



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 05:07 AM EST

PDB ID : 7RE2  
EMDB ID : EMD-24431  
Title : SARS-CoV-2 replication-transcription complex bound to nsp13 helicase - nsp13(1)-RTC  
Authors : Chen, J.; Malone, B.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2021-07-12  
Resolution : 3.17 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

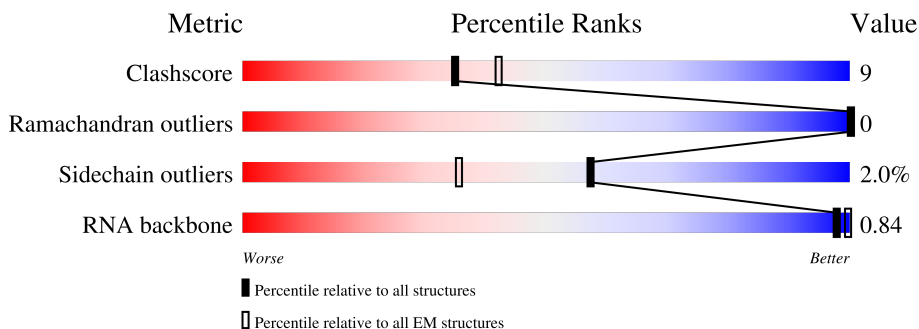
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.17 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  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	932	
2	B	199	
2	D	199	
3	C	88	
4	E	605	
5	P	35	
6	T	55	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	1N7	A	1005	X	-	-	-
11	AF3	E	706	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 17096 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	927	7470	4770	1253	1393	54	0	0

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	186	1408	884	241	272	11	0	0
2	D	185	1415	889	242	273	11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P0DTD1
D	0	MET	-	initiating methionine	UNP P0DTD1

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	75	576	362	94	113	7	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP P0DTD1
C	-3	PRO	-	expression tag	UNP P0DTD1
C	-2	VAL	-	expression tag	UNP P0DTD1
C	-1	ASP	-	expression tag	UNP P0DTD1
C	0	MET	-	expression tag	UNP P0DTD1

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	590	4557	2896	771	856	34	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP P0DTD1
E	-2	PRO	-	expression tag	UNP P0DTD1
E	-1	HIS	-	expression tag	UNP P0DTD1
E	0	MET	-	expression tag	UNP P0DTD1

- Molecule 5 is a RNA chain called Product RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	P	34	719	322	125	238	34	0	0

- Molecule 6 is a RNA chain called Template RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	T	37	789	353	141	258	37	0	0

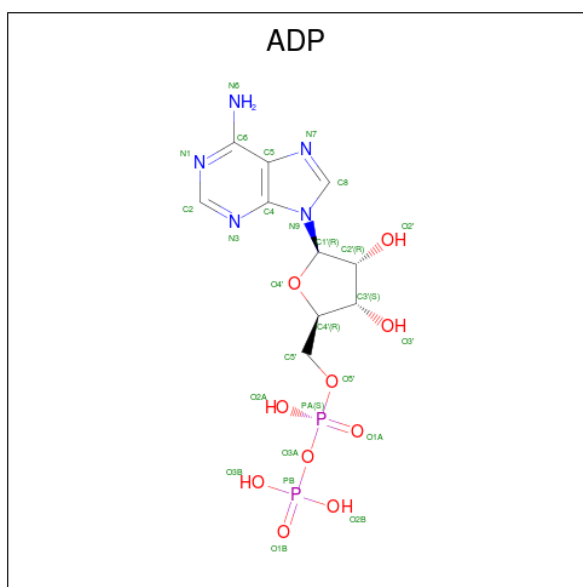
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	A	2	2	2	0
7	E	3	3	3	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

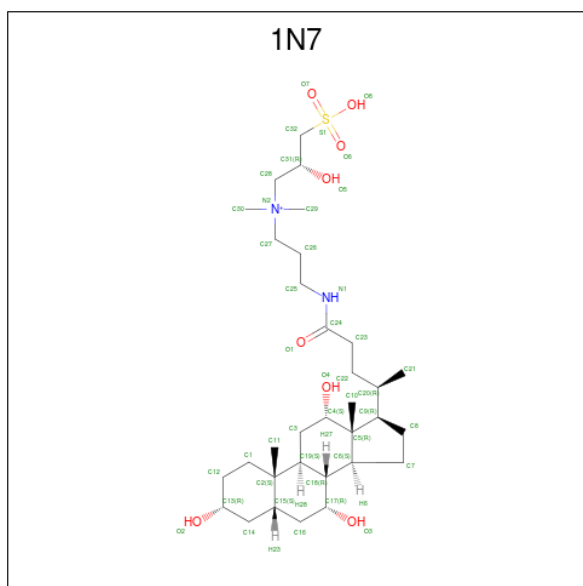
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	A	1	1	1	0
8	E	1	1	1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula:  $C_{32}H_{59}N_2O_8S$ ).



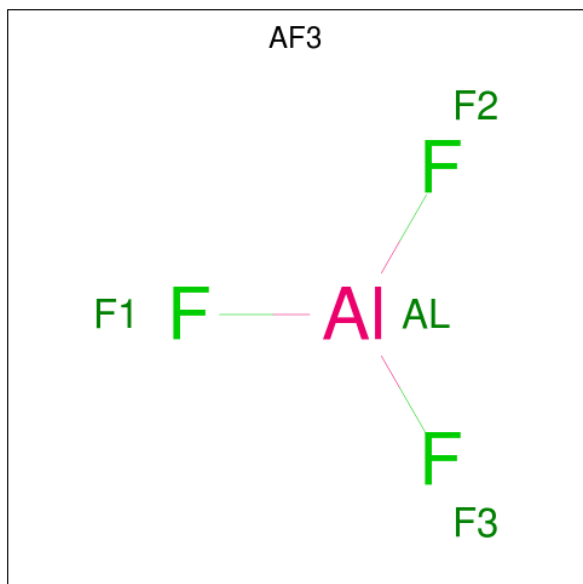
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	A	1	Total	C	N	O	0
			61	52	2	7	
10	A	1	Total	C	N	O	0
			61	52	2	7	

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Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
10	E	1	36	30	2	4	0

- Molecule 11 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $\text{AlF}_3$ ).

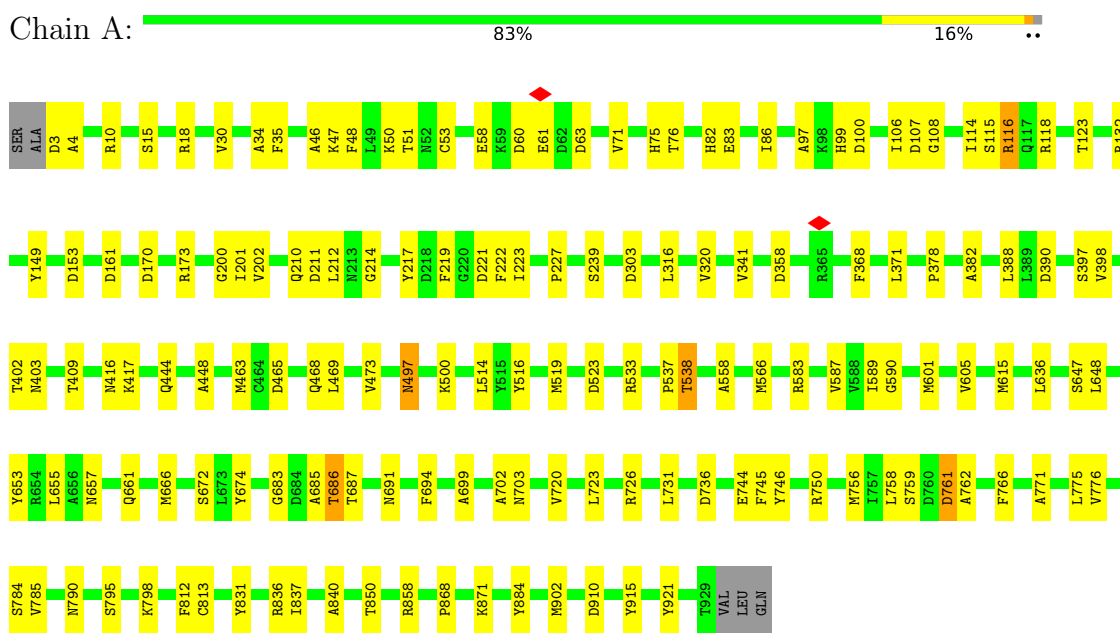


Mol	Chain	Residues	Atoms		AltConf	
			Total	Al		F
11	E	1	4	1	3	0

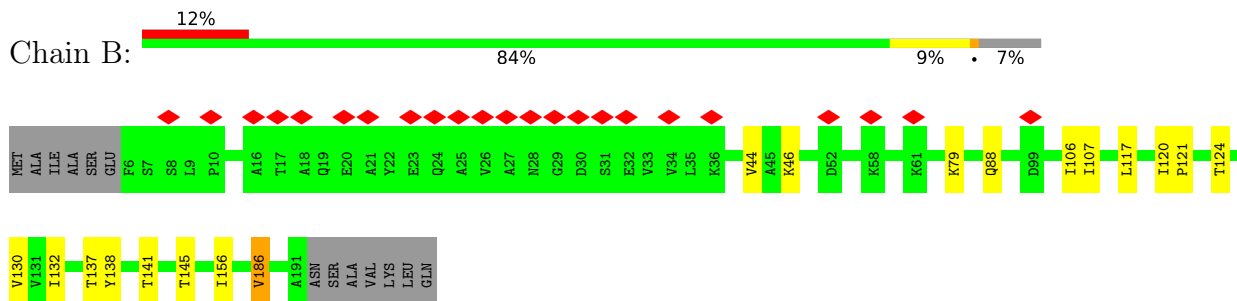
### 3 Residue-property plots [i](#)

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

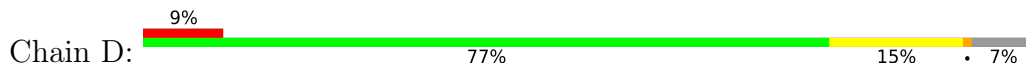
- Molecule 1: RNA-directed RNA polymerase



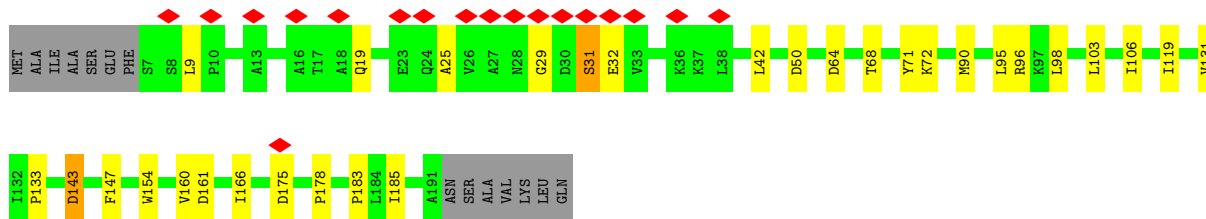
- Molecule 2: Non-structural protein 8



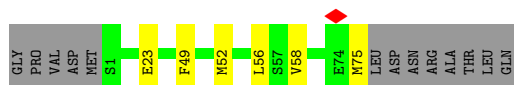
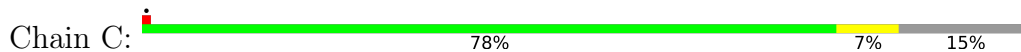
- Molecule 2: Non-structural protein 8



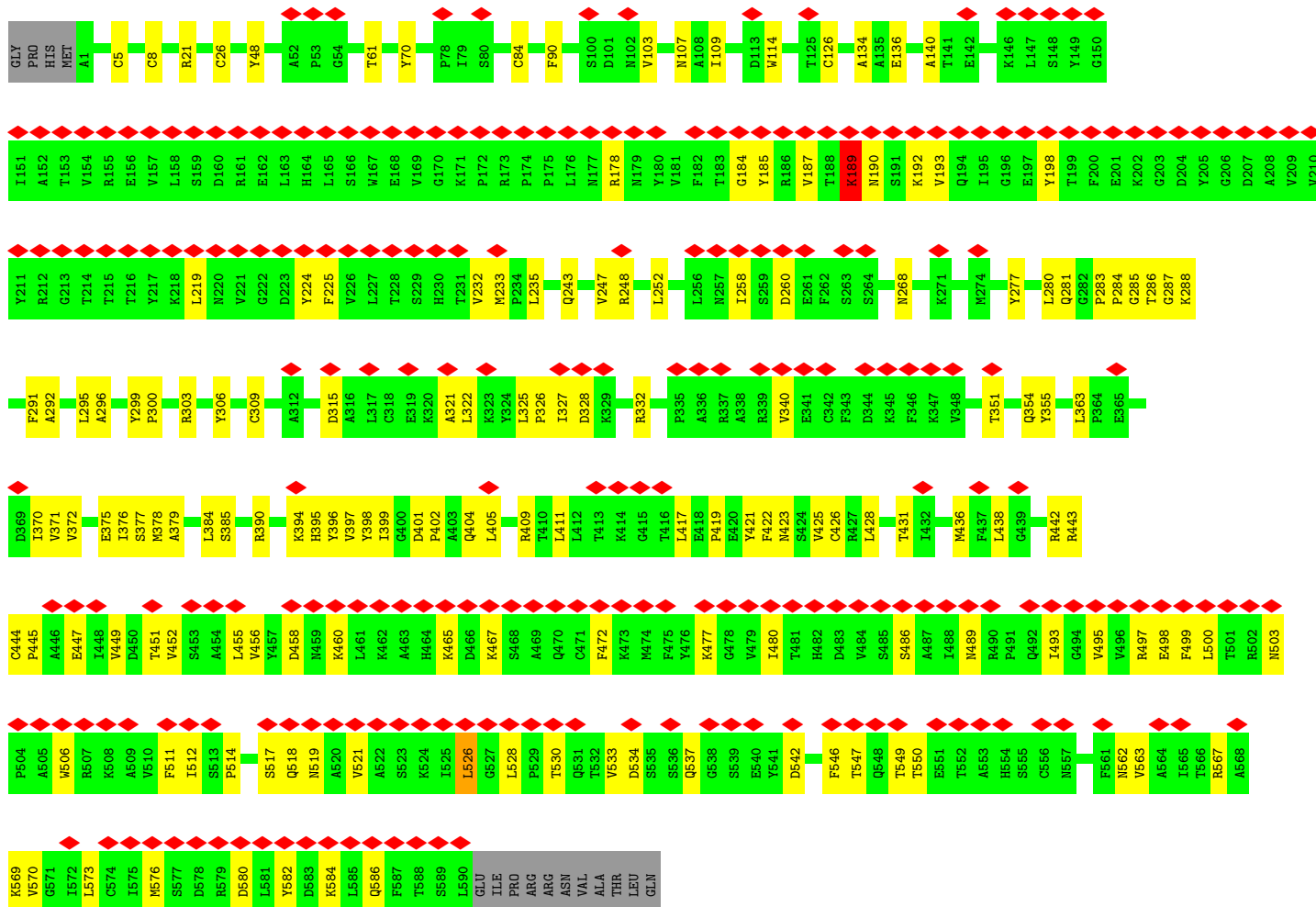




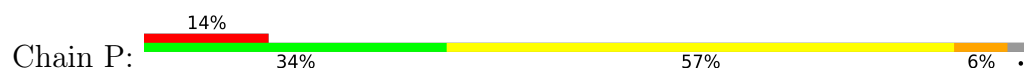
• Molecule 3: Non-structural protein 7



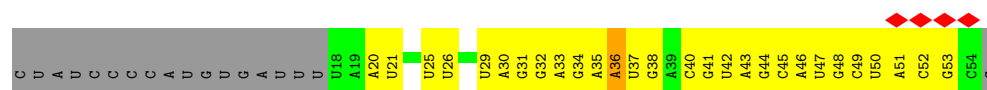
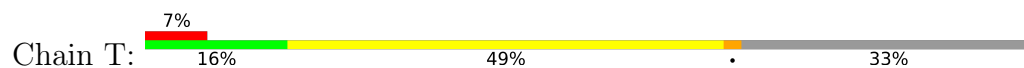
• Molecule 4: Helicase



• Molecule 5: Product RNA



● Molecule 6: Template RNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85187	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.065	Depositor
Minimum map value	-2.260	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	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: ADP, AF3, MG, ZN, 1N7

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	0.36	0/7659	0.48	0/10394
2	B	0.28	0/1427	0.46	0/1937
2	D	0.27	0/1434	0.46	0/1943
3	C	0.29	0/579	0.44	0/779
4	E	0.26	0/4659	0.49	1/6344 (0.0%)
5	P	0.31	0/802	0.76	0/1246
6	T	0.33	0/882	0.77	0/1372
All	All	0.32	0/17442	0.52	1/24015 (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
2	D	0	1
4	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	189	LYS	C-N-CA	5.04	134.30	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	31	SER	Peptide
4	E	189	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7470	0	7206	91	0
2	B	1408	0	1407	12	0
2	D	1415	0	1431	20	0
3	C	576	0	608	6	0
4	E	4557	0	4503	104	0
5	P	719	0	366	30	0
6	T	789	0	398	35	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
9	A	27	0	12	1	0
9	E	27	0	12	3	0
10	A	61	0	86	6	0
10	E	36	0	52	5	0
11	E	4	0	0	2	0
All	All	17096	0	16081	289	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 9.

All (289) 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)
4:E:5:CYS:HB3	4:E:8:CYS:SG	2.19	0.81
4:E:458:ASP:H	4:E:460:LYS:HE3	1.46	0.80
4:E:5:CYS:CB	4:E:8:CYS:SG	2.72	0.77
1:A:116:ARG:NH2	9:A:1004:ADP:O3B	2.17	0.76
4:E:189:LYS:H	4:E:190:ASN:HB2	1.50	0.76
2:D:25:ALA:O	2:D:29:GLY:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:NZ	1:A:53:CYS:SG	2.63	0.71
1:A:653:TYR:O	1:A:657:ASN:ND2	2.23	0.71
2:D:50:ASP:OD2	5:P:19:A:O2'	2.11	0.69
1:A:15:SER:OG	1:A:118:ARG:NH2	2.26	0.68
4:E:178:ARG:HD3	4:E:340:VAL:HG22	1.74	0.68
4:E:379:ALA:O	4:E:423:ASN:ND2	2.26	0.68
4:E:549:THR:HG22	4:E:550:THR:HG23	1.76	0.67
1:A:83:GLU:HG3	1:A:219:PHE:HB2	1.76	0.67
1:A:239:SER:OG	1:A:465:ASP:OD1	2.12	0.67
5:P:24:C:H2'	5:P:25:C:H6	1.61	0.65
5:P:24:C:H2'	5:P:25:C:C6	2.34	0.63
4:E:465:LYS:NZ	4:E:569:LYS:O	2.31	0.63
5:P:13:U:H2'	5:P:14:A:H8	1.64	0.62
4:E:303:ARG:NH2	4:E:351:THR:O	2.31	0.62
4:E:443:ARG:NH2	11:E:706:AF3:F1	2.23	0.62
6:T:42:U:H2'	6:T:43:A:H8	1.65	0.62
4:E:405:LEU:HD11	4:E:534:ASP:HA	1.81	0.61
6:T:50:U:H2'	6:T:51:A:H8	1.64	0.61
4:E:189:LYS:N	4:E:190:ASN:HB2	2.15	0.61
4:E:497:ARG:HH12	4:E:500:LEU:HD22	1.65	0.61
4:E:300:PRO:O	4:E:354:GLN:NE2	2.32	0.61
1:A:100:ASP:HB3	1:A:115:SER:HB3	1.83	0.61
4:E:198:TYR:HE2	4:E:219:LEU:HD11	1.66	0.61
1:A:589:ILE:HG12	1:A:758:LEU:HD13	1.82	0.60
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.83	0.60
1:A:615:MET:HB2	1:A:766:PHE:HE1	1.65	0.60
1:A:583:ARG:NH2	1:A:590:GLY:O	2.35	0.60
1:A:691:ASN:HB3	1:A:759:SER:O	2.00	0.60
4:E:114:TRP:HB2	4:E:411:LEU:HD11	1.83	0.60
2:B:130:VAL:HB	2:B:186:VAL:HG13	1.83	0.59
6:T:35:A:H2'	6:T:36:A:H8	1.66	0.59
6:T:52:C:H2'	6:T:53:G:C8	2.37	0.59
1:A:58:GLU:OE1	1:A:118:ARG:NH1	2.36	0.59
4:E:184:GLY:HA2	4:E:225:PHE:HA	1.85	0.58
1:A:116:ARG:HG2	1:A:217:TYR:HB2	1.85	0.58
4:E:321:ALA:O	4:E:325:LEU:N	2.36	0.58
6:T:34:G:H2'	6:T:35:A:H8	1.67	0.58
1:A:221:ASP:HB2	10:A:1005:1N7:H2	1.85	0.58
4:E:486:SER:HB2	4:E:517:SER:HB3	1.86	0.58
1:A:18:ARG:NH2	1:A:63:ASP:OD1	2.36	0.58
5:P:25:C:H2'	5:P:26:U:H6	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:42:U:H2'	6:T:43:A:C8	2.38	0.58
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.86	0.58
4:E:280:LEU:HB3	4:E:399:ILE:HG22	1.86	0.58
1:A:18:ARG:HH12	1:A:61:GLU:HA	1.69	0.57
4:E:70:TYR:OH	10:E:707:1N7:O2	2.22	0.57
4:E:109:ILE:HD13	4:E:134:ALA:HB2	1.85	0.57
4:E:576:MET:HB2	4:E:582:TYR:HD2	1.69	0.57
6:T:47:U:H2'	6:T:48:G:H8	1.69	0.57
1:A:149:TYR:HE2	1:A:212:LEU:HD13	1.69	0.57
2:D:143:ASP:OD1	2:D:143:ASP:N	2.38	0.57
1:A:720:VAL:HG11	1:A:775:LEU:HD13	1.87	0.56
1:A:468:GLN:HA	1:A:731:LEU:HD22	1.87	0.56
6:T:35:A:H2'	6:T:36:A:C8	2.39	0.56
1:A:123:THR:HA	1:A:211:ASP:HA	1.88	0.56
4:E:103:VAL:O	4:E:107:ASN:ND2	2.38	0.56
5:P:13:U:H2'	5:P:14:A:C8	2.40	0.55
1:A:30:VAL:HG22	1:A:51:THR:HG22	1.88	0.55
1:A:107:ASP:OD1	1:A:108:GLY:N	2.39	0.55
1:A:726:ARG:NH2	1:A:744:GLU:OE1	2.33	0.55
1:A:35:PHE:CZ	1:A:50:LYS:HB3	2.42	0.55
4:E:315:ASP:OD1	4:E:332:ARG:NH2	2.33	0.55
1:A:685:ALA:O	6:T:21:U:O2'	2.25	0.55
4:E:287:GLY:O	4:E:291:PHE:N	2.39	0.55
6:T:36:A:H2'	6:T:37:U:H6	1.72	0.55
4:E:292:ALA:HB1	4:E:306:TYR:HE2	1.72	0.54
1:A:35:PHE:HZ	1:A:50:LYS:HB3	1.73	0.54
1:A:3:ASP:OD1	1:A:4:ALA:N	2.41	0.54
4:E:185:TYR:N	4:E:224:TYR:O	2.34	0.54
4:E:295:LEU:HD21	4:E:370:ILE:HD13	1.89	0.54
4:E:451:THR:HG22	4:E:586:GLN:H	1.72	0.54
1:A:358:ASP:OD1	1:A:533:ARG:NH1	2.40	0.53
4:E:404:GLN:HG2	4:E:537:GLN:HE21	1.73	0.53
4:E:518:GLN:NE2	4:E:547:THR:OG1	2.42	0.53
4:E:187:VAL:HG12	4:E:192:LYS:HG3	1.91	0.53
4:E:283:PRO:HG2	4:E:286:THR:HG21	1.90	0.52
4:E:493:ILE:O	4:E:497:ARG:HG2	2.10	0.52
4:E:140:ALA:HA	4:E:232:VAL:HG21	1.91	0.52
6:T:52:C:H2'	6:T:53:G:H8	1.73	0.52
3:C:58:VAL:HG22	2:D:119:ILE:HG12	1.90	0.52
4:E:233:MET:SD	4:E:233:MET:N	2.83	0.52
6:T:32:G:H2'	6:T:33:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:LEU:HD21	1:A:655:LEU:HD22	1.92	0.52
1:A:538:THR:HB	1:A:661:GLN:HG2	1.92	0.52
1:A:746:TYR:CZ	1:A:750:ARG:HD2	2.45	0.52
4:E:284:PRO:HD3	4:E:404:GLN:HE22	1.75	0.52
4:E:495:VAL:HA	4:E:498:GLU:HG2	1.92	0.52
4:E:519:ASN:OD1	4:E:530:THR:OG1	2.27	0.52
1:A:409:THR:OG1	3:C:23:GLU:OE2	2.21	0.51
6:T:41:G:H2'	6:T:42:U:C6	2.46	0.51
1:A:469:LEU:O	1:A:473:VAL:HG23	2.10	0.51
10:A:1005:1N7:H6	10:A:1005:1N7:H15	1.91	0.51
4:E:563:VAL:O	4:E:567:ARG:NH1	2.43	0.51
2:B:120:ILE:O	2:B:124:THR:OG1	2.19	0.51
5:P:26:U:H2'	5:P:27:A:H8	1.75	0.51
1:A:378:PRO:HD2	1:A:537:PRO:HB2	1.93	0.51
4:E:449:VAL:HA	4:E:452:VAL:HG12	1.92	0.51
6:T:36:A:H2'	6:T:37:U:C6	2.46	0.51
6:T:50:U:H2'	6:T:51:A:C8	2.44	0.51
1:A:316:LEU:HB2	1:A:463:MET:SD	2.50	0.50
4:E:136:GLU:HB2	4:E:235:LEU:HD21	1.93	0.50
4:E:409:ARG:NH2	4:E:422:PHE:O	2.45	0.50
5:P:25:C:H2'	5:P:26:U:C6	2.46	0.50
1:A:795:SER:HG	1:A:798:LYS:HZ3	1.54	0.50
1:A:615:MET:HB2	1:A:766:PHE:CE1	2.46	0.50
4:E:322:LEU:HD12	4:E:327:ILE:HG12	1.93	0.50
1:A:388:LEU:HD23	1:A:397:SER:HB2	1.92	0.50
4:E:394:LYS:O	4:E:395:HIS:ND1	2.45	0.50
4:E:489:ASN:HB2	4:E:549:THR:HG23	1.93	0.50
4:E:375:GLU:OE2	11:E:706:AF3:F3	2.20	0.50
2:D:31:SER:HB3	2:D:32:GLU:HB2	1.93	0.50
4:E:428:LEU:HA	4:E:431:THR:HG22	1.92	0.50
4:E:493:ILE:HD11	4:E:518:GLN:HG3	1.94	0.50
1:A:836:ARG:NH1	1:A:840:ALA:HB2	2.27	0.49
4:E:325:LEU:HD12	4:E:326:PRO:HD2	1.94	0.49
4:E:187:VAL:HA	4:E:192:LYS:HA	1.94	0.49
6:T:41:G:H2'	6:T:42:U:H6	1.77	0.49
4:E:21:ARG:NE	4:E:136:GLU:OE2	2.43	0.49
5:P:23:U:H2'	5:P:24:C:H6	1.78	0.49
6:T:37:U:H2'	6:T:38:G:H8	1.77	0.49
1:A:915:TYR:O	1:A:921:TYR:OH	2.16	0.49
6:T:34:G:H2'	6:T:35:A:C8	2.47	0.49
1:A:587:VAL:HG12	1:A:589:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:THR:O	1:A:686:THR:OG1	2.31	0.49
2:B:137:THR:O	2:B:141:THR:HG22	2.13	0.48
1:A:516:TYR:CZ	1:A:566:MET:HG2	2.49	0.48
1:A:75:HIS:CG	1:A:76:THR:H	2.32	0.48
1:A:97:ALA:O	1:A:99:HIS:ND1	2.43	0.48
4:E:281:GLN:HE21	4:E:402:PRO:HD2	1.78	0.48
5:P:23:U:H2'	5:P:24:C:C6	2.49	0.47
6:T:37:U:C2	6:T:38:G:C8	3.02	0.47
1:A:223:ILE:HD13	10:A:1005:1N7:H25	1.96	0.47
1:A:416:ASN:HA	1:A:850:THR:HG23	1.96	0.47
1:A:523:ASP:OD1	1:A:523:ASP:N	2.45	0.47
5:P:8:C:H2'	5:P:9:A:H8	1.79	0.47
1:A:390:ASP:OD2	1:A:674:TYR:OH	2.19	0.47
4:E:288:LYS:N	9:E:704:ADP:O2B	2.47	0.47
6:T:32:G:H2'	6:T:33:A:C8	2.49	0.47
1:A:759:SER:OG	5:P:35:A:O3'	2.33	0.47
10:A:1005:1N7:H14	10:A:1005:1N7:H29	1.70	0.47
4:E:503:ASN:HB3	4:E:506:TRP:CD1	2.50	0.47
4:E:48:TYR:OH	4:E:90:PHE:O	2.29	0.47
4:E:243:GLN:HB2	4:E:277:TYR:CE2	2.49	0.47
5:P:18:C:H2'	5:P:19:A:H8	1.79	0.47
4:E:328:ASP:OD1	4:E:328:ASP:N	2.48	0.47
6:T:47:U:H2'	6:T:48:G:C8	2.49	0.47
1:A:388:LEU:HD22	1:A:672:SER:HB3	1.96	0.46
6:T:25:U:H2'	6:T:26:U:H6	1.81	0.46
6:T:45:C:H2'	6:T:46:A:H8	1.80	0.46
5:P:22:C:H2'	5:P:23:U:H6	1.81	0.46
1:A:53:CYS:HB3	1:A:71:VAL:HG13	1.97	0.46
4:E:285:GLY:HA2	4:E:443:ARG:HE	1.81	0.46
1:A:161:ASP:OD1	1:A:161:ASP:N	2.47	0.46
4:E:419:PRO:HA	4:E:422:PHE:CZ	2.51	0.46
4:E:511:PHE:HZ	4:E:518:GLN:HE21	1.64	0.46
4:E:472:PHE:HB2	4:E:573:LEU:HG	1.96	0.46
2:D:160:VAL:HG12	2:D:166:ILE:HD13	1.97	0.46
4:E:285:GLY:O	4:E:442:ARG:N	2.42	0.46
6:T:20:A:H2'	6:T:21:U:C6	2.51	0.46
1:A:86:ILE:HG23	1:A:201:ILE:HD13	1.98	0.46
4:E:285:GLY:N	9:E:704:ADP:O1B	2.48	0.45
1:A:858:ARG:HG2	5:P:32:G:H5'	1.97	0.45
2:B:132:ILE:HG21	2:B:138:TYR:HB2	1.97	0.45
2:D:147:PHE:N	2:D:154:TRP:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:518:GLN:HA	4:E:521:VAL:HG12	1.97	0.45
4:E:247:VAL:HG13	4:E:248:ARG:HG3	1.98	0.45
5:P:26:U:H2'	5:P:27:A:C8	2.52	0.45
1:A:444:GLN:HB3	1:A:448:ALA:HB2	1.98	0.45
2:D:161:ASP:OD1	2:D:161:ASP:N	2.49	0.45
4:E:497:ARG:HA	4:E:497:ARG:NH1	2.31	0.45
10:E:707:1N7:H41	10:E:707:1N7:H9	1.81	0.45
4:E:419:PRO:HA	4:E:422:PHE:CE1	2.51	0.45
2:B:120:ILE:HB	2:B:121:PRO:HD3	1.98	0.45
1:A:132:ARG:NH2	1:A:465:ASP:OD2	2.50	0.45
2:D:175:ASP:O	2:D:178:PRO:HD2	2.16	0.45
4:E:376:ILE:HG21	4:E:398:TYR:HB3	1.99	0.45
1:A:170:ASP:OD2	1:A:173:ARG:NH2	2.39	0.45
1:A:371:LEU:HD21	2:B:88:GLN:HG3	1.97	0.45
3:C:49:PHE:HE1	2:D:98:LEU:HD23	1.82	0.45
6:T:42:U:C2	6:T:43:A:C8	3.05	0.45
1:A:647:SER:OG	1:A:648:LEU:N	2.50	0.44
1:A:558:ALA:O	1:A:683:GLY:HA3	2.18	0.44
2:D:68:THR:O	2:D:72:LYS:HG2	2.17	0.44
4:E:401:ASP:HB3	4:E:404:GLN:OE1	2.18	0.44
5:P:15:C:H2'	5:P:16:G:H8	1.82	0.44
1:A:699:ALA:O	1:A:703:ASN:ND2	2.50	0.44
3:C:52:MET:HG3	2:D:103:LEU:HD21	1.98	0.44
2:D:19:GLN:HA	2:D:42:LEU:HD12	2.00	0.44
4:E:61:THR:HA	4:E:84:CYS:HB3	2.00	0.44
4:E:377:SER:OG	4:E:401:ASP:O	2.29	0.44
1:A:723:LEU:HD21	1:A:745:PHE:HD1	1.83	0.44
5:P:32:G:H2'	5:P:33:C:C6	2.53	0.44
2:B:46:LYS:HE3	2:B:46:LYS:HB2	1.88	0.44
1:A:82:HIS:NE2	1:A:222:PHE:O	2.49	0.43
1:A:382:ALA:HB3	2:B:117:LEU:HD11	2.00	0.43
4:E:260:ASP:OD1	4:E:260:ASP:N	2.49	0.43
1:A:116:ARG:HD3	1:A:116:ARG:N	2.33	0.43
4:E:580:ASP:O	4:E:584:LYS:HD3	2.18	0.43
10:E:707:1N7:H14	10:E:707:1N7:H29	1.85	0.43
6:T:43:A:H2'	6:T:44:G:H8	1.82	0.43
1:A:758:LEU:HD23	1:A:813:CYS:SG	2.57	0.43
5:P:22:C:H2'	5:P:23:U:C6	2.54	0.43
6:T:31:G:H2'	6:T:32:G:H8	1.84	0.43
1:A:35:PHE:HD2	1:A:48:PHE:HB2	1.83	0.43
1:A:153:ASP:OD1	1:A:153:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:24:C:O2'	5:P:25:C:OP1	2.33	0.43
1:A:398:VAL:HG21	1:A:666:MET:SD	2.58	0.43
5:P:8:C:C2	5:P:9:A:C8	3.07	0.43
1:A:303:ASP:N	1:A:303:ASP:OD1	2.51	0.43
1:A:601:MET:O	1:A:605:VAL:HG23	2.19	0.43
4:E:417:LEU:HD11	4:E:421:TYR:HB2	2.00	0.43
10:E:707:1N7:H10	10:E:707:1N7:H33	1.71	0.43
1:A:605:VAL:HG22	1:A:756:MET:HB2	2.00	0.43
5:P:27:A:H2'	5:P:28:A:H8	1.84	0.43
6:T:29:U:H2'	6:T:30:A:H8	1.84	0.42
1:A:200:GLY:HA3	1:A:227:PRO:HA	2.00	0.42
4:E:268:ASN:HB3	4:E:436:MET:SD	2.59	0.42
5:P:27:A:H2'	5:P:28:A:C8	2.54	0.42
6:T:40:C:C2	6:T:41:G:C8	3.06	0.42
4:E:90:PHE:HZ	10:E:707:1N7:H7	1.84	0.42
4:E:372:VAL:HA	4:E:397:VAL:HG13	2.01	0.42
5:P:19:A:H2'	5:P:20:U:C6	2.55	0.42
4:E:287:GLY:HA2	9:E:704:ADP:H5'1	2.01	0.42
1:A:202:VAL:HB	1:A:223:ILE:HG13	2.01	0.42
1:A:831:TYR:HB3	1:A:868:PRO:HB2	2.01	0.42
10:A:1006:1N7:H29	10:A:1006:1N7:H14	1.74	0.42
3:C:75:MET:HG2	2:D:96:ARG:HH21	1.84	0.42
2:B:106:ILE:HG13	2:B:107:ILE:N	2.34	0.42
6:T:48:G:H2'	6:T:49:C:H6	1.85	0.42
1:A:46:ALA:HB3	1:A:48:PHE:CE2	2.55	0.42
1:A:771:ALA:HB2	1:A:776:VAL:HG12	2.01	0.42
4:E:252:LEU:HD13	4:E:299:TYR:CE2	2.55	0.42
4:E:296:ALA:HB1	4:E:355:TYR:HE1	1.85	0.42
4:E:443:ARG:NH1	4:E:567:ARG:HH21	2.17	0.42
4:E:309:CYS:SG	4:E:378:MET:HB3	2.60	0.42
4:E:526:LEU:HD13	4:E:528:LEU:HB2	2.00	0.42
1:A:837:ILE:HG22	1:A:884:TYR:CE1	2.55	0.42
4:E:444:CYS:SG	4:E:449:VAL:HB	2.60	0.42
6:T:49:C:H2'	6:T:50:U:H6	1.85	0.42
1:A:34:ALA:HA	1:A:47:LYS:HA	2.01	0.42
1:A:761:ASP:HB3	1:A:812:PHE:CE1	2.55	0.42
10:A:1006:1N7:H10	10:A:1006:1N7:H33	1.87	0.41
4:E:477:LYS:HD2	4:E:477:LYS:HA	1.80	0.41
1:A:210:GLN:HE21	1:A:214:GLY:HA2	1.85	0.41
1:A:702:ALA:HA	1:A:785:VAL:HG21	2.03	0.41
4:E:514:PRO:HA	4:E:533:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:18:C:H2'	5:P:19:A:C8	2.54	0.41
2:D:160:VAL:HG22	2:D:185:ILE:HB	2.02	0.41
4:E:512:ILE:O	4:E:546:PHE:HA	2.20	0.41
5:P:21:U:H2'	5:P:22:C:H6	1.86	0.41
1:A:106:ILE:HG23	1:A:107:ASP:H	1.85	0.41
1:A:417:LYS:HD2	2:D:90:MET:HG3	2.01	0.41
2:D:133:PRO:HA	2:D:183:PRO:HB3	2.01	0.41
5:P:21:U:H2'	5:P:22:C:C6	2.56	0.41
1:A:902:MET:SD	2:D:71:TYR:HD1	2.43	0.41
5:P:3:C:H2'	5:P:4:G:C8	2.56	0.41
1:A:514:LEU:HD13	2:B:79:LYS:HE3	2.01	0.41
4:E:363:LEU:O	4:E:390:ARG:HD3	2.21	0.41
4:E:404:GLN:HG2	4:E:537:GLN:NE2	2.36	0.41
4:E:452:VAL:HA	4:E:455:LEU:HG	2.02	0.41
4:E:497:ARG:HH22	4:E:500:LEU:HD22	1.86	0.41
6:T:25:U:H2'	6:T:26:U:C6	2.56	0.41
1:A:497:ASN:OD1	1:A:500:LYS:NZ	2.52	0.41
4:E:445:PRO:O	4:E:449:VAL:HG12	2.21	0.41
4:E:542:ASP:O	4:E:570:VAL:HG12	2.21	0.41
5:P:32:G:H2'	5:P:33:C:H6	1.86	0.41
6:T:51:A:H2'	6:T:52:C:C6	2.56	0.41
4:E:277:TYR:HA	4:E:396:TYR:O	2.21	0.40
4:E:325:LEU:HD21	4:E:355:TYR:CG	2.56	0.40
4:E:443:ARG:CZ	4:E:567:ARG:HH21	2.34	0.40
4:E:447:GLU:HB2	4:E:467:LYS:HB3	2.02	0.40
6:T:49:C:C2	6:T:50:U:C5	3.09	0.40
2:B:44:VAL:HG12	6:T:42:U:H4'	2.02	0.40
4:E:235:LEU:HD12	4:E:385:SER:HB3	2.02	0.40
1:A:368:PHE:CE2	1:A:519:MET:HG2	2.57	0.40
1:A:694:PHE:HZ	1:A:790:ASN:HD21	1.69	0.40
1:A:756:MET:O	1:A:762:ALA:HA	2.21	0.40
4:E:384:LEU:HD11	4:E:425:VAL:HG12	2.03	0.40
4:E:480:ILE:HG12	4:E:550:THR:HG22	2.03	0.40
4:E:489:ASN:ND2	4:E:549:THR:O	2.36	0.40
5:P:26:U:C2	5:P:27:A:C8	3.09	0.40
2:B:145:THR:O	2:B:156:ILE:HG12	2.21	0.40
4:E:451:THR:CG2	4:E:586:GLN:H	2.34	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	A	925/932 (99%)	877 (95%)	48 (5%)	0	100	100
2	B	184/199 (92%)	182 (99%)	2 (1%)	0	100	100
2	D	183/199 (92%)	178 (97%)	5 (3%)	0	100	100
3	C	73/88 (83%)	73 (100%)	0	0	100	100
4	E	588/605 (97%)	545 (93%)	43 (7%)	0	100	100
All	All	1953/2023 (96%)	1855 (95%)	98 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	819/823 (100%)	802 (98%)	17 (2%)	53	79
2	B	149/168 (89%)	148 (99%)	1 (1%)	84	93
2	D	152/168 (90%)	147 (97%)	5 (3%)	38	70
3	C	70/81 (86%)	70 (100%)	0	100	100
4	E	504/526 (96%)	493 (98%)	11 (2%)	52	78
All	All	1694/1766 (96%)	1660 (98%)	34 (2%)	57	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	60	ASP
1	A	114	ILE
1	A	116	ARG
1	A	320	VAL
1	A	341	VAL
1	A	402	THR
1	A	403	ASN
1	A	497	ASN
1	A	538	THR
1	A	686	THR
1	A	687	THR
1	A	736	ASP
1	A	761	ASP
1	A	784	SER
1	A	871	LYS
1	A	910	ASP
2	B	186	VAL
2	D	9	LEU
2	D	64	ASP
2	D	95	LEU
2	D	131	VAL
2	D	143	ASP
4	E	26	CYS
4	E	126	CYS
4	E	193	VAL
4	E	258	ILE
4	E	371	VAL
4	E	426	CYS
4	E	438	LEU
4	E	456	VAL
4	E	499	PHE
4	E	526	LEU
4	E	562	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	33/35 (94%)	1 (3%)	1 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	T	36/55 (65%)	1 (2%)	0
All	All	69/90 (76%)	2 (2%)	1 (1%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	25	C
6	T	36	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	P	24	C

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
9	ADP	E	704	8	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
9	ADP	A	1004	8	24,29,29	0.94	1 (4%)	29,45,45	1.57	4 (13%)
10	1N7	A	1006	-	29,29,46	2.71	16 (55%)	47,47,72	2.35	20 (42%)
11	AF3	E	706	-	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	1N7	A	1005	-	38,38,46	2.84	20 (52%)	58,58,72	3.01	23 (39%)
10	1N7	E	707	-	39,39,46	2.74	21 (53%)	61,61,72	2.51	27 (44%)

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
9	ADP	E	704	8	-	1/12/32/32	0/3/3/3
9	ADP	A	1004	8	-	3/12/32/32	0/3/3/3
10	1N7	A	1006	-	-	4/6/71/92	0/4/4/4
10	1N7	A	1005	-	2/2/13/16	7/16/81/92	0/4/4/4
10	1N7	E	707	-	-	10/17/82/92	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1005	1N7	C18-C17	6.21	1.64	1.53
10	A	1006	1N7	C18-C17	5.88	1.63	1.53
10	E	707	1N7	C18-C17	5.83	1.63	1.53
10	A	1005	1N7	C23-C24	5.06	1.60	1.51
10	E	707	1N7	C23-C24	4.94	1.60	1.51
10	A	1005	1N7	C24-N1	4.86	1.44	1.33
10	E	707	1N7	C24-N1	4.85	1.44	1.33
10	A	1005	1N7	C2-C19	4.64	1.64	1.56
10	A	1005	1N7	C16-C17	4.41	1.60	1.52
10	A	1006	1N7	C2-C19	4.41	1.64	1.56
10	E	707	1N7	C2-C19	4.37	1.64	1.56
10	E	707	1N7	C16-C17	4.31	1.60	1.52
10	A	1006	1N7	C3-C19	4.23	1.60	1.53
10	A	1006	1N7	C16-C17	4.18	1.60	1.52
10	E	707	1N7	C3-C19	4.13	1.60	1.53
10	A	1005	1N7	C3-C19	4.08	1.60	1.53
10	A	1006	1N7	C14-C13	4.06	1.59	1.51
10	E	707	1N7	C14-C13	4.06	1.59	1.51
10	A	1005	1N7	C14-C13	3.97	1.59	1.51
10	A	1005	1N7	C28-N2	3.96	1.58	1.46
10	A	1005	1N7	C20-C9	3.82	1.61	1.54
10	E	707	1N7	C20-C9	3.65	1.60	1.54
10	A	1006	1N7	C20-C9	3.62	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	707	1N7	C28-N2	3.61	1.60	1.50
10	A	1005	1N7	C5-C4	3.51	1.60	1.54
10	A	1006	1N7	C5-C4	3.45	1.59	1.54
10	E	707	1N7	C5-C4	3.38	1.59	1.54
10	A	1006	1N7	C14-C15	3.30	1.59	1.53
10	E	707	1N7	C14-C15	3.29	1.59	1.53
10	A	1005	1N7	C14-C15	3.20	1.59	1.53
10	A	1005	1N7	C18-C6	3.01	1.59	1.53
10	E	707	1N7	C16-C15	2.99	1.58	1.53
10	A	1005	1N7	C25-N1	2.97	1.53	1.46
10	E	707	1N7	C25-N1	2.95	1.52	1.46
10	A	1005	1N7	C16-C15	2.92	1.58	1.53
10	A	1005	1N7	C1-C2	2.91	1.59	1.54
10	A	1006	1N7	C16-C15	2.89	1.58	1.53
10	E	707	1N7	C29-N2	2.89	1.58	1.50
10	A	1005	1N7	C5-C6	2.84	1.60	1.55
10	A	1006	1N7	C1-C2	2.80	1.59	1.54
10	E	707	1N7	C2-C15	2.73	1.59	1.55
10	A	1005	1N7	C2-C15	2.72	1.59	1.55
10	E	707	1N7	C1-C2	2.70	1.59	1.54
10	A	1006	1N7	C18-C6	2.69	1.59	1.53
10	A	1006	1N7	C2-C15	2.66	1.59	1.55
10	E	707	1N7	C18-C6	2.63	1.59	1.53
10	E	707	1N7	C18-C19	2.62	1.59	1.53
10	A	1006	1N7	C3-C4	2.62	1.57	1.53
10	A	1005	1N7	C18-C19	2.60	1.58	1.53
10	A	1005	1N7	C3-C4	2.57	1.57	1.53
10	E	707	1N7	C3-C4	2.56	1.57	1.53
10	A	1006	1N7	C18-C19	2.51	1.58	1.53
10	A	1005	1N7	C12-C13	2.47	1.57	1.51
10	E	707	1N7	C12-C13	2.46	1.57	1.51
9	E	704	ADP	C5-C4	2.46	1.47	1.40
10	A	1006	1N7	C12-C13	2.45	1.57	1.51
9	A	1004	ADP	C5-C4	2.40	1.47	1.40
10	A	1006	1N7	C5-C6	2.27	1.59	1.55
10	E	707	1N7	C5-C6	2.16	1.59	1.55

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1005	1N7	C9-C5-C4	-12.86	105.93	117.67
10	A	1006	1N7	C9-C5-C4	-6.42	111.81	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	707	1N7	C9-C5-C4	-6.36	111.86	117.67
10	A	1005	1N7	C6-C5-C4	5.97	112.96	107.40
10	E	707	1N7	C8-C9-C5	-5.93	97.74	103.55
10	A	1005	1N7	C9-C5-C6	5.75	105.89	100.09
10	E	707	1N7	C5-C9-C20	-5.58	112.83	119.50
10	A	1005	1N7	C23-C24-N1	5.49	125.66	116.42
10	A	1006	1N7	C6-C18-C17	5.47	119.06	111.81
10	A	1005	1N7	C5-C9-C20	-5.23	113.26	119.50
10	E	707	1N7	C6-C18-C17	4.99	118.43	111.81
10	E	707	1N7	C3-C4-C5	-4.98	106.13	111.24
10	E	707	1N7	C23-C24-N1	4.94	124.74	116.42
10	A	1005	1N7	C6-C18-C17	4.67	118.00	111.81
10	A	1005	1N7	C8-C9-C5	-4.50	99.14	103.55
10	A	1005	1N7	C11-C2-C1	-4.48	101.04	108.26
10	A	1006	1N7	C5-C9-C20	-4.45	114.18	119.50
10	A	1006	1N7	C8-C9-C5	-4.42	99.22	103.55
10	E	707	1N7	C6-C5-C4	4.15	111.26	107.40
10	A	1006	1N7	C11-C2-C1	-4.10	101.65	108.26
10	E	707	1N7	C8-C9-C20	3.87	118.14	112.15
9	A	1004	ADP	PA-O3A-PB	-3.87	119.55	132.83
10	A	1006	1N7	C3-C4-C5	-3.86	107.28	111.24
10	A	1005	1N7	C19-C2-C15	3.85	113.99	108.58
10	E	707	1N7	C11-C2-C1	-3.83	102.08	108.26
10	A	1005	1N7	C8-C9-C20	3.83	118.08	112.15
9	E	704	ADP	PA-O3A-PB	-3.79	119.81	132.83
10	A	1005	1N7	C7-C6-C18	-3.56	113.36	118.33
10	A	1005	1N7	C2-C19-C18	3.49	115.56	111.82
10	E	707	1N7	C29-N2-C28	-3.39	100.26	108.97
9	A	1004	ADP	C3'-C2'-C1'	3.25	105.87	100.98
9	E	704	ADP	C3'-C2'-C1'	3.24	105.85	100.98
9	A	1004	ADP	N3-C2-N1	-3.23	123.63	128.68
10	A	1005	1N7	O1-C24-C23	-3.16	116.23	122.02
9	E	704	ADP	N3-C2-N1	-3.16	123.74	128.68
10	E	707	1N7	C19-C2-C15	3.15	113.01	108.58
10	E	707	1N7	C27-C26-C25	3.13	117.08	111.04
10	A	1006	1N7	C19-C2-C15	3.13	112.97	108.58
10	A	1006	1N7	C6-C5-C4	3.05	110.24	107.40
10	A	1006	1N7	C1-C12-C13	2.96	114.27	110.47
10	A	1005	1N7	C1-C12-C13	2.96	114.26	110.47
10	E	707	1N7	O1-C24-C23	-2.94	116.64	122.02
10	A	1005	1N7	C3-C19-C2	-2.80	110.84	113.73
9	A	1004	ADP	C4-C5-N7	-2.74	106.55	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	707	1N7	C7-C6-C5	-2.68	100.92	103.55
10	A	1005	1N7	C10-C5-C4	2.67	111.79	109.07
10	E	707	1N7	C3-C19-C2	-2.63	111.01	113.73
10	A	1005	1N7	C23-C22-C20	2.63	119.32	114.52
9	E	704	ADP	C4-C5-N7	-2.61	106.68	109.40
10	A	1006	1N7	C7-C8-C9	2.60	110.29	105.13
10	E	707	1N7	C1-C12-C13	2.60	113.80	110.47
10	A	1005	1N7	O1-C24-N1	-2.60	118.11	123.01
10	A	1005	1N7	C15-C16-C17	2.53	117.25	114.46
10	A	1006	1N7	C19-C3-C4	2.50	117.60	114.30
10	A	1006	1N7	C7-C6-C5	-2.50	101.10	103.55
10	A	1006	1N7	C10-C5-C9	-2.49	107.32	111.21
10	E	707	1N7	C10-C5-C9	-2.49	107.32	111.21
10	A	1005	1N7	C19-C3-C4	2.49	117.58	114.30
10	E	707	1N7	C11-C2-C19	-2.48	107.76	111.18
10	E	707	1N7	C30-N2-C28	-2.43	102.72	108.97
10	A	1006	1N7	C10-C5-C4	2.42	111.53	109.07
10	A	1005	1N7	C16-C17-C18	2.41	114.05	111.48
10	E	707	1N7	C15-C14-C13	2.39	116.27	112.76
10	E	707	1N7	O1-C24-N1	-2.33	118.61	123.01
10	E	707	1N7	C7-C8-C9	2.31	109.72	105.13
10	A	1005	1N7	C10-C5-C9	-2.31	107.60	111.21
10	E	707	1N7	C1-C2-C15	2.29	111.16	107.77
10	A	1005	1N7	C7-C6-C5	2.28	105.79	103.55
10	A	1006	1N7	C9-C5-C6	2.25	102.36	100.09
10	A	1006	1N7	C8-C9-C20	2.21	115.56	112.15
10	A	1006	1N7	C15-C14-C13	2.20	115.99	112.76
10	E	707	1N7	C25-N1-C24	2.18	126.88	122.84
10	A	1006	1N7	C15-C16-C17	2.18	116.86	114.46
10	A	1006	1N7	O3-C17-C16	-2.17	104.57	109.94
10	E	707	1N7	C10-C5-C4	2.13	111.23	109.07
10	A	1006	1N7	C11-C2-C19	-2.10	108.28	111.18
10	E	707	1N7	C26-C25-N1	2.05	118.06	112.21
10	E	707	1N7	C16-C15-C2	-2.00	110.53	112.66

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1005	1N7	C18
10	A	1005	1N7	C6

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1004	ADP	C5'-O5'-PA-O1A
9	A	1004	ADP	C5'-O5'-PA-O2A
10	A	1005	1N7	C21-C20-C9-C5
10	A	1005	1N7	C22-C20-C9-C5
10	A	1005	1N7	C22-C20-C9-C8
10	E	707	1N7	C21-C20-C9-C5
10	E	707	1N7	C22-C20-C9-C5
10	E	707	1N7	C22-C20-C9-C8
10	A	1005	1N7	C21-C20-C9-C8
10	E	707	1N7	C21-C20-C9-C8
10	E	707	1N7	C21-C20-C22-C23
10	A	1006	1N7	C22-C20-C9-C5
10	A	1006	1N7	C21-C20-C9-C5
10	E	707	1N7	C9-C20-C22-C23
10	E	707	1N7	C22-C23-C24-N1
10	A	1005	1N7	C26-C27-N2-C28
10	E	707	1N7	C22-C23-C24-O1
10	A	1005	1N7	C9-C20-C22-C23
10	E	707	1N7	C25-C26-C27-N2
10	A	1006	1N7	C21-C20-C9-C8
10	A	1006	1N7	C22-C20-C9-C8
10	A	1005	1N7	C20-C22-C23-C24
9	E	704	ADP	O4'-C4'-C5'-O5'
10	E	707	1N7	C20-C22-C23-C24
9	A	1004	ADP	C5'-O5'-PA-O3A

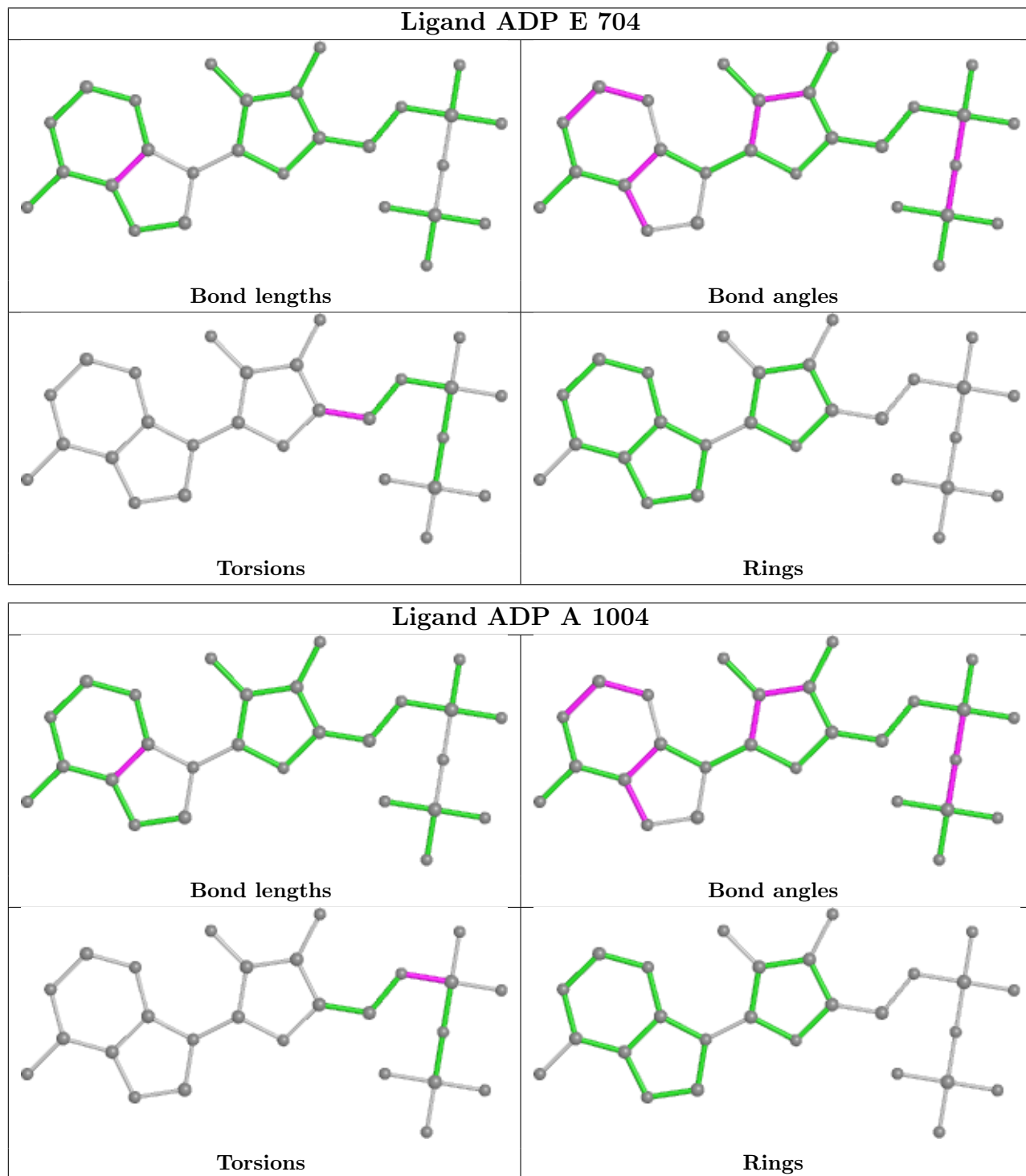
There are no ring outliers.

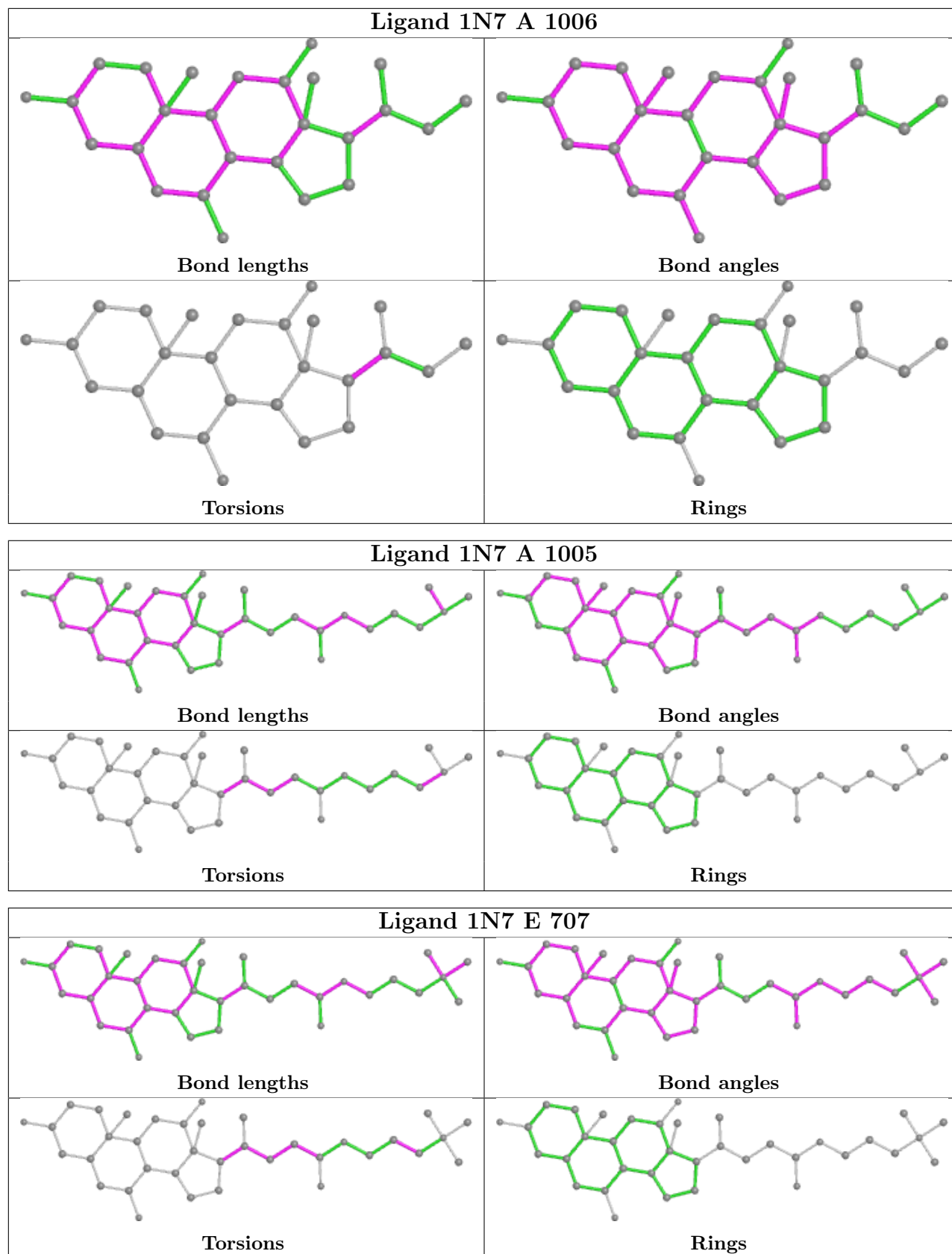
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	704	ADP	3	0
9	A	1004	ADP	1	0
10	A	1006	1N7	2	0
11	E	706	AF3	2	0
10	A	1005	1N7	4	0
10	E	707	1N7	5	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

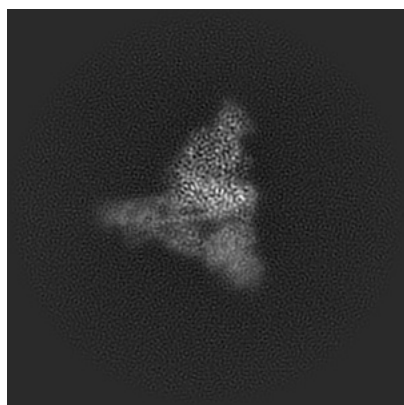
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24431. These allow visual inspection of the internal detail of the map and identification of artifacts.

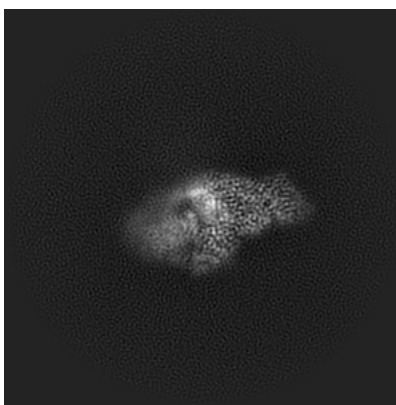
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

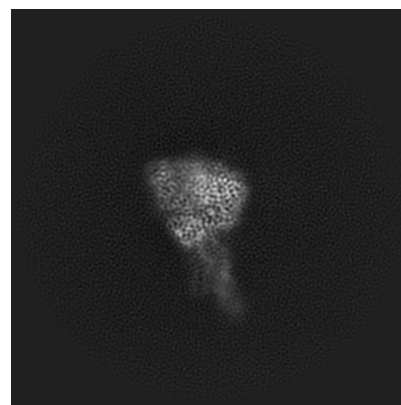
#### 6.1.1 Primary map



X



Y

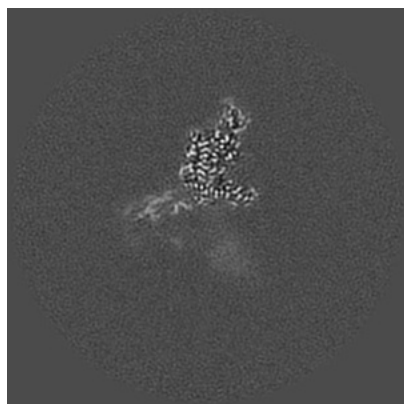


Z

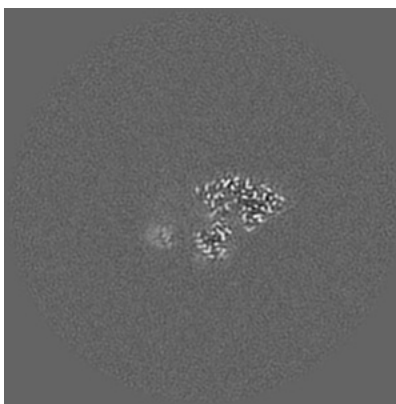
The images above show the map projected in three orthogonal directions.

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

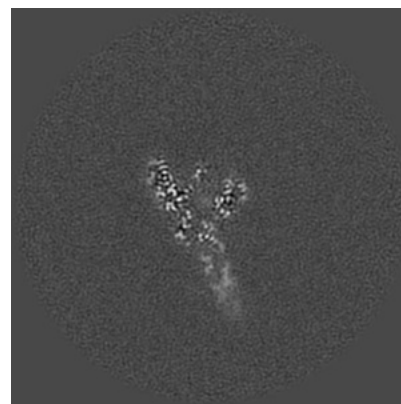
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



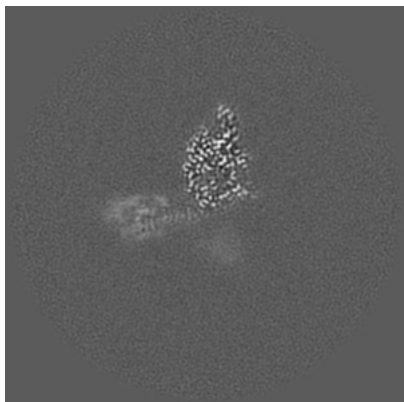
Z Index: 160



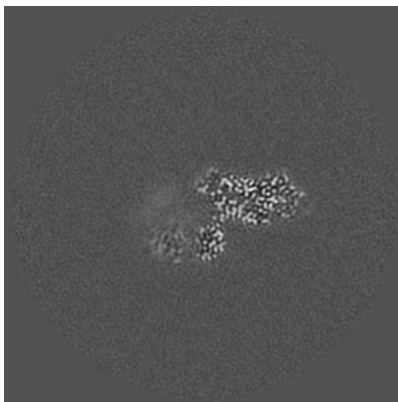
The images above show central slices of the map in three orthogonal directions.

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

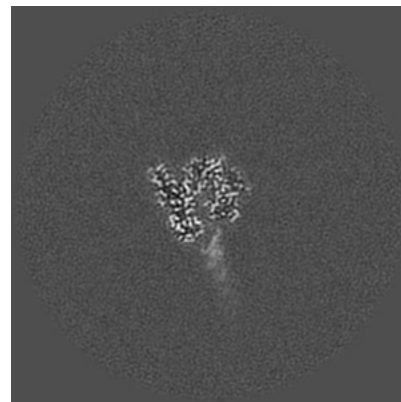
### 6.3.1 Primary map



X Index: 169



Y Index: 172



Z Index: 167

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

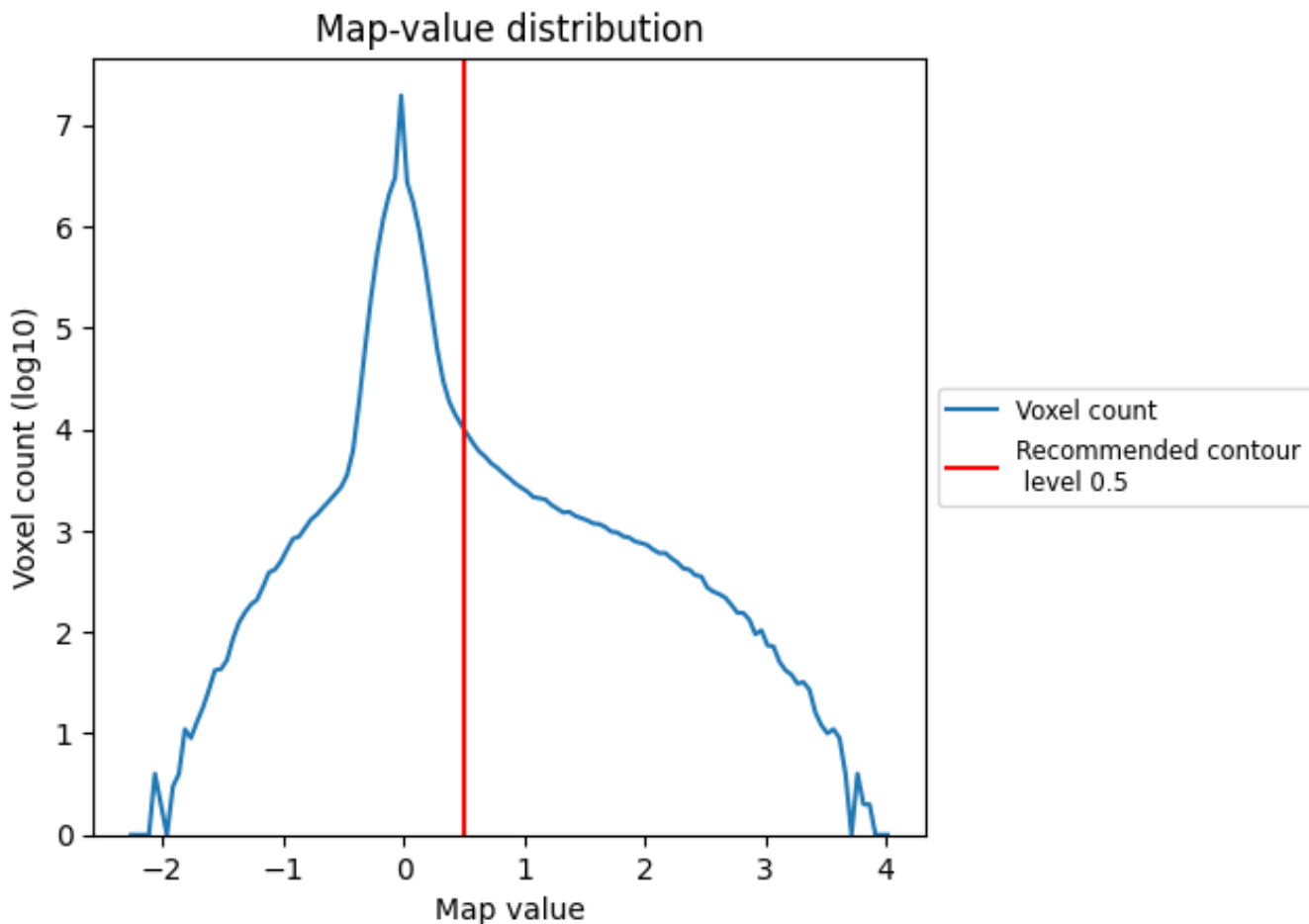
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

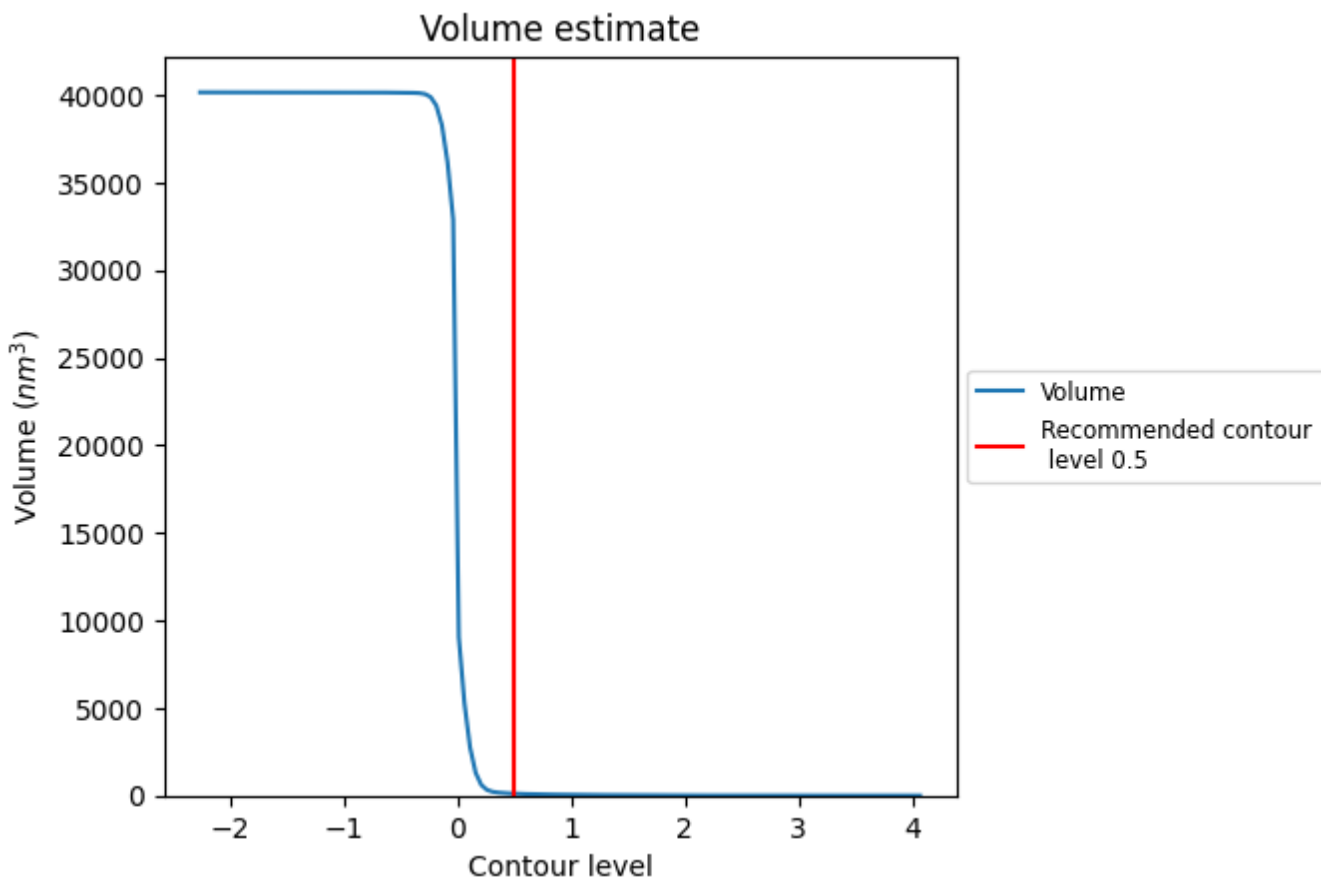
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

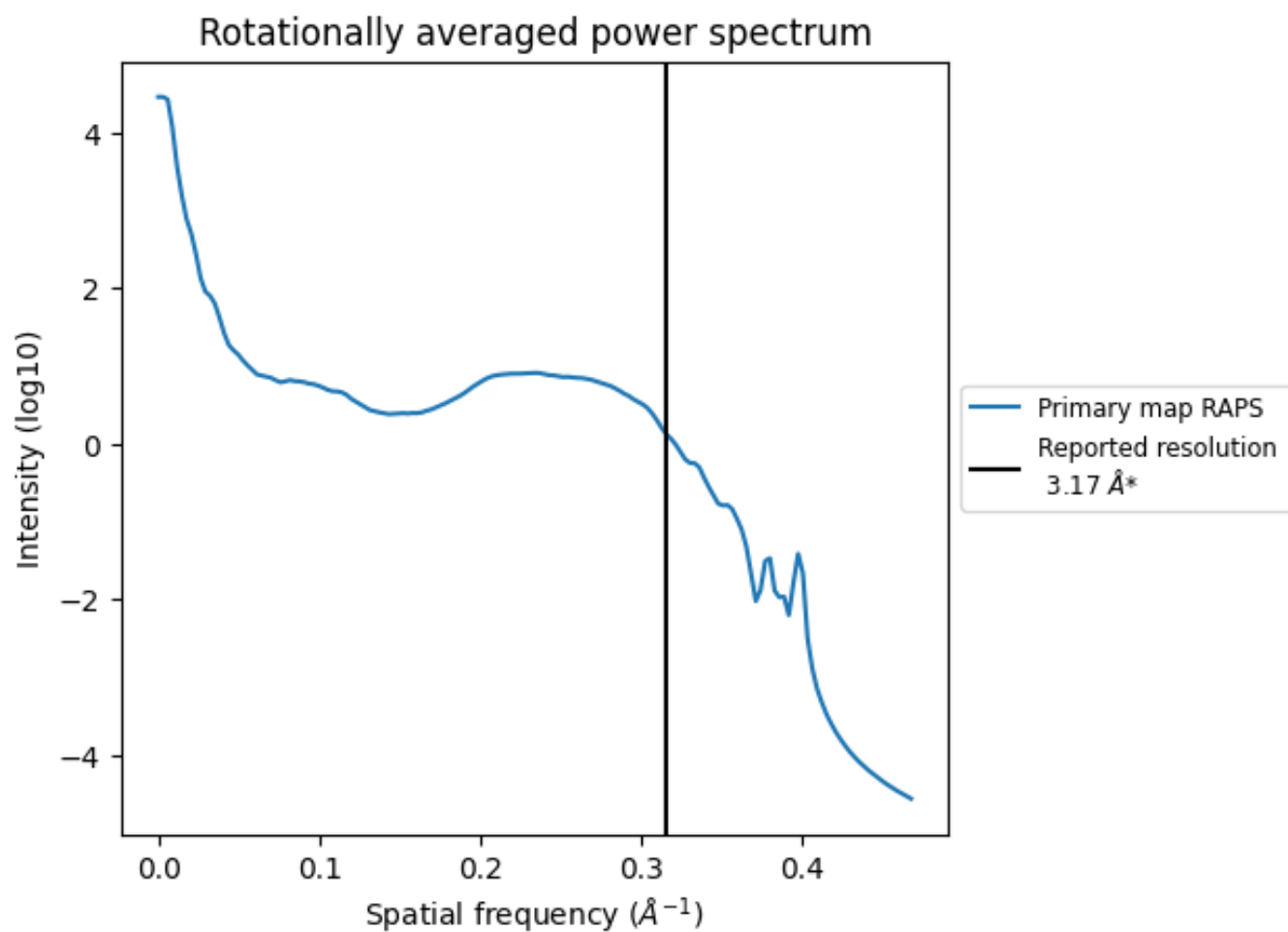
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm<sup>3</sup>; this corresponds to an approximate mass of 100 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

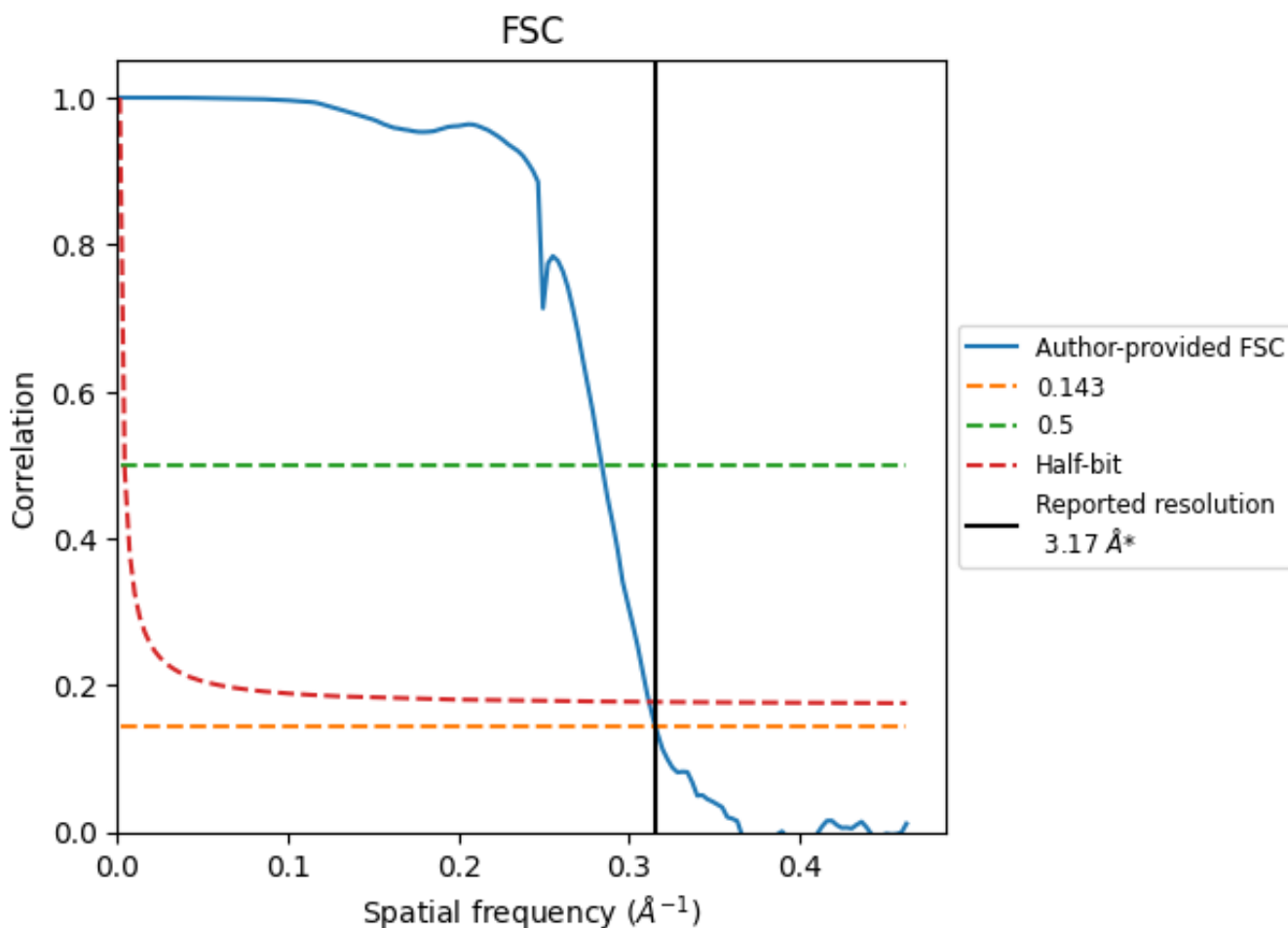


\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

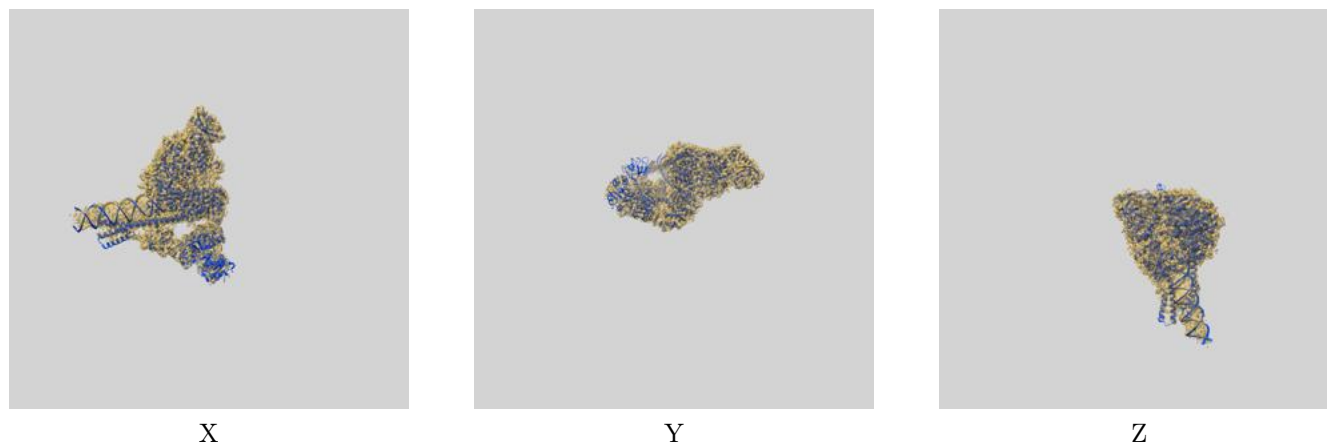
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.52	3.21
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-24431 and PDB model 7RE2. Per-residue inclusion information can be found in section 3 on page 8.

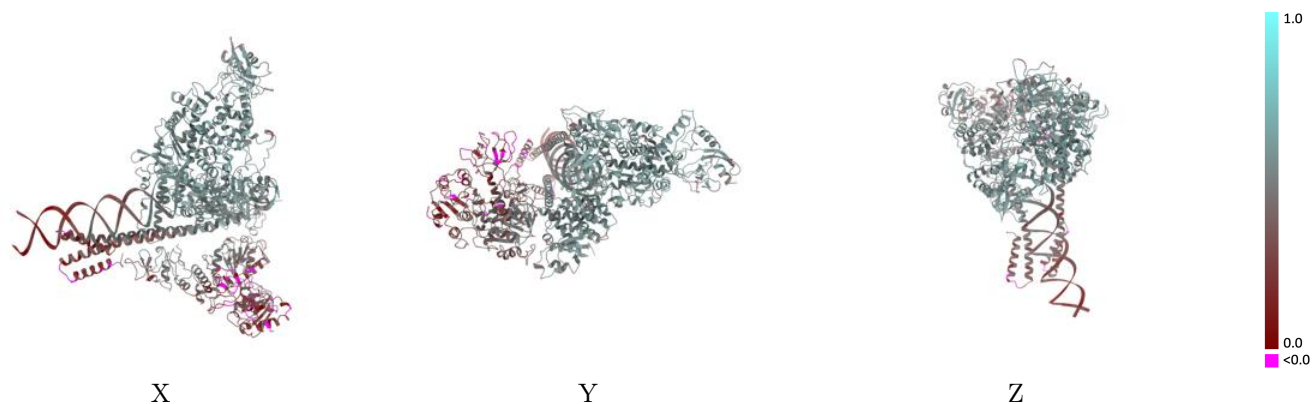
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

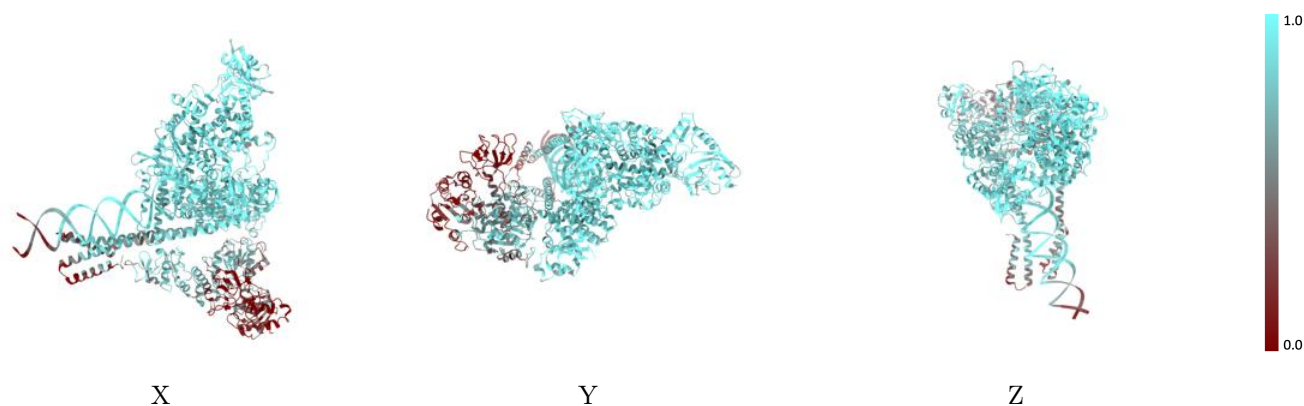


## 9.2 Q-score mapped to coordinate model [i](#)



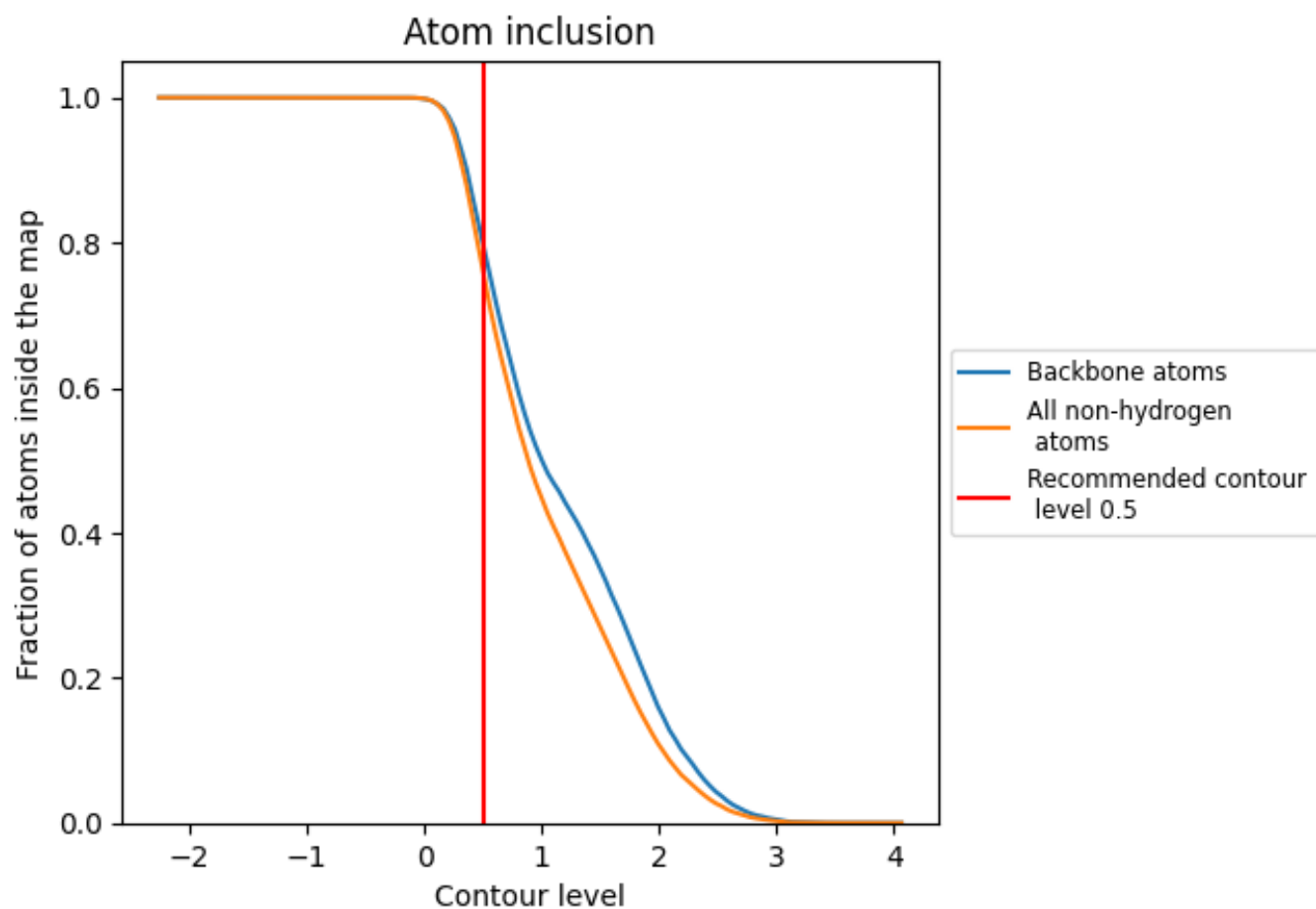
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7595	 0.4640
A	 0.9185	 0.5620
B	 0.7641	 0.4560
C	 0.8569	 0.5360
D	 0.7961	 0.4700
E	 0.4630	 0.3310
P	 0.7914	 0.3490
T	 0.8010	 0.3620

