SU, 5MU, H2U, PSU, 3AU, GTP

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	C	0.26	0/2987	0.51	0/4060
2	B	0.42	1/1318 (0.1%)	0.90	3/2048 (0.1%)
3	A	0.25	0/9163	0.44	1/12405 (0.0%)
4	D	0.26	0/1569	0.51	0/2124
All	All	0.27	1/15037 (0.0%)	0.53	4/20637 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.71	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	C	C2-N1-C1'	7.34	126.87	118.80
3	A	1586	LEU	CA-CB-CG	6.44	130.11	115.30
2	B	74	C	N1-C2-O2	6.31	122.68	118.90
2	B	74	C	C6-N1-C1'	-5.20	114.56	120.80

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	C	2937	0	2899	53	0
2	B	1309	0	672	16	0
3	A	9015	0	8710	161	0
4	D	1535	0	1578	56	0
5	C	1	0	0	0	0
6	C	32	0	12	1	0
All	All	14829	0	13871	278	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 10.

All (278) 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:C:284:ARG:HH12	2:B:74:C:H42	1.24	0.84
2:B:51:U:H3	2:B:63:G:H1	0.86	0.82
3:A:314:GLY:HA2	3:A:317:THR:HG22	1.67	0.77
4:D:174:GLU:HG3	4:D:175:THR:HG23	1.70	0.73
3:A:1529:ASP:O	3:A:1535:ASN:ND2	2.19	0.73
3:A:767:PHE:HA	3:A:770:ILE:HG12	1.71	0.73
3:A:403:ASN:ND2	3:A:584:ASN:OD1	2.24	0.71
3:A:972:LEU:HB2	3:A:994:ILE:HG21	1.73	0.71
3:A:999:ASN:OD1	3:A:1003:ARG:NH2	2.22	0.69
4:D:33:HIS:HD2	4:D:34:PRO:HD2	1.58	0.69
1:C:53:ALA:HB3	1:C:56:GLU:HG3	1.75	0.68
3:A:1428:PHE:O	3:A:1432:TYR:HB3	1.93	0.68
4:D:24:GLU:HA	4:D:27:LEU:HG	1.75	0.67
3:A:763:GLU:OE2	3:A:763:GLU:N	2.29	0.66
1:C:213:LEU:HD12	1:C:232:VAL:HG22	1.78	0.65
3:A:600:PHE:HE1	3:A:668:VAL:HA	1.60	0.65
3:A:311:LEU:HD13	3:A:315:LEU:HD23	1.79	0.65
3:A:795:MET:HE1	3:A:839:VAL:HG21	1.79	0.64
3:A:936:SER:OG	3:A:940:LYS:NZ	2.30	0.64
4:D:23:ARG:HH21	4:D:27:LEU:HB3	1.61	0.64
3:A:320:ALA:O	3:A:324:MET:HG2	1.98	0.63
3:A:623:GLU:OE1	3:A:626:ARG:NH1	2.31	0.63
3:A:1344:ASN:OD1	3:A:1403:ARG:NH2	2.32	0.63
3:A:300:SER:O	3:A:304:MET:HG3	1.97	0.63
3:A:840:MET:HG2	3:A:856:LEU:HD11	1.82	0.62
3:A:575:TYR:HB2	3:A:696:GLU:OE1	2.00	0.62
4:D:149:VAL:HG22	4:D:184:VAL:HG12	1.81	0.62
3:A:30:LEU:O	3:A:34:THR:OG1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:HIS:CD2	4:D:34:PRO:HD2	2.35	0.61
4:D:33:HIS:HE1	4:D:150:ILE:HG23	1.65	0.61
3:A:478:THR:HG21	3:A:709:LEU:HB3	1.82	0.60
1:C:104:LEU:HD11	1:C:116:THR:HG23	1.82	0.60
3:A:955:LEU:HD21	3:A:1024:ILE:HG13	1.84	0.60
1:C:14:ASN:ND2	1:C:272:GLY:O	2.36	0.58
4:D:101:ARG:O	4:D:104:GLU:HG3	2.02	0.58
1:C:339:THR:OG1	2:B:65:G:O2'	2.16	0.58
3:A:1399:ARG:HH21	3:A:1403:ARG:HB2	1.68	0.58
3:A:15:ASP:OD2	3:A:1564:ARG:NH1	2.35	0.58
4:D:33:HIS:HB3	4:D:36:THR:HG23	1.85	0.57
3:A:1583:GLU:HA	3:A:1586:LEU:HD23	1.85	0.57
3:A:1018:GLY:O	3:A:1022:ASN:ND2	2.37	0.57
2:B:8:4SU:O2'	2:B:21:A:N1	2.29	0.57
4:D:100:ASN:OD1	4:D:101:ARG:N	2.37	0.57
3:A:1582:ASP:O	3:A:1586:LEU:HD22	2.06	0.56
3:A:843:GLY:HA3	3:A:852:VAL:HG11	1.87	0.56
4:D:23:ARG:NH2	4:D:27:LEU:HB3	2.20	0.56
3:A:724:GLN:HA	3:A:727:LYS:HE3	1.87	0.56
4:D:23:ARG:NE	4:D:23:ARG:O	2.39	0.56
1:C:289:ARG:NE	2:B:1:G:OP2	2.36	0.56
1:C:17:THR:HG23	1:C:79:HIS:CE1	2.41	0.56
3:A:1543:TYR:OH	3:A:1558:ASP:O	2.20	0.56
3:A:962:VAL:HA	3:A:965:ILE:HG12	1.87	0.56
3:A:566:LEU:HD11	3:A:695:LYS:HD3	1.88	0.56
3:A:628:ALA:O	3:A:631:THR:OG1	2.23	0.56
3:A:1595:ASP:OD1	3:A:1598:ARG:NH2	2.39	0.56
3:A:531:ILE:O	3:A:535:MET:HG3	2.06	0.55
3:A:1583:GLU:O	3:A:1587:GLN:HG2	2.05	0.55
1:C:91:ASN:ND2	2:B:2:C:OP1	2.29	0.55
4:D:190:LEU:O	4:D:194:ILE:HG12	2.06	0.55
3:A:23:LYS:NZ	3:A:27:ASP:OD2	2.37	0.55
3:A:589:LEU:HD23	3:A:635:GLN:HE21	1.72	0.55
3:A:676:ASP:OD1	3:A:677:TYR:N	2.39	0.55
3:A:837:TYR:HA	3:A:840:MET:HE3	1.89	0.55
1:C:135:LEU:HD21	1:C:150:VAL:HG11	1.88	0.55
3:A:1421:PHE:HA	3:A:1516:SER:HB2	1.88	0.54
3:A:1568:THR:OG1	3:A:1571:ASP:OD1	2.23	0.54
4:D:70:TRP:NE1	4:D:76:GLU:O	2.35	0.54
3:A:327:TYR:O	3:A:330:GLN:HG3	2.08	0.54
4:D:50:LEU:HD22	4:D:53:PRO:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:PHE:HA	3:A:86:ILE:HD12	1.88	0.54
1:C:245:ILE:O	1:C:251:THR:HA	2.07	0.54
3:A:792:MET:HA	3:A:795:MET:HE3	1.89	0.54
1:C:45:ARG:HH11	1:C:50:ILE:HD13	1.73	0.53
3:A:296:PRO:HG3	3:A:390:PHE:CD2	2.43	0.53
4:D:107:THR:O	4:D:111:LYS:N	2.37	0.53
3:A:387:ASP:N	3:A:387:ASP:OD1	2.41	0.53
1:C:327:TYR:OH	1:C:379:GLU:OE1	2.26	0.52
3:A:971:LYS:HD3	3:A:994:ILE:HG12	1.91	0.52
3:A:1390:THR:HG22	3:A:1618:GLN:NE2	2.25	0.52
1:C:59:ARG:NH2	1:C:88:TYR:OH	2.42	0.52
3:A:317:THR:O	3:A:321:LEU:HB2	2.10	0.52
1:C:75:ARG:NH2	1:C:200:ILE:O	2.42	0.52
3:A:938:ARG:O	3:A:941:ILE:HG13	2.09	0.52
1:C:22:ASP:OD2	3:A:437:LYS:NZ	2.30	0.51
1:C:254:SER:HB2	1:C:282:ILE:HD11	1.92	0.51
3:A:747:LYS:HD3	3:A:763:GLU:HA	1.91	0.51
3:A:1355:THR:OG1	3:A:1356:TYR:N	2.44	0.51
1:C:357:ILE:HD11	3:A:156:PRO:HG3	1.92	0.51
3:A:475:ASP:OD2	3:A:494:TYR:OH	2.21	0.51
4:D:32:SER:OG	4:D:36:THR:OG1	2.28	0.51
3:A:1354:GLY:HA3	3:A:1358:ARG:HH21	1.76	0.51
1:C:20:HIS:ND1	1:C:115:GLN:HB2	2.26	0.51
4:D:60:PHE:HE2	4:D:80:SER:HB3	1.76	0.51
1:C:301:PRO:HB2	1:C:366:PRO:HB2	1.92	0.51
2:B:63:G:H2'	2:B:64:A:C8	2.46	0.51
3:A:952:ILE:HG23	3:A:955:LEU:HD12	1.93	0.51
3:A:1032:CYS:HA	3:A:1035:LEU:HG	1.93	0.50
2:B:63:G:H2'	2:B:64:A:H8	1.75	0.50
4:D:33:HIS:CD2	4:D:152:ALA:HA	2.46	0.50
1:C:338:VAL:HG21	1:C:367:ILE:HG21	1.93	0.50
3:A:12:LEU:HD22	3:A:18:ILE:HD12	1.92	0.50
1:C:117:ARG:NH1	1:C:161:TYR:OH	2.41	0.50
3:A:948:PHE:O	3:A:952:ILE:HG12	2.11	0.50
3:A:746:LEU:O	3:A:750:LEU:HB2	2.11	0.50
3:A:1602:LYS:O	3:A:1605:GLU:HG2	2.11	0.50
3:A:775:PHE:CE1	3:A:787:GLN:HG2	2.48	0.49
3:A:910:GLN:NE2	3:A:953:SER:O	2.45	0.49
4:D:76:GLU:HA	4:D:84:LEU:H	1.76	0.49
3:A:291:LYS:HD3	3:A:328:TYR:CZ	2.48	0.49
4:D:54:VAL:HG11	4:D:64:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:LEU:HD12	4:D:69:LYS:HG3	1.94	0.49
4:D:157:TYR:HD1	4:D:162:LEU:HD13	1.78	0.49
3:A:1255:GLN:HA	3:A:1258:VAL:HG12	1.94	0.49
3:A:635:GLN:N	3:A:635:GLN:OE1	2.46	0.48
3:A:1608:ILE:O	3:A:1612:ILE:HG23	2.13	0.48
4:D:165:PHE:O	4:D:169:THR:HG22	2.14	0.48
1:C:206:ALA:HB1	1:C:209:LYS:HG3	1.94	0.48
4:D:84:LEU:HD13	4:D:89:LEU:HD21	1.95	0.48
4:D:164:ASN:OD1	4:D:165:PHE:N	2.46	0.48
2:B:69:G:O2'	2:B:70:G:H5'	2.13	0.48
4:D:173:ASP:O	4:D:177:LYS:NZ	2.47	0.48
3:A:1410:ASP:OD2	3:A:1411:THR:N	2.47	0.48
4:D:33:HIS:ND1	4:D:185:VAL:HG12	2.29	0.48
1:C:6:PHE:HB2	1:C:264:LYS:HB3	1.96	0.48
3:A:795:MET:SD	3:A:859:LEU:HD21	2.54	0.48
4:D:150:ILE:O	4:D:184:VAL:HG13	2.14	0.48
3:A:1355:THR:O	3:A:1358:ARG:HG2	2.14	0.48
4:D:182:ASP:OD2	4:D:182:ASP:N	2.45	0.48
3:A:547:ASN:HB3	3:A:549:THR:HG23	1.95	0.47
1:C:349:GLU:HB2	3:A:154:PHE:HB3	1.96	0.47
4:D:153:GLN:NE2	4:D:155:LYS:HB2	2.29	0.47
4:D:158:ASP:HB3	4:D:161:ALA:HB3	1.97	0.47
1:C:307:SER:HA	1:C:390:ALA:H	1.79	0.47
1:C:391:LYS:NZ	1:C:392:VAL:O	2.47	0.47
2:B:51:U:O4	2:B:63:G:O6	2.31	0.47
3:A:1538:GLN:HA	3:A:1538:GLN:OE1	2.14	0.47
3:A:1422:GLY:H	3:A:1516:SER:HB3	1.80	0.47
1:C:37:ALA:HA	1:C:42:GLY:HA3	1.97	0.46
3:A:400:SER:O	3:A:404:GLU:HG2	2.14	0.46
3:A:433:LYS:HG2	3:A:503:PHE:CD1	2.50	0.46
3:A:1284:PHE:HD1	3:A:1363:ARG:HH12	1.63	0.46
3:A:191:LEU:HD12	3:A:248:LEU:HD12	1.96	0.46
3:A:429:ASN:OD1	3:A:429:ASN:N	2.41	0.46
3:A:921:GLN:NE2	3:A:925:ASP:OD2	2.48	0.46
3:A:1346:GLU:OE2	3:A:1357:SER:N	2.43	0.46
3:A:67:ALA:O	3:A:71:LYS:HG3	2.15	0.46
3:A:937:ALA:HA	3:A:940:LYS:HE2	1.98	0.46
3:A:40:SER:HB3	3:A:312:LYS:HA	1.98	0.46
3:A:474:VAL:HG22	3:A:709:LEU:HG	1.98	0.46
1:C:295:LYS:HG3	1:C:296:PRO:HD2	1.98	0.46
4:D:114:ASN:OD1	4:D:114:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:130:GLN:HB3	3:A:866:PRO:HG2	1.98	0.46
3:A:636:LEU:HD12	3:A:674:ILE:HD11	1.97	0.46
3:A:1607:ARG:O	3:A:1611:PHE:CD1	2.68	0.46
3:A:325:ASN:HA	3:A:385:LEU:HD22	1.98	0.45
3:A:1604:CYS:O	3:A:1608:ILE:HG23	2.16	0.45
3:A:1410:ASP:OD2	3:A:1412:SER:N	2.45	0.45
3:A:116:TYR:HD1	3:A:119:LEU:HD12	1.82	0.45
3:A:253:SER:O	3:A:257:ILE:HD12	2.16	0.45
3:A:1246:LEU:HD23	3:A:1246:LEU:HA	1.80	0.45
4:D:53:PRO:HG2	4:D:92:PHE:O	2.17	0.45
3:A:456:LYS:HG3	3:A:709:LEU:HD13	1.99	0.45
3:A:972:LEU:HA	3:A:994:ILE:HD13	1.97	0.45
4:D:54:VAL:HG23	4:D:62:TYR:HB2	1.99	0.45
4:D:127:LYS:HB2	4:D:127:LYS:HE2	1.85	0.45
3:A:388:ASP:O	3:A:392:GLN:HG2	2.17	0.45
2:B:23:A:H2'	2:B:24:G:C8	2.52	0.45
3:A:26:LYS:HE2	3:A:77:GLU:HG2	1.99	0.45
3:A:257:ILE:HD12	3:A:257:ILE:H	1.82	0.45
3:A:718:LYS:HZ3	3:A:808:TYR:H	1.65	0.45
3:A:51:ASN:OD1	3:A:51:ASN:N	2.50	0.45
3:A:751:SER:HA	3:A:1352:LYS:HG3	1.98	0.45
3:A:1245:TYR:HE1	3:A:1298:VAL:HG13	1.82	0.45
1:C:378:ARG:HG2	1:C:383:THR:HA	1.97	0.44
3:A:253:SER:O	3:A:256:SER:OG	2.25	0.44
3:A:65:GLN:HA	3:A:68:VAL:HG12	1.99	0.44
3:A:919:LYS:O	3:A:922:GLU:HG3	2.17	0.44
3:A:970:THR:O	3:A:973:GLU:HG3	2.17	0.44
4:D:23:ARG:HH21	4:D:27:LEU:CB	2.28	0.44
4:D:187:PHE:CD1	4:D:190:LEU:HB2	2.52	0.44
1:C:304:LYS:HG2	1:C:393:LEU:HD12	1.98	0.44
1:C:332:TYR:HE1	1:C:378:ARG:HB2	1.83	0.44
3:A:578:ARG:HB3	3:A:692:LEU:HD13	1.98	0.44
3:A:26:LYS:HB3	3:A:26:LYS:HE3	1.72	0.44
3:A:681:LYS:HD3	3:A:681:LYS:HA	1.88	0.44
4:D:119:ASN:OD1	4:D:120:ALA:N	2.51	0.44
3:A:1342:ALA:HB2	3:A:1360:VAL:HG11	1.99	0.44
2:B:23:A:H2'	2:B:24:G:H8	1.82	0.44
1:C:122:LEU:O	1:C:126:VAL:HG22	2.17	0.43
2:B:1:G:HO2'	2:B:2:C:P	2.40	0.43
3:A:924:ILE:HD11	3:A:976:LEU:HD13	1.99	0.43
4:D:164:ASN:HA	4:D:167:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLU:O	1:C:156:GLU:HG2	2.18	0.43
4:D:20:LYS:O	4:D:24:GLU:HG3	2.18	0.43
1:C:14:ASN:O	1:C:100:ASP:N	2.50	0.43
3:A:145:ALA:O	3:A:149:LYS:HG3	2.19	0.43
3:A:257:ILE:HG23	3:A:294:ILE:CG2	2.48	0.43
3:A:289:ASP:OD1	3:A:293:ASN:ND2	2.47	0.43
3:A:593:GLN:HA	3:A:596:VAL:HG12	1.99	0.43
3:A:727:LYS:HB3	3:A:727:LYS:HE2	1.80	0.43
4:D:62:TYR:OH	4:D:77:ASP:OD1	2.29	0.43
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.83	0.43
3:A:1552:LYS:HB2	3:A:1589:LEU:HD11	1.99	0.43
4:D:51:LYS:HA	4:D:51:LYS:HD3	1.65	0.43
1:C:216:GLU:HG3	1:C:217:ASP:N	2.33	0.43
3:A:453:LYS:HE2	3:A:453:LYS:HB3	1.81	0.43
4:D:153:GLN:HE21	4:D:155:LYS:HB2	1.84	0.43
4:D:36:THR:OG1	4:D:36:THR:O	2.37	0.43
1:C:114:PRO:HG3	3:A:496:GLN:HG3	2.01	0.42
1:C:182:ASP:O	1:C:186:GLU:HG3	2.19	0.42
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.87	0.42
4:D:190:LEU:HD12	4:D:190:LEU:HA	1.79	0.42
3:A:393:LYS:HE2	3:A:393:LYS:HB2	1.86	0.42
3:A:1003:ARG:HG3	3:A:1025:SER:OG	2.19	0.42
3:A:1590:ILE:HG13	3:A:1591:THR:N	2.33	0.42
2:B:58:A:O2'	2:B:60:U:OP2	2.28	0.42
3:A:985:GLU:O	3:A:988:LEU:HG	2.19	0.42
3:A:1400:GLU:HG3	3:A:1611:PHE:CE1	2.54	0.42
4:D:130:THR:OG1	4:D:131:GLU:OE1	2.37	0.42
3:A:706:LYS:HD3	3:A:706:LYS:HA	1.75	0.42
3:A:933:VAL:O	3:A:938:ARG:NH1	2.53	0.42
4:D:177:LYS:HB2	4:D:179:LEU:HD23	2.00	0.42
4:D:188:ASP:O	4:D:192:GLN:HG2	2.19	0.42
2:B:70:G:O2'	2:B:71:G:O5'	2.32	0.42
1:C:295:LYS:O	1:C:298:THR:HG22	2.18	0.42
3:A:303:GLU:OE2	3:A:394:ARG:NH2	2.47	0.42
1:C:218:VAL:HG21	1:C:287:ILE:HG22	2.02	0.42
4:D:157:TYR:CD1	4:D:162:LEU:HD13	2.55	0.42
1:C:34:THR:HG21	1:C:179:LEU:HD12	2.02	0.42
3:A:304:MET:HG2	3:A:401:ARG:HD3	2.01	0.42
3:A:261:LEU:HD23	3:A:290:ILE:HD12	2.00	0.42
3:A:328:TYR:HE2	3:A:383:GLY:HA2	1.85	0.42
3:A:1253:LEU:HD23	3:A:1253:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1245:TYR:O	3:A:1248:LEU:HG	2.20	0.41
4:D:35:GLU:HB3	4:D:109:TYR:HE2	1.85	0.41
1:C:329:PRO:HG2	1:C:331:PHE:CE1	2.56	0.41
3:A:455:TYR:CE2	3:A:459:GLN:HG3	2.55	0.41
3:A:909:ASP:N	3:A:909:ASP:OD1	2.52	0.41
1:C:27:THR:OG1	6:C:402:GTP:O1A	2.26	0.41
1:C:132:ILE:HD13	1:C:196:LEU:HD12	2.02	0.41
1:C:332:TYR:CE1	1:C:378:ARG:HB2	2.56	0.41
3:A:64:THR:H	3:A:523:GLN:HB2	1.85	0.41
3:A:295:LEU:HD23	3:A:295:LEU:HA	1.87	0.41
3:A:940:LYS:HB3	3:A:1038:ASN:HD22	1.85	0.41
3:A:1390:THR:HG22	3:A:1618:GLN:HE21	1.86	0.41
3:A:1399:ARG:HH21	3:A:1403:ARG:CB	2.33	0.41
3:A:1502:ASP:O	3:A:1505:PHE:HB2	2.20	0.41
1:C:90:LYS:HD2	1:C:289:ARG:NH2	2.35	0.41
1:C:331:PHE:O	1:C:337:ASP:HA	2.21	0.41
4:D:64:LYS:HA	4:D:67:ILE:HG22	2.03	0.41
4:D:100:ASN:O	4:D:103:VAL:HG22	2.20	0.41
2:B:46:G:OP1	2:B:47:3AU:H5'A	2.20	0.41
1:C:15:VAL:HA	1:C:101:GLY:O	2.20	0.41
3:A:191:LEU:HD21	3:A:305:VAL:HG11	2.03	0.41
3:A:587:LEU:HD23	3:A:587:LEU:HA	1.88	0.41
3:A:1533:GLU:HA	3:A:1536:LYS:HD3	2.02	0.41
4:D:60:PHE:CE2	4:D:80:SER:HB3	2.55	0.41
3:A:110:LYS:HE3	3:A:110:LYS:HB3	1.80	0.41
3:A:910:GLN:HA	3:A:913:ILE:HG12	2.03	0.41
3:A:1399:ARG:O	3:A:1399:ARG:NE	2.52	0.41
3:A:1609:GLY:O	3:A:1612:ILE:HG13	2.21	0.41
3:A:462:PHE:HE1	3:A:469:ILE:HB	1.85	0.41
3:A:731:SER:OG	3:A:803:GLU:OE1	2.24	0.41
3:A:1613:ASP:O	3:A:1616:LYS:HG3	2.21	0.40
3:A:426:GLY:HA2	3:A:507:LEU:HD11	2.02	0.40
3:A:129:ILE:HD13	3:A:129:ILE:HA	1.96	0.40
3:A:254:TYR:O	3:A:258:VAL:HG13	2.21	0.40
3:A:933:VAL:HB	3:A:938:ARG:CZ	2.51	0.40
3:A:1396:ARG:O	3:A:1400:GLU:HG2	2.21	0.40
1:C:15:VAL:O	1:C:79:HIS:HA	2.22	0.40
3:A:251:ILE:HG22	3:A:301:GLU:HB3	2.03	0.40
1:C:143:ASP:OD1	1:C:145:GLU:N	2.53	0.40
1:C:227:VAL:HA	1:C:277:VAL:O	2.21	0.40
3:A:407:LEU:HD23	3:A:407:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:467:PRO:HG2	3:A:815:TYR:O	2.22	0.40
3:A:965:ILE:HG13	3:A:966:LEU:N	2.37	0.40
4:D:117:VAL:O	4:D:120:ALA:HB3	2.21	0.40
4:D:155:LYS:HD2	4:D:157:TYR:CE2	2.57	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 PDB entries followed by that with respect to all EM entries.

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	C	391/394 (99%)	379 (97%)	12 (3%)	0	100 100
3	A	1153/2244 (51%)	1113 (96%)	40 (4%)	0	100 100
4	D	187/264 (71%)	182 (97%)	4 (2%)	1 (0%)	29 64
All	All	1731/2902 (60%)	1674 (97%)	56 (3%)	1 (0%)	54 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	174	GLU

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 PDB entries followed by that with respect to all EM entries.

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	C	301/327 (92%)	294 (98%)	7 (2%)	50 77
3	A	932/2015 (46%)	918 (98%)	14 (2%)	65 85
4	D	174/241 (72%)	170 (98%)	4 (2%)	50 77
All	All	1407/2583 (54%)	1382 (98%)	25 (2%)	61 82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	75	ARG
1	C	166	ASP
1	C	167	ASP
1	C	197	ASP
1	C	208	ASP
1	C	216	GLU
1	C	256	CYS
3	A	543	TYR
3	A	688	ASP
3	A	768	ASP
3	A	849	LYS
3	A	950	LYS
3	A	1012	HIS
3	A	1254	TYR
3	A	1419	SER
3	A	1428	PHE
3	A	1508	ARG
3	A	1571	ASP
3	A	1573	LYS
3	A	1616	LYS
3	A	1618	GLN
4	D	23	ARG
4	D	47	SER
4	D	125	ARG
4	D	187	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1022	ASN

5.3.3 RNA [\(i\)](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	59/76 (77%)	15 (25%)	3 (5%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	C
2	B	9	A
2	B	14	A
2	B	16	H2U
2	B	19	G
2	B	20	H2U
2	B	21	A
2	B	23	A
2	B	45	U
2	B	48	C
2	B	52	G
2	B	70	G
2	B	71	G
2	B	73	A
2	B	74	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	G
2	B	13	C
2	B	70	G

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	PSU	B	55	2	18,21,22	1.03	1 (5%)	22,30,33	1.78	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4SU	B	8	2	18,21,22	3.64	7 (38%)	26,30,33	2.30	4 (15%)
2	5MU	B	54	2	19,22,23	0.47	0	28,32,35	0.61	0
2	H2U	B	16	2	18,21,22	0.49	0	21,30,33	0.98	1 (4%)
2	3AU	B	47	2	24,28,29	2.74	9 (37%)	33,40,43	1.35	4 (12%)
2	H2U	B	20	2	18,21,22	0.57	0	21,30,33	1.43	3 (14%)

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
2	PSU	B	55	2	-	0/7/25/26	0/2/2/2
2	4SU	B	8	2	-	0/7/25/26	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	H2U	B	16	2	-	3/7/38/39	0/2/2/2
2	3AU	B	47	2	-	6/16/34/35	0/2/2/2
2	H2U	B	20	2	-	6/7/38/39	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	4SU	C2-N3	7.07	1.50	1.38
2	B	8	4SU	C2-N1	7.02	1.49	1.38
2	B	8	4SU	C4-N3	6.81	1.44	1.37
2	B	47	3AU	C2-N1	6.30	1.47	1.38
2	B	47	3AU	C6-C5	6.11	1.49	1.35
2	B	47	3AU	C2-N3	5.95	1.49	1.38
2	B	8	4SU	C5-C4	5.63	1.49	1.42
2	B	8	4SU	C6-C5	5.44	1.47	1.35
2	B	8	4SU	C4-S4	-4.39	1.60	1.68
2	B	47	3AU	O2-C2	-3.63	1.15	1.22
2	B	47	3AU	C4-N3	3.62	1.46	1.40
2	B	47	3AU	C6-N1	3.52	1.46	1.38
2	B	55	PSU	C6-C5	3.17	1.39	1.35
2	B	47	3AU	C11-C10	3.00	1.58	1.52
2	B	8	4SU	C6-N1	2.78	1.44	1.38
2	B	47	3AU	O4-C4	-2.33	1.18	1.23
2	B	47	3AU	O30-C13	2.30	1.29	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	4SU	C4-N3-C2	-7.97	119.59	127.34
2	B	8	4SU	C5-C4-N3	5.90	120.16	114.69
2	B	55	PSU	C4-N3-C2	-4.78	119.45	126.34
2	B	55	PSU	N1-C2-N3	4.44	120.16	115.13
2	B	8	4SU	C5-C4-S4	-3.88	119.47	124.47
2	B	47	3AU	C4-N3-C2	-3.73	119.95	124.63
2	B	20	H2U	C5-C4-N3	-3.62	112.58	116.65
2	B	8	4SU	N3-C2-N1	3.59	119.65	114.89
2	B	20	H2U	O2-C2-N1	3.56	127.57	123.11
2	B	16	H2U	C5-C4-N3	-3.13	113.14	116.65
2	B	47	3AU	C5-C4-N3	3.08	119.56	115.50
2	B	55	PSU	O2-C2-N1	-2.54	120.00	122.79
2	B	47	3AU	O2-C2-N3	-2.46	118.57	121.99
2	B	20	H2U	O2-C2-N3	-2.39	117.05	121.50
2	B	47	3AU	C6-N1-C2	-2.38	119.65	121.79

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	47	3AU	C10-C11-C12-N40
2	B	47	3AU	O4'-C4'-C5'-O5'
2	B	16	H2U	O4'-C4'-C5'-O5'
2	B	16	H2U	C3'-C4'-C5'-O5'
2	B	20	H2U	C2'-C1'-N1-C2
2	B	47	3AU	C3'-C4'-C5'-O5'
2	B	20	H2U	C2'-C1'-N1-C6
2	B	47	3AU	C11-C12-C13-O31
2	B	47	3AU	C11-C12-C13-O30
2	B	20	H2U	O4'-C4'-C5'-O5'
2	B	20	H2U	C4'-C5'-O5'-P
2	B	20	H2U	C3'-C4'-C5'-O5'
2	B	47	3AU	C10-C11-C12-C13
2	B	16	H2U	C4'-C5'-O5'-P
2	B	20	H2U	O4'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	4SU	1	0
2	B	47	3AU	1	0

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GTP	C	402	5	26,34,34	1.15	1 (3%)	32,54,54	1.62	7 (21%)

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
6	GTP	C	402	5	-	8/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	402	GTP	C5-C6	-4.07	1.39	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	402	GTP	PB-O3B-PG	-3.76	119.91	132.83
6	C	402	GTP	C5-C6-N1	3.36	119.88	113.95
6	C	402	GTP	C2-N1-C6	-2.99	119.58	125.10
6	C	402	GTP	C8-N7-C5	2.97	108.65	102.99
6	C	402	GTP	C3'-C2'-C1'	2.94	105.40	100.98
6	C	402	GTP	PA-O3A-PB	-2.82	123.15	132.83
6	C	402	GTP	O6-C6-C5	-2.24	120.00	124.37

There are no chirality outliers.

All (8) torsion outliers are listed below:

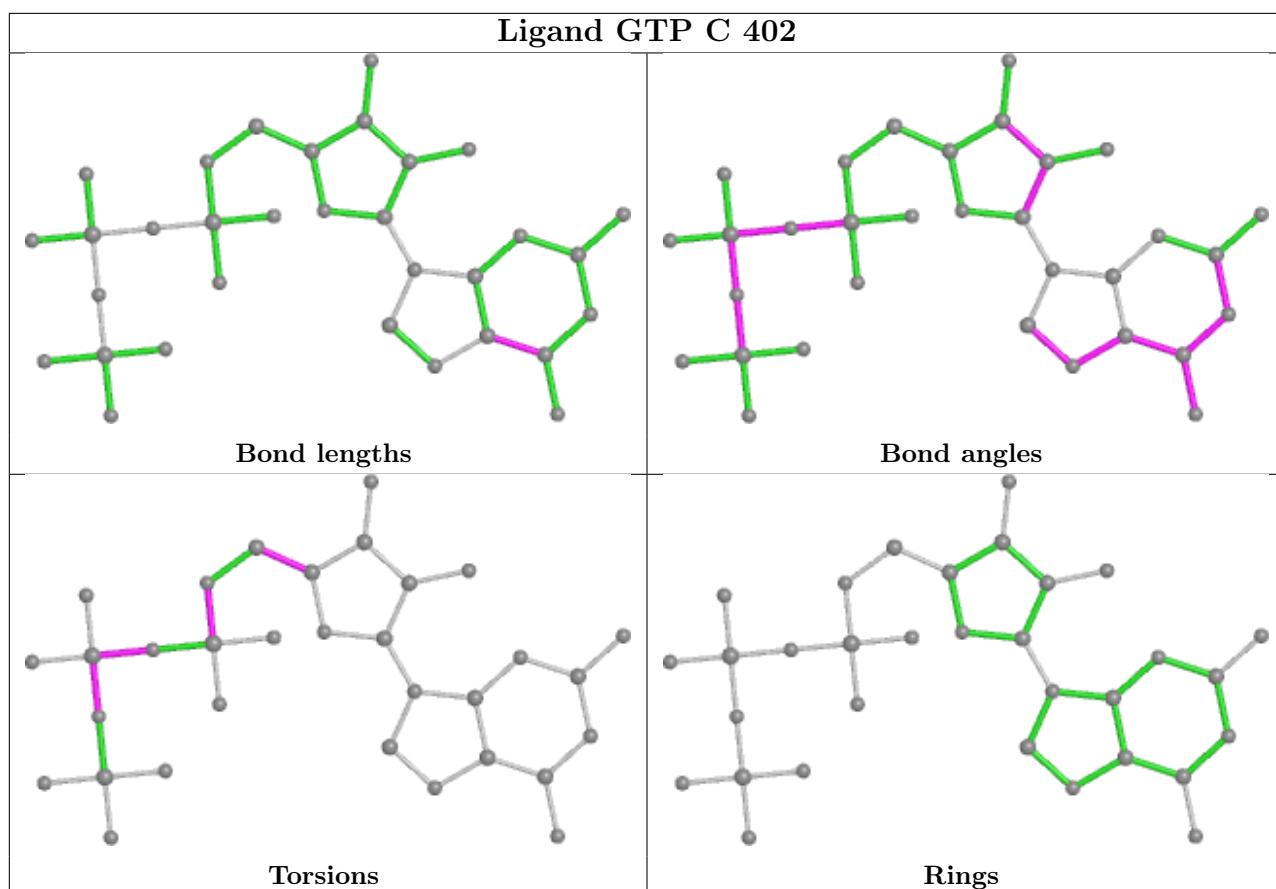
Mol	Chain	Res	Type	Atoms
6	C	402	GTP	C5'-O5'-PA-O1A
6	C	402	GTP	O4'-C4'-C5'-O5'
6	C	402	GTP	C3'-C4'-C5'-O5'
6	C	402	GTP	PG-O3B-PB-O2B
6	C	402	GTP	C5'-O5'-PA-O3A
6	C	402	GTP	PG-O3B-PB-O1B
6	C	402	GTP	PA-O3A-PB-O1B
6	C	402	GTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	GTP	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 Map visualisation [\(i\)](#)

This section contains visualisations of the EMDB entry EMD-18407. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [\(i\)](#)

This section was not generated.

6.2 Central slices [\(i\)](#)

This section was not generated.

6.3 Largest variance slices [\(i\)](#)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

This section was not generated.

6.5 Orthogonal surface views [\(i\)](#)

This section was not generated.

6.6 Mask visualisation [\(i\)](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [\(i\)](#)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [\(i\)](#)

This section was not generated.

7.2 Volume estimate versus contour level [\(i\)](#)

This section was not generated.

7.3 Rotationally averaged power spectrum [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [\(i\)](#)

This section was not generated.