Full wwPDB EM Validation Report ⓘ

Mar 8, 2025 – 06:13 am GMT

PDB ID	:	9GJU
EMDB ID	:	EMD-51403
Title	:	Structure of replicating Nipah Virus RNA Polymerase Complex - RNA-bound state
Authors	:	Sala, F.; Ditter, K.; Dybkov, O.; Urlaub, H.; Hillen, H.S.
Deposited on	:	2024-08-22
Resolution	:	2.80 Å(reported)
Based on initial model	:	.

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 ⓘ 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:

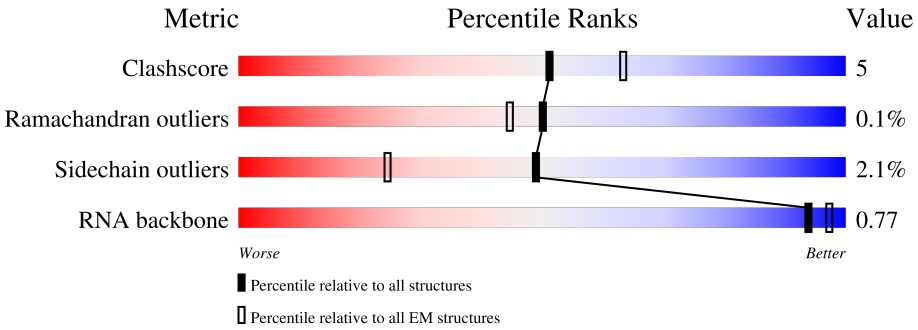
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=5%

Mol	Chain	Length	Quality of chain
1	B	709	21% 6% 72%
1	C	709	11% · 86%
1	D	709	14% · 83%
1	E	709	12% · 85%
2	F	9	44% 44% 11%
3	G	12	50% 50%
4	A	2246	78% 12% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20935 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	101	Total	C	N	O	S	0	0
			806	508	133	158	7		
1	D	118	Total	C	N	O	S	0	0
			935	587	160	181	7		
1	E	106	Total	C	N	O	S	0	0
			840	530	140	163	7		
1	B	195	Total	C	N	O	S	0	0
			1572	985	263	316	8		

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*CP*CP*AP*AP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	9	Total	C	N	O	P	0	0
			192	87	39	57	9		

- Molecule 3 is a RNA chain called RNA (5'-R(P*CP*CP*CP*UP*UP*GP*UP*UP*UP*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	12	Total	C	N	O	P	0	0
			249	111	36	90	12		

- Molecule 4 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2020	Total	C	N	O	S	0	0
			16306	10422	2777	3016	91		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q997F0
A	0	ASN	-	expression tag	UNP Q997F0

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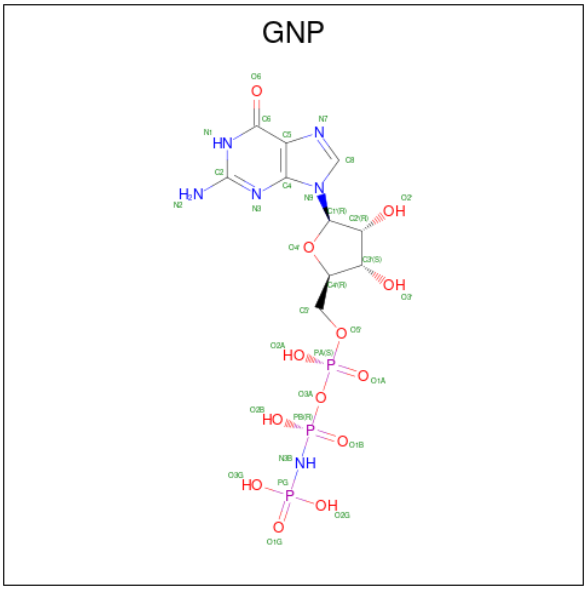
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q997F0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Zn	0
			2	2	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

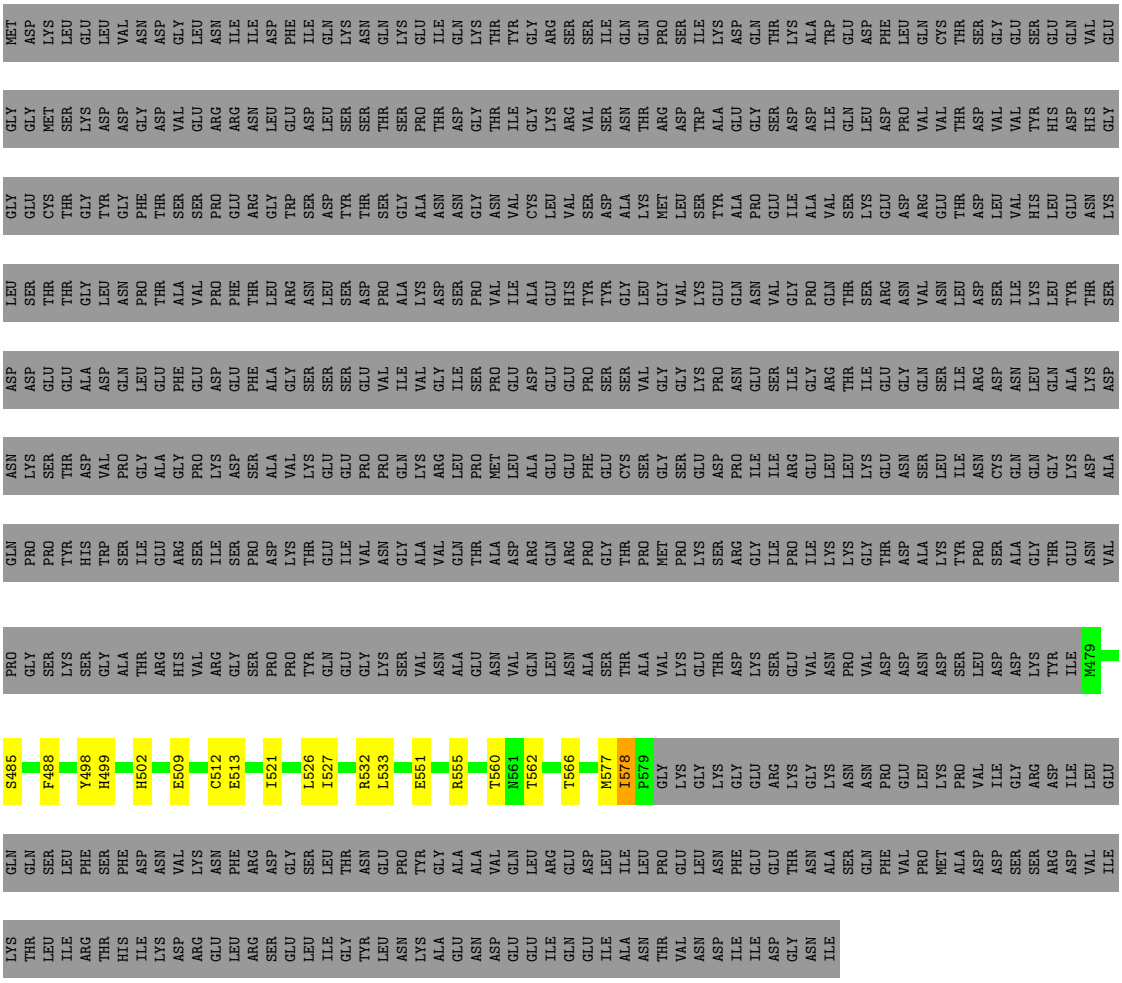
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

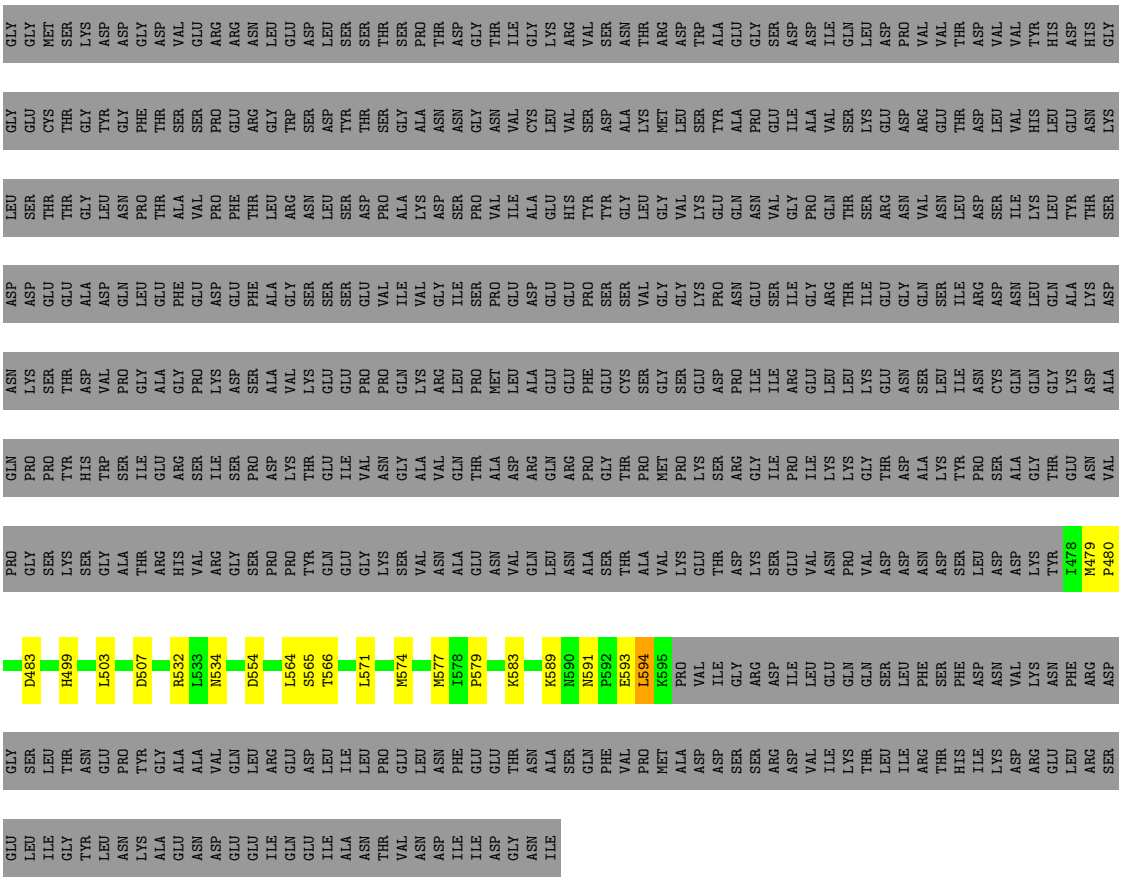
• Molecule 1: Phosphoprotein

Chain C:



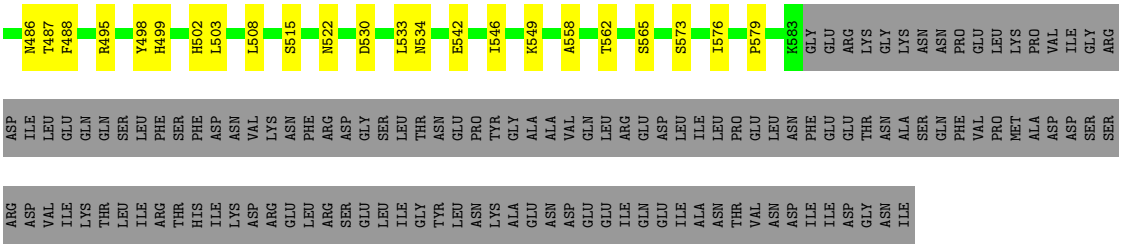
• Molecule 1: Phosphoprotein

Chain D:



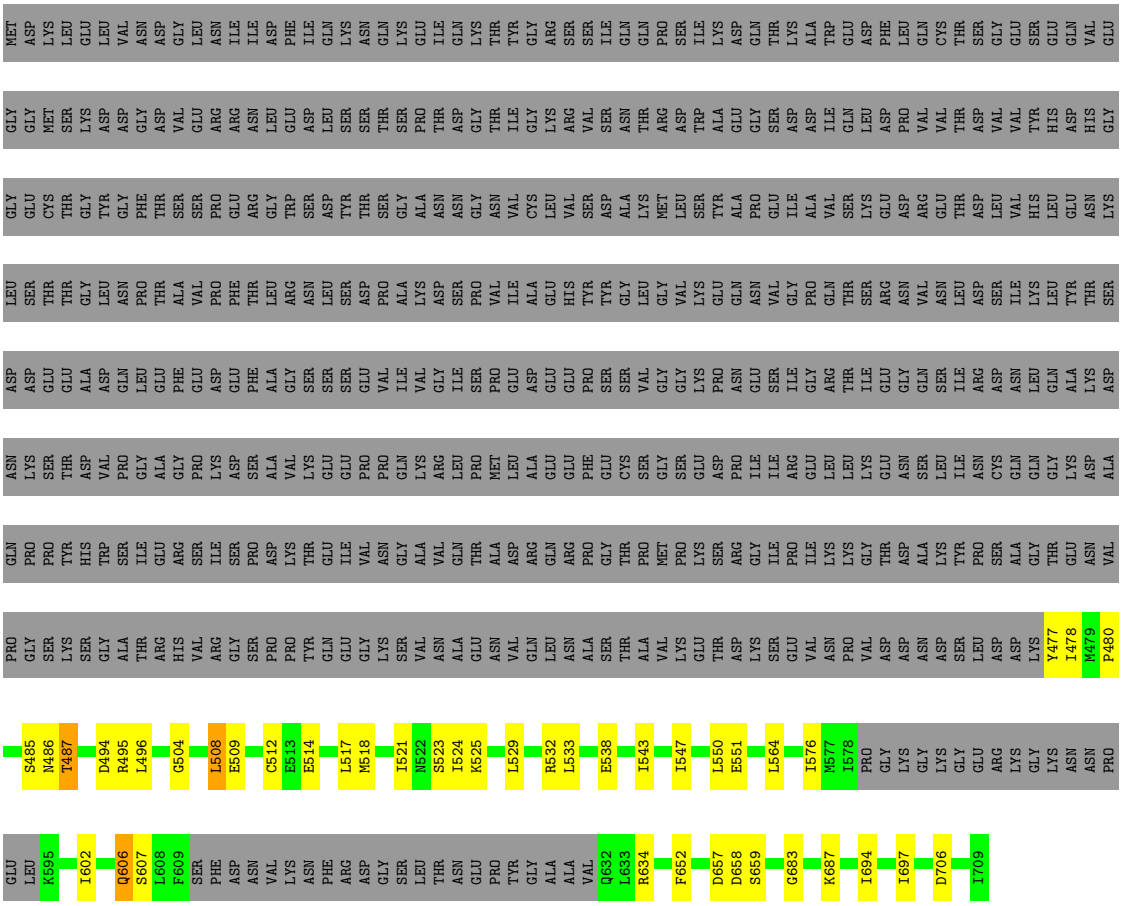
• Molecule 1: Phosphoprotein

Chain E:



• Molecule 1: Phosphoprotein

Chain B:

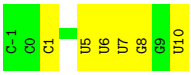


• Molecule 2: RNA (5'-R(P*AP*CP*CP*AP*AP*AP*CP*AP*A)-3')

Chain F:

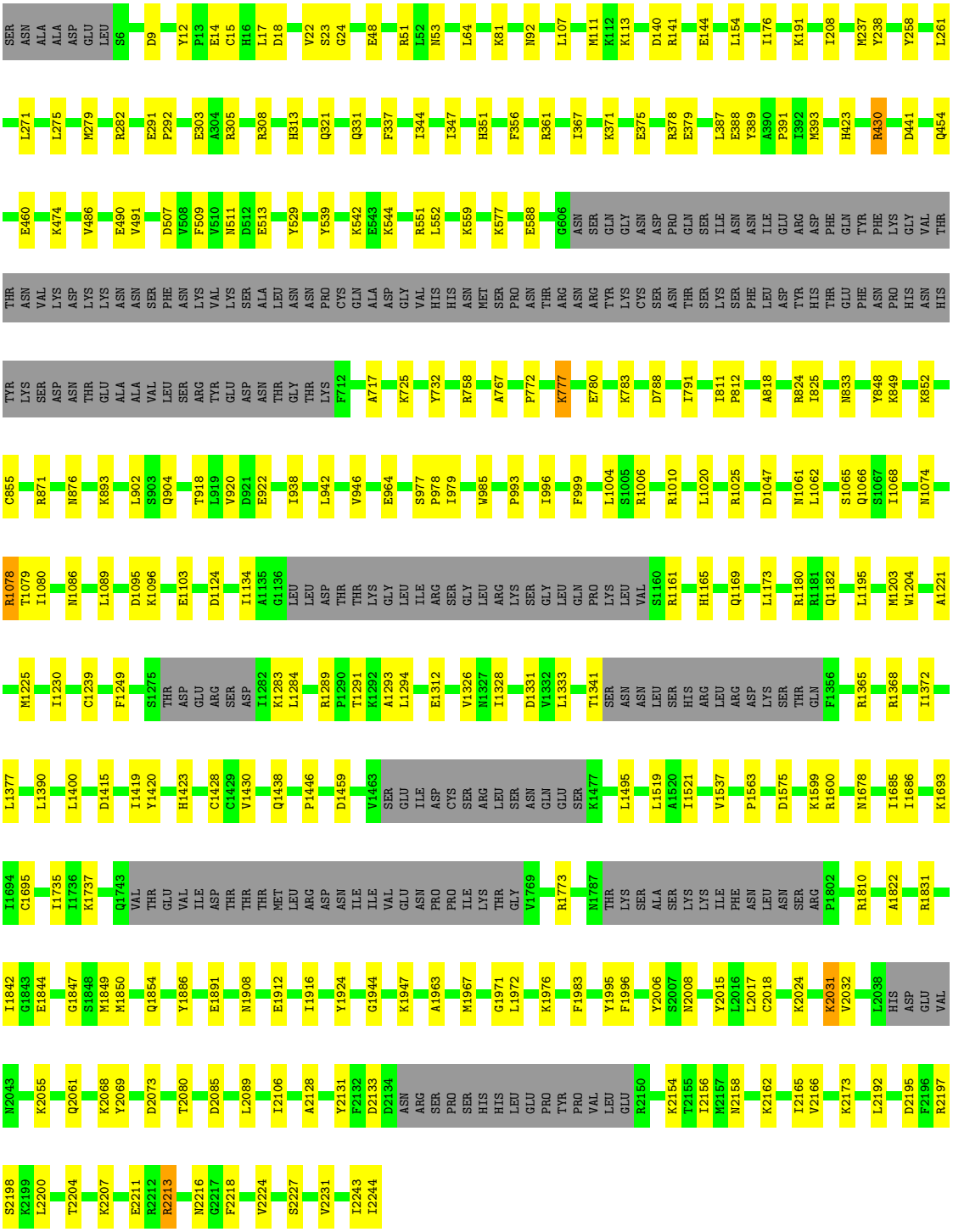
• Molecule 3: RNA (5'-R(P*CP*CP*CP*UP*UP*GP*UP*UP*UP*GP*GP*U)-3')

Chain G:



• Molecule 4: RNA-directed RNA polymerase L

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330750	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.26	0/1591	0.47	0/2147
1	C	0.26	0/819	0.42	0/1108
1	D	0.25	0/949	0.47	1/1277 (0.1%)
1	E	0.25	0/853	0.45	0/1151
2	F	0.19	0/215	0.67	0/332
3	G	0.17	0/275	0.67	0/425
4	A	0.24	0/16643	0.46	0/22499
All	All	0.24	0/21345	0.46	1/28939 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	554	ASP	CB-CG-OD1	5.48	123.23	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	578	ILE	Mainchain

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	B	1572	0	1561	55	0
1	C	806	0	803	33	0
1	D	935	0	946	22	0
1	E	840	0	846	24	0
2	F	192	0	100	4	0
3	G	249	0	127	7	0
4	A	16306	0	16434	146	0
5	A	32	0	13	2	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
All	All	20935	0	20830	222	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 5.

All (222) 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:509:GLU:HG3	1:B:508:LEU:HD21	1.17	1.16
3:G:7:U:O2'	4:A:1006:ARG:NH2	1.90	1.03
4:A:305:ARG:NH2	1:B:706:ASP:OD2	1.99	0.94
1:E:480:PRO:HD2	1:B:514:GLU:OE1	1.70	0.92
1:E:522:ASN:OD1	1:B:523:SER:OG	1.87	0.91
1:C:509:GLU:HG3	1:B:508:LEU:CD2	2.01	0.91
1:C:532:ARG:HH22	1:D:534:ASN:HA	1.37	0.90
1:D:579:PRO:HG3	4:A:732:TYR:CD1	2.17	0.80
4:A:1062:LEU:HB2	4:A:1065:SER:HB3	1.72	0.72
4:A:2133:ASP:OD1	4:A:2216:ASN:ND2	2.22	0.71
4:A:305:ARG:NE	1:B:706:ASP:OD2	2.23	0.71
4:A:305:ARG:CZ	1:B:706:ASP:OD2	2.38	0.70
4:A:1822:ALA:HB2	4:A:1849:MET:HG2	1.72	0.69
1:C:499:HIS:CE1	1:B:480:PRO:HA	2.26	0.69
1:C:498:TYR:OH	1:B:478:ILE:HG22	1.92	0.69
1:C:527:ILE:HG13	1:B:525:LYS:NZ	2.08	0.69
3:G:1:C:H5"	4:A:474:LYS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:480:PRO:CD	1:B:514:GLU:OE1	2.44	0.66
1:D:532:ARG:NH1	1:E:530:ASP:OD1	2.28	0.66
1:E:549:LYS:HD2	1:B:550:LEU:HB3	1.77	0.65
4:A:1773:ARG:NH1	4:A:2061:GLN:OE1	2.30	0.65
4:A:1079:THR:HG22	4:A:1080:ILE:HD13	1.79	0.64
4:A:824:ARG:HH11	4:A:824:ARG:HA	1.62	0.64
4:A:979:ILE:HD13	4:A:985:TRP:HB3	1.81	0.63
1:D:565:SER:HB3	4:A:423:HIS:HB3	1.80	0.63
1:C:526:LEU:HD13	1:B:525:LYS:HB2	1.82	0.62
4:A:361:ARG:NH1	4:A:544:LYS:O	2.33	0.61
4:A:1495:LEU:HB2	4:A:1735:ILE:HG21	1.83	0.60
4:A:780:GLU:HG3	4:A:783:LYS:HG2	1.85	0.58
1:C:499:HIS:CE1	1:B:480:PRO:CA	2.86	0.58
1:E:546:ILE:HG23	1:B:550:LEU:HD11	1.86	0.58
3:G:6:U:H4'	4:A:1010:ARG:NH1	2.19	0.57
1:E:558:ALA:O	1:E:562:THR:HG23	2.05	0.57
4:A:551:ARG:NH2	5:A:2301:GNP:O2A	2.33	0.57
4:A:993:PRO:HD2	4:A:996:ILE:HD11	1.87	0.57
1:D:483:ASP:OD2	1:E:499:HIS:NE2	2.36	0.57
4:A:48:GLU:HG3	4:A:51:ARG:HH21	1.70	0.56
1:C:578:ILE:HG23	1:B:576:ILE:HD11	1.87	0.56
4:A:1537:VAL:O	4:A:1600:ARG:NH2	2.30	0.56
4:A:1341:THR:HG22	4:A:1737:LYS:HD3	1.87	0.56
4:A:1239:CYS:SG	4:A:1423:HIS:HE1	2.28	0.56
4:A:1810:ARG:NH2	4:A:2006:TYR:O	2.39	0.55
1:D:480:PRO:HG3	1:E:503:LEU:HD21	1.88	0.55
4:A:486:VAL:HG21	4:A:767:ALA:HB1	1.88	0.55
4:A:509:PHE:O	4:A:1086:ASN:ND2	2.40	0.55
1:C:527:ILE:CG1	1:B:525:LYS:NZ	2.70	0.55
1:C:499:HIS:HE1	1:B:480:PRO:HA	1.72	0.55
1:C:533:LEU:HD13	1:B:532:ARG:HD2	1.90	0.54
4:A:818:ALA:HB2	4:A:825:ILE:HG12	1.90	0.54
1:C:527:ILE:HG13	1:B:525:LYS:HZ2	1.72	0.54
1:C:532:ARG:HH22	1:D:534:ASN:CA	2.17	0.54
4:A:2008:ASN:O	4:A:2055:LYS:NZ	2.40	0.54
1:C:562:THR:O	1:C:566:THR:HG23	2.07	0.54
4:A:14:GLU:HA	4:A:918:THR:HG21	1.89	0.53
3:G:6:U:O3'	4:A:1010:ARG:NH1	2.39	0.53
1:B:517:LEU:O	1:B:521:ILE:HG13	2.08	0.53
4:A:717:ALA:HB2	4:A:855:CYS:HB3	1.91	0.53
4:A:1844:GLU:OE2	4:A:1850:MET:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1:A:H61	3:G:10:U:H3	1.58	0.52
3:G:5:U:O3'	4:A:588:GLU:HB2	2.09	0.52
4:A:460:GLU:HG2	4:A:1289:ARG:HB3	1.92	0.52
4:A:1293:ALA:HB3	4:A:1459:ASP:HB2	1.91	0.52
1:D:593:GLU:HG2	4:A:1289:ARG:HD2	1.91	0.52
4:A:1842:ILE:HD12	4:A:1916:ILE:HD11	1.91	0.52
4:A:2195:ASP:O	4:A:2198:SER:OG	2.27	0.52
1:C:502:HIS:CE1	1:B:477:TYR:HB2	2.44	0.51
4:A:922:GLU:OE2	4:A:922:GLU:N	2.28	0.51
4:A:1249:PHE:HB2	4:A:1420:TYR:HB3	1.91	0.51
1:C:502:HIS:ND1	1:B:477:TYR:CG	2.78	0.51
1:C:577:MET:HG2	1:B:606:GLN:NE2	2.25	0.51
2:F:8:A:OP2	4:A:361:ARG:NH2	2.43	0.51
4:A:1103:GLU:HG3	4:A:1446:PRO:HB3	1.91	0.51
1:E:549:LYS:HB3	1:B:550:LEU:HD13	1.91	0.51
1:C:509:GLU:CG	1:B:508:LEU:HD21	2.11	0.51
1:C:577:MET:HG2	1:B:606:GLN:HE22	1.75	0.51
1:B:547:ILE:O	1:B:551:GLU:HG2	2.11	0.51
4:A:388:GLU:HB3	4:A:391:PRO:HD2	1.92	0.51
4:A:378:ARG:NH1	4:A:788:ASP:O	2.27	0.51
4:A:1074:ASN:O	4:A:1078:ARG:HB2	2.10	0.51
4:A:258:TYR:HD2	4:A:261:LEU:HD12	1.76	0.50
4:A:529:TYR:O	4:A:758:ARG:NH1	2.44	0.50
1:D:574:MET:HG3	4:A:389:TYR:CE1	2.47	0.50
1:D:566:THR:HA	4:A:423:HIS:CD2	2.47	0.50
1:E:576:ILE:HB	4:A:387:LEU:HB2	1.94	0.50
1:B:658:ASP:OD1	1:B:659:SER:N	2.44	0.50
4:A:22:VAL:HG12	4:A:24:GLY:H	1.77	0.50
1:C:527:ILE:HG13	1:B:525:LYS:HZ3	1.77	0.49
4:A:1291:THR:OG1	4:A:1459:ASP:OD2	2.29	0.49
4:A:313:HIS:CD2	1:B:652:PHE:HE1	2.30	0.49
4:A:1844:GLU:HG3	4:A:1847:GLY:HA2	1.94	0.49
4:A:113:LYS:NZ	4:A:964:GLU:OE2	2.45	0.49
4:A:1061:ASN:ND2	4:A:1203:MET:O	2.30	0.49
1:C:502:HIS:ND1	1:B:477:TYR:HB2	2.26	0.49
1:E:533:LEU:HG	1:B:533:LEU:HD21	1.95	0.48
4:A:375:GLU:O	4:A:379:GLU:HG2	2.12	0.48
1:D:480:PRO:CG	1:E:503:LEU:HD21	2.42	0.48
4:A:1068:ILE:HD11	4:A:1165:HIS:CG	2.48	0.48
4:A:371:LYS:HB2	4:A:371:LYS:HE2	1.60	0.48
1:E:499:HIS:O	1:E:503:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:491:VAL:HG12	4:A:772:PRO:HB3	1.96	0.48
4:A:17:LEU:HD22	4:A:237:MET:HB2	1.94	0.48
4:A:378:ARG:HG3	4:A:791:ILE:HG12	1.96	0.47
1:B:518:MET:HE1	1:B:521:ILE:HD12	1.96	0.47
1:D:566:THR:HA	4:A:423:HIS:CG	2.50	0.47
1:D:583:LYS:HG2	4:A:454:GLN:NE2	2.29	0.47
4:A:1967:MET:HG2	4:A:1971:GLY:HA3	1.95	0.47
4:A:1972:LEU:HD21	4:A:2017:LEU:HG	1.96	0.47
1:C:512:CYS:SG	1:B:512:CYS:SG	3.10	0.47
1:C:578:ILE:CG2	1:B:576:ILE:HD11	2.44	0.47
4:A:999:PHE:HE1	4:A:1173:LEU:HD22	1.80	0.47
4:A:291:GLU:HB2	4:A:292:PRO:HD3	1.97	0.47
4:A:2106:ILE:HG13	4:A:2166:VAL:HG21	1.96	0.46
4:A:871:ARG:NH1	4:A:876:ASN:OD1	2.48	0.46
1:E:486:ASN:OD1	1:E:487:THR:N	2.49	0.46
1:D:532:ARG:NH2	1:E:534:ASN:OD1	2.47	0.46
4:A:507:ASP:O	4:A:511:ASN:ND2	2.48	0.46
4:A:1061:ASN:HB2	4:A:1204:TRP:CE2	2.50	0.46
4:A:1326:VAL:HG12	4:A:1459:ASP:HB3	1.97	0.46
1:B:657:ASP:OD2	1:B:658:ASP:N	2.48	0.46
1:D:507:ASP:OD1	1:D:507:ASP:N	2.42	0.46
2:F:2:C:H2'	2:F:3:C:C6	2.51	0.46
4:A:1230:ILE:HB	4:A:1419:ILE:HB	1.98	0.46
4:A:1519:LEU:HD23	4:A:1519:LEU:HA	1.80	0.46
4:A:1328:ILE:HG21	4:A:1333:LEU:HD13	1.98	0.45
4:A:539:TYR:HB3	4:A:552:LEU:HD22	1.97	0.45
1:B:538:GLU:OE1	1:B:538:GLU:HA	2.16	0.45
4:A:92:ASN:OD1	4:A:238:TYR:OH	2.21	0.45
4:A:1428:CYS:O	4:A:1430:VAL:N	2.48	0.45
4:A:2213:ARG:HD2	4:A:2218:PHE:HB3	1.98	0.45
4:A:308:ARG:NH2	1:B:706:ASP:OD1	2.48	0.45
4:A:938:ILE:HA	4:A:942:LEU:HB3	1.98	0.45
4:A:2031:LYS:HA	4:A:2031:LYS:HD3	1.86	0.45
4:A:1221:ALA:O	4:A:1225:MET:HG2	2.17	0.45
4:A:1563:PRO:O	4:A:1678:ASN:ND2	2.45	0.45
4:A:2200:LEU:O	4:A:2204:THR:HG23	2.15	0.45
1:D:483:ASP:OD1	1:E:495:ARG:NH2	2.46	0.45
4:A:347:ILE:HD11	4:A:356:PHE:HE2	1.82	0.44
4:A:542:LYS:HD2	4:A:551:ARG:HD2	2.00	0.44
4:A:893:LYS:O	4:A:904:GLN:NE2	2.51	0.44
4:A:1365:ARG:O	4:A:1368:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1976:LYS:HB2	4:A:2015:TYR:CE2	2.53	0.44
4:A:2213:ARG:NH1	4:A:2218:PHE:O	2.45	0.44
1:D:499:HIS:O	1:D:503:LEU:HG	2.18	0.44
4:A:1095:ASP:OD1	4:A:1095:ASP:N	2.50	0.44
4:A:430:ARG:NH2	4:A:1686:ILE:HD12	2.33	0.44
1:C:521:ILE:HD11	1:B:496:LEU:HD13	2.00	0.43
1:E:579:PRO:HG2	1:B:602:ILE:HD11	2.01	0.43
3:G:7:U:H2'	3:G:8:G:C8	2.53	0.43
4:A:848:TYR:O	4:A:852:LYS:HG2	2.18	0.43
4:A:1372:ILE:HD11	4:A:1400:LEU:HD21	2.00	0.43
4:A:1996:PHE:CG	4:A:2018:CYS:HB3	2.54	0.43
1:C:498:TYR:CE1	1:B:477:TYR:HD1	2.37	0.43
1:C:551:GLU:OE2	1:C:555:ARG:NH2	2.51	0.43
4:A:53:ASN:ND2	4:A:490:GLU:O	2.51	0.43
4:A:2158:ASN:O	4:A:2162:LYS:HD3	2.18	0.43
4:A:1377:LEU:HD22	4:A:1390:LEU:HD21	2.01	0.43
4:A:1294:LEU:HA	4:A:1326:VAL:HG11	2.00	0.43
1:E:549:LYS:HD2	1:B:550:LEU:CB	2.45	0.43
4:A:23:SER:HA	4:A:367:ILE:HD11	2.01	0.43
4:A:1944:GLY:HA3	4:A:1947:LYS:HD3	2.01	0.43
4:A:559:LYS:HB3	4:A:559:LYS:HE3	1.77	0.42
1:B:694:ILE:HA	1:B:697:ILE:HG22	2.00	0.42
4:A:1908:ASN:HB3	4:A:1924:TYR:CE1	2.54	0.42
4:A:725:LYS:H	5:A:2301:GNP:HNB3	1.66	0.42
4:A:1372:ILE:HD11	4:A:1400:LEU:HD11	2.02	0.42
4:A:1685:ILE:O	4:A:1693:LYS:HE3	2.20	0.42
4:A:2068:LYS:HG2	4:A:2069:TYR:CD1	2.54	0.42
4:A:577:LYS:H	4:A:577:LYS:HG2	1.68	0.42
4:A:1020:LEU:HD13	4:A:1195:LEU:HB3	2.00	0.42
1:C:532:ARG:NH1	1:D:534:ASN:OD1	2.52	0.42
1:C:560:THR:HG23	1:D:564:LEU:HD11	2.02	0.42
4:A:1912:GLU:OE1	4:A:1912:GLU:N	2.52	0.42
1:B:564:LEU:HD12	1:B:564:LEU:HA	1.87	0.42
4:A:154:LEU:HD21	4:A:946:VAL:HA	2.02	0.42
4:A:920:VAL:HG12	4:A:920:VAL:O	2.19	0.42
4:A:2173:LYS:HD2	4:A:2244:ILE:HD12	2.02	0.42
1:E:542:GLU:HB2	1:B:543:ILE:HG21	2.01	0.42
2:F:3:C:H2'	2:F:4:A:C8	2.54	0.42
4:A:140:ASP:O	4:A:144:GLU:HG2	2.19	0.42
1:C:513:GLU:OE2	1:B:504:GLY:HA2	2.19	0.41
4:A:271:LEU:HD22	4:A:344:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:777:LYS:HB2	4:A:777:LYS:HE2	1.80	0.41
4:A:1004:LEU:HD13	4:A:1025:ARG:HD2	2.02	0.41
4:A:2165:ILE:HG13	4:A:2192:LEU:HD22	2.02	0.41
4:A:2207:LYS:O	4:A:2211:GLU:HG3	2.19	0.41
4:A:275:LEU:HB3	4:A:279:MET:HG3	2.02	0.41
4:A:2085:ASP:O	4:A:2089:LEU:HG	2.20	0.41
4:A:2128:ALA:HB2	4:A:2156:ILE:HG21	2.01	0.41
1:B:494:ASP:OD1	1:B:495:ARG:N	2.53	0.41
4:A:282:ARG:HE	4:A:282:ARG:HB3	1.54	0.41
4:A:303:GLU:HG3	4:A:849:LYS:HD3	2.02	0.41
1:C:533:LEU:HD12	1:B:529:LEU:HD22	2.02	0.41
1:B:607:SER:O	1:B:634:ARG:NH1	2.49	0.41
1:D:591:ASN:O	1:D:594:LEU:HB2	2.20	0.41
1:E:508:LEU:HD13	1:B:509:GLU:CD	2.41	0.41
4:A:1963:ALA:O	4:A:1967:MET:HB2	2.21	0.41
4:A:2080:THR:O	4:A:2243:ILE:HG22	2.20	0.41
4:A:1995:TYR:HE2	4:A:2032:VAL:HA	1.86	0.41
4:A:351:HIS:CE1	4:A:902:LEU:HA	2.56	0.41
4:A:977:SER:OG	4:A:978:PRO:HD3	2.21	0.41
1:C:485:SER:HA	1:C:488:PHE:CD2	2.56	0.41
1:C:526:LEU:HD13	1:B:525:LYS:CB	2.49	0.41
1:D:577:MET:HE3	4:A:393:MET:SD	2.61	0.41
4:A:1089:LEU:HD22	4:A:1134:ILE:HG21	2.02	0.41
4:A:2213:ARG:HE	4:A:2213:ARG:HB3	1.71	0.41
1:B:486:ASN:OD1	1:B:487:THR:N	2.53	0.41
4:A:1854:GLN:HG3	4:A:1886:TYR:HE2	1.87	0.41
1:E:488:PHE:CZ	1:B:524:ILE:HG21	2.57	0.40
4:A:275:LEU:HD11	4:A:337:PHE:CZ	2.55	0.40
4:A:811:ILE:N	4:A:812:PRO:HD2	2.37	0.40
4:A:1165:HIS:O	4:A:1169:GLN:HG2	2.21	0.40
4:A:2227:SER:O	4:A:2231:VAL:HG23	2.21	0.40
1:B:683:GLY:O	1:B:687:LYS:NZ	2.48	0.40
1:E:502:HIS:ND1	1:E:503:LEU:HD22	2.36	0.40
4:A:1074:ASN:HB3	4:A:1078:ARG:NH2	2.36	0.40
4:A:1599:LYS:NZ	4:A:1891:GLU:OE1	2.54	0.40
4:A:2192:LEU:HB2	4:A:2224:VAL:HG12	2.02	0.40
1:D:571:LEU:HD23	1:D:571:LEU:HA	1.91	0.40
1:E:549:LYS:HE2	1:E:549:LYS:HB2	1.80	0.40
4:A:12:TYR:HB2	4:A:918:THR:O	2.21	0.40
4:A:107:LEU:O	4:A:111:MET:HG2	2.22	0.40
4:A:176:ILE:HD11	4:A:208:ILE:HD13	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 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	B	189/709 (27%)	187 (99%)	2 (1%)	0	100 100
1	C	99/709 (14%)	99 (100%)	0	0	100 100
1	D	116/709 (16%)	113 (97%)	2 (2%)	1 (1%)	14 42
1	E	104/709 (15%)	103 (99%)	1 (1%)	0	100 100
4	A	2000/2246 (89%)	1966 (98%)	32 (2%)	2 (0%)	48 77
All	All	2508/5082 (49%)	2468 (98%)	37 (2%)	3 (0%)	50 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	479	MET
4	A	1521	ILE
4	A	1983	PHE

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	B	182/625 (29%)	178 (98%)	4 (2%)	47 79
1	C	95/625 (15%)	95 (100%)	0	100 100
1	D	108/625 (17%)	106 (98%)	2 (2%)	52 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	98/625 (16%)	94 (96%)	4 (4%)	26 59
4	A	1836/2047 (90%)	1798 (98%)	38 (2%)	48 80
All	All	2319/4547 (51%)	2271 (98%)	48 (2%)	49 80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	589	LYS
1	D	594	LEU
1	E	498	TYR
1	E	515	SER
1	E	565	SER
1	E	573	SER
4	A	9	ASP
4	A	15	CYS
4	A	18	ASP
4	A	64	LEU
4	A	81	LYS
4	A	141	ARG
4	A	191	LYS
4	A	321	GLN
4	A	331	GLN
4	A	430	ARG
4	A	441	ASP
4	A	513	GLU
4	A	777	LYS
4	A	833	ASN
4	A	1047	ASP
4	A	1066	GLN
4	A	1078	ARG
4	A	1096	LYS
4	A	1124	ASP
4	A	1161	ARG
4	A	1180	ARG
4	A	1182	GLN
4	A	1283	LYS
4	A	1284	LEU
4	A	1312	GLU
4	A	1331	ASP
4	A	1415	ASP
4	A	1438	GLN

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Mol	Chain	Res	Type
4	A	1575	ASP
4	A	1695	CYS
4	A	1831	ARG
4	A	2024	LYS
4	A	2031	LYS
4	A	2073	ASP
4	A	2131	TYR
4	A	2154	LYS
4	A	2197	ARG
4	A	2213	ARG
1	B	485	SER
1	B	487	THR
1	B	508	LEU
1	B	606	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	534	ASN
1	C	570	HIS
4	A	313	HIS
1	B	606	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	8/9 (88%)	1 (12%)	0
3	G	11/12 (91%)	0	0
All	All	19/21 (90%)	1 (5%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	2	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are 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	$\#\|Z\| > 2$
5	GNP	A	2301	7	29,34,34	2.55	7 (24%)	33,54,54	2.74	8 (24%)

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
5	GNP	A	2301	7	-	3/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2301	GNP	PB-O3A	8.15	1.69	1.59
5	A	2301	GNP	PG-N3B	6.46	1.80	1.63
5	A	2301	GNP	PG-O1G	4.55	1.53	1.46
5	A	2301	GNP	C6-N1	4.26	1.40	1.33
5	A	2301	GNP	PB-O1B	2.96	1.50	1.46
5	A	2301	GNP	C8-N7	-2.71	1.29	1.34
5	A	2301	GNP	PB-O2B	-2.24	1.50	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2301	GNP	C5-C6-N1	-9.36	110.63	123.43
5	A	2301	GNP	O1G-PG-N3B	-7.21	101.16	111.77
5	A	2301	GNP	C2-N1-C6	6.36	126.04	115.93
5	A	2301	GNP	O2B-PB-O1B	4.54	119.44	109.92
5	A	2301	GNP	N3-C2-N1	-3.17	123.00	127.22
5	A	2301	GNP	O3A-PB-N3B	-2.43	99.84	106.59
5	A	2301	GNP	O2G-PG-O3G	2.33	113.84	107.64
5	A	2301	GNP	C4-C5-C6	-2.08	118.81	120.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2301	GNP	PB-N3B-PG-O1G
5	A	2301	GNP	PG-N3B-PB-O3A
5	A	2301	GNP	PA-O3A-PB-O2B

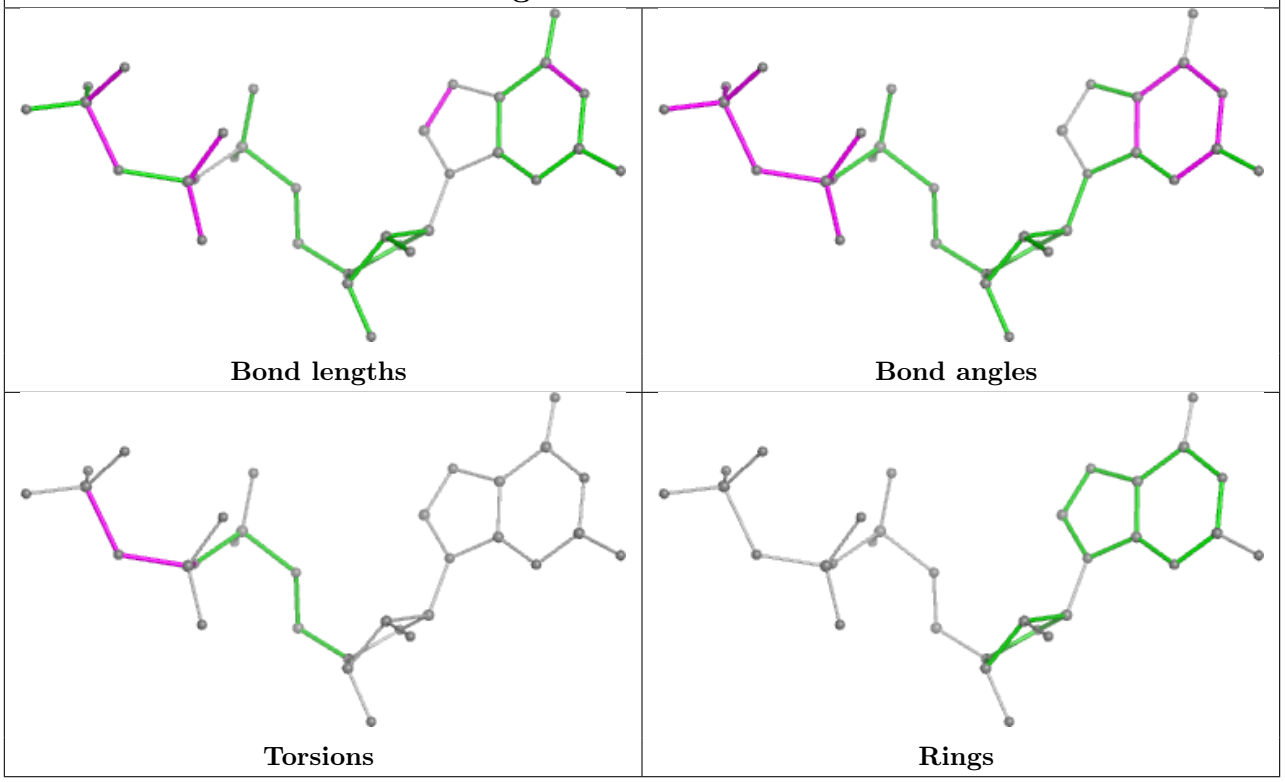
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2301	GNP	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 then 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.

Ligand GNP A 2301



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

This section contains visualisations of the EMDB entry EMD-51403. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

This section was not generated.