Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 05:58 AM EST

PDB ID	:	7RE3
EMDB ID	:	EMD-24432
Title	:	SARS-CoV-2 replication-transcription complex bound to nsp13 helicase - nsp13(2)-RTC dimer
Authors	:	Chen, J.; Malone, B.; Campbell, E.A.; Darst, S.A.
Deposited on	:	2021-07-12
Resolution	:	3.33 Å(reported)

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

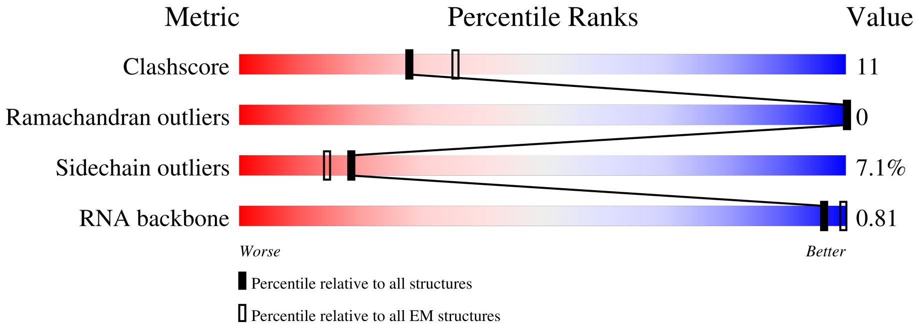
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

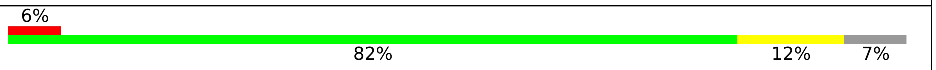
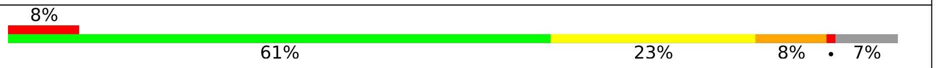
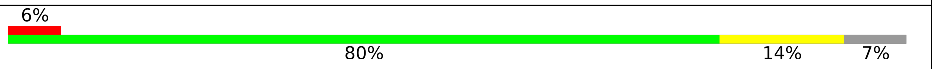
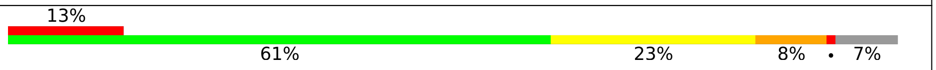
The reported resolution of this entry is 3.33 Å.

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 <=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	
1	G	932	
2	B	199	
2	D	199	
2	H	199	
2	J	199	
3	C	88	

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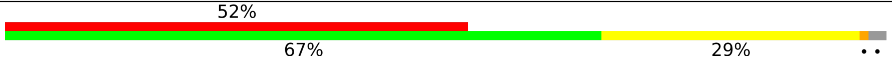
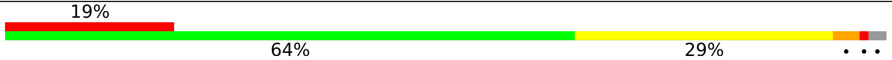
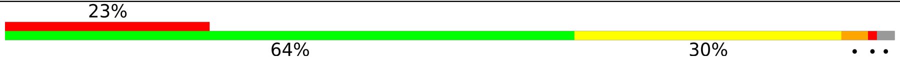
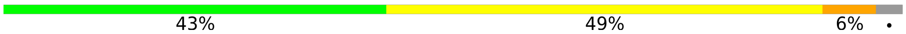
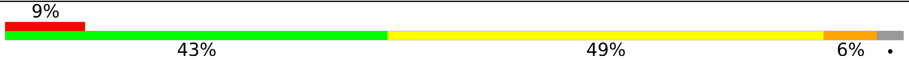
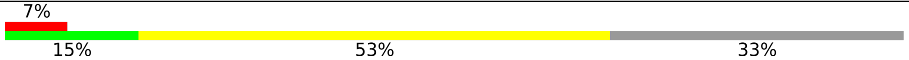
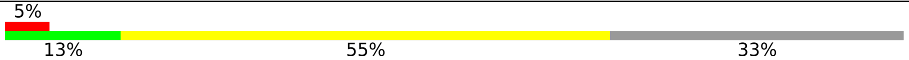
Mol	Chain	Length	Quality of chain
3	I	88	
4	E	605	
4	F	605	
4	K	605	
4	L	605	
5	P	35	
5	Q	35	
6	T	55	
6	U	55	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 43154 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
1	G	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
2	H	186	1405	883	241	270	11	0	0
2	J	185	1406	885	239	271	11	0	0

There are 4 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
H	0	MET	-	initiating methionine	UNP P0DTD1
J	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
3	I	75	576	362	94	113	7	0	0

There are 10 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
I	-4	GLY	-	expression tag	UNP P0DTD1
I	-3	PRO	-	expression tag	UNP P0DTD1
I	-2	VAL	-	expression tag	UNP P0DTD1
I	-1	ASP	-	expression tag	UNP P0DTD1
I	0	MET	-	expression tag	UNP P0DTD1

- Molecule 4 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	590	Total 4507	C 2861	N 761	O 851	S 34	0	0
4	F	590	Total 4563	C 2899	N 774	O 856	S 34	0	0
4	K	590	Total 4507	C 2861	N 761	O 851	S 34	0	0
4	L	590	Total 4563	C 2899	N 774	O 856	S 34	0	0

There are 16 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
F	-3	GLY	-	expression tag	UNP P0DTD1
F	-2	PRO	-	expression tag	UNP P0DTD1
F	-1	HIS	-	expression tag	UNP P0DTD1
F	0	MET	-	expression tag	UNP P0DTD1
K	-3	GLY	-	expression tag	UNP P0DTD1
K	-2	PRO	-	expression tag	UNP P0DTD1
K	-1	HIS	-	expression tag	UNP P0DTD1
K	0	MET	-	expression tag	UNP P0DTD1
L	-3	GLY	-	expression tag	UNP P0DTD1
L	-2	PRO	-	expression tag	UNP P0DTD1
L	-1	HIS	-	expression tag	UNP P0DTD1
L	0	MET	-	expression tag	UNP P0DTD1

- Molecule 5 is a RNA chain called Product RNA.

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

- Molecule 6 is a RNA chain called Template RNA.

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

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

Mol	Chain	Residues	Atoms	AltConf
7	A	2	Total Zn 2 2	0
7	E	3	Total Zn 3 3	0
7	F	3	Total Zn 3 3	0
7	G	2	Total Zn 2 2	0
7	K	3	Total Zn 3 3	0
7	L	3	Total Zn 3 3	0

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

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

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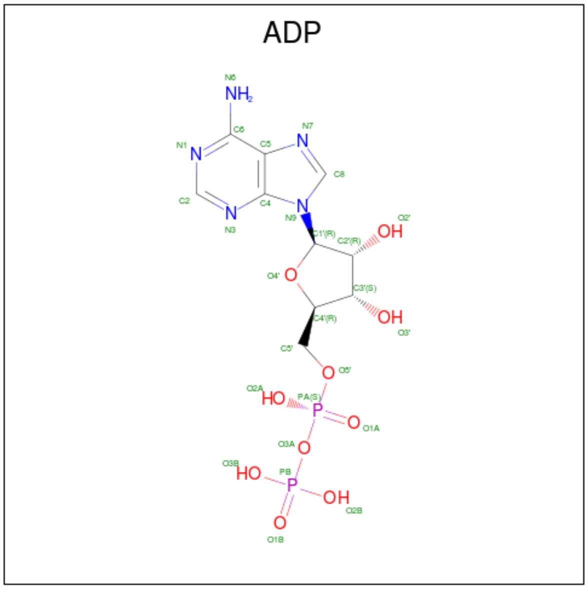
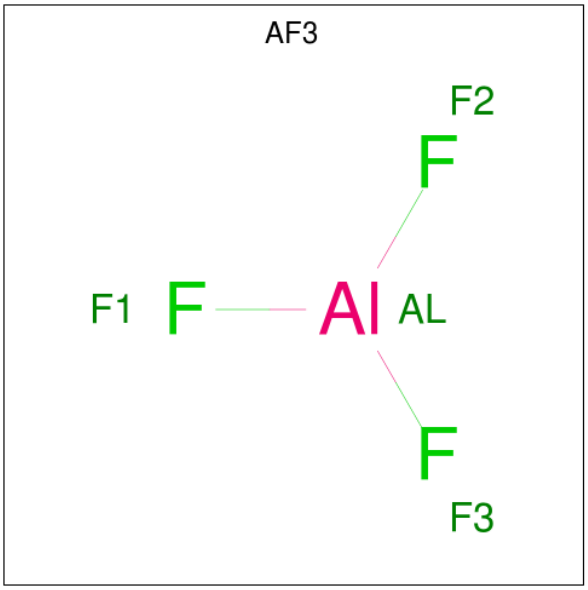
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	L	1	1	1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



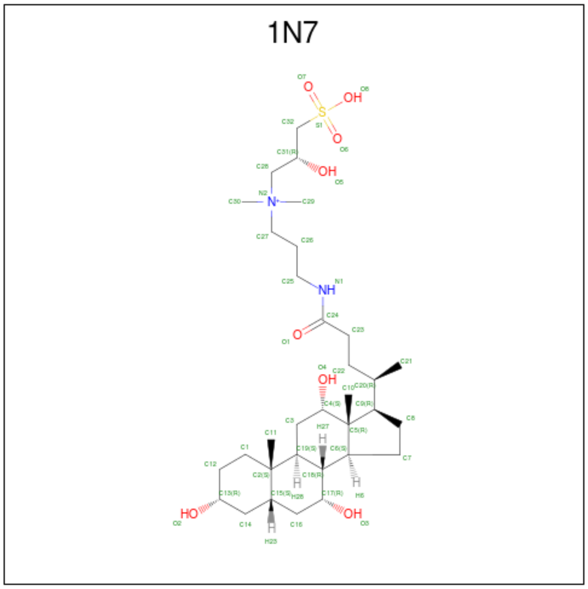
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	27	10	5	10	2	0
9	E	1	27	10	5	10	2	0
9	F	1	27	10	5	10	2	0
9	G	1	27	10	5	10	2	0
9	K	1	27	10	5	10	2	0
9	L	1	27	10	5	10	2	0

- Molecule 10 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	AltConf
10	E	1	Total Al F 4 1 3	0
10	F	1	Total Al F 4 1 3	0
10	K	1	Total Al F 4 1 3	0
10	L	1	Total Al F 4 1 3	0

- Molecule 11 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).

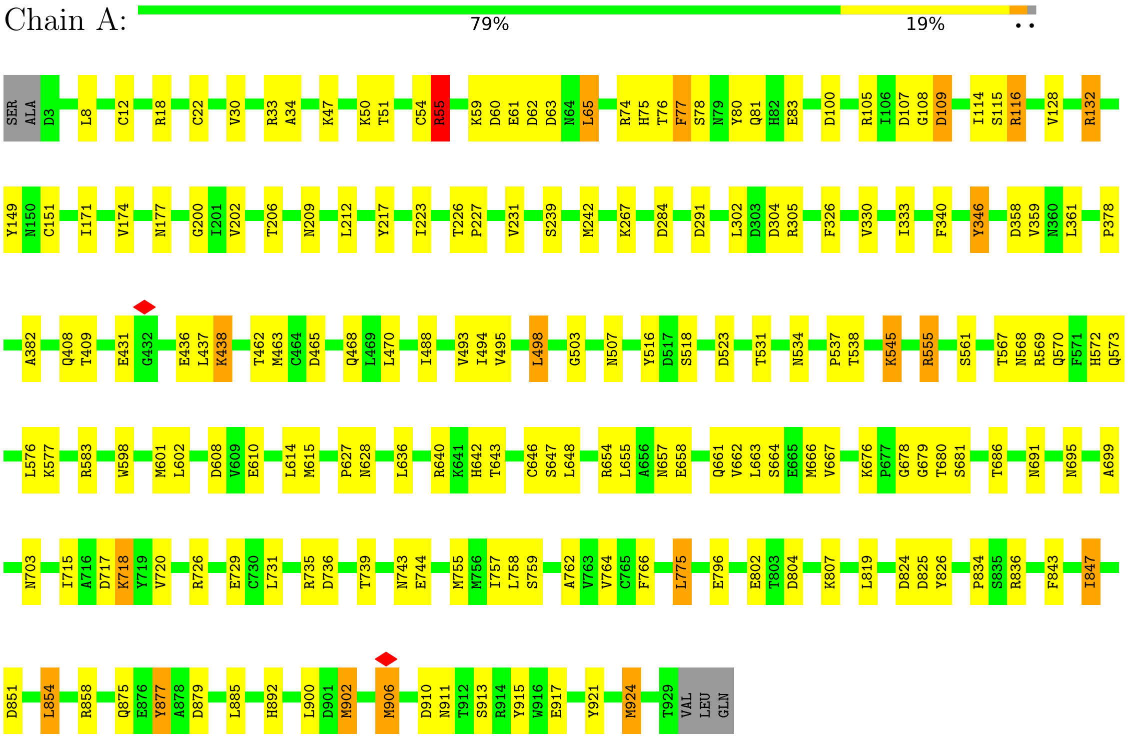


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	E	1	36	30	2	4	0
			Total	C	N	O	
11	K	1	36	30	2	4	0

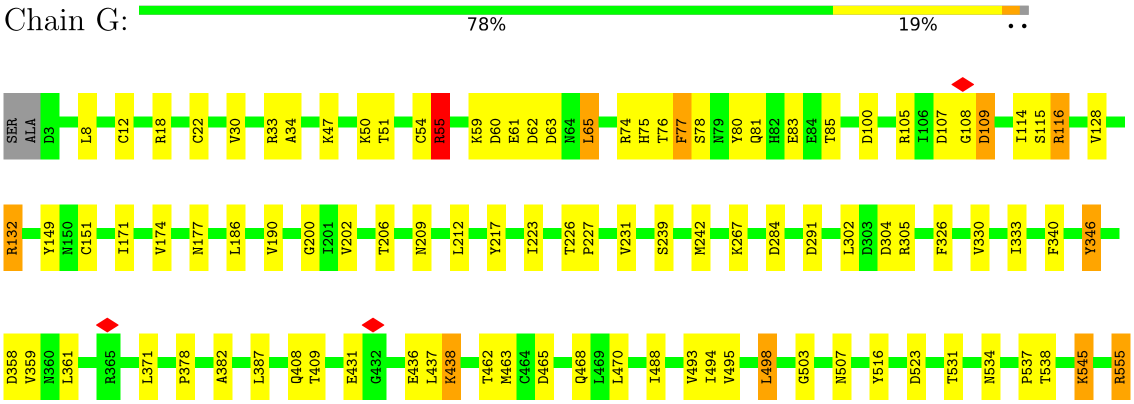
3 Residue-property plots ⓘ

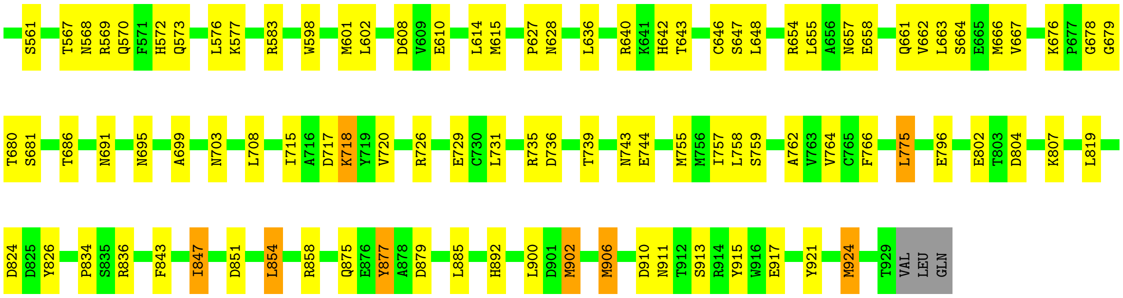
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



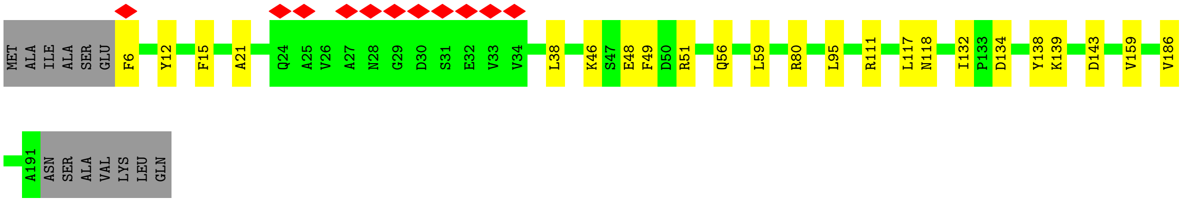
- Molecule 1: RNA-directed RNA polymerase





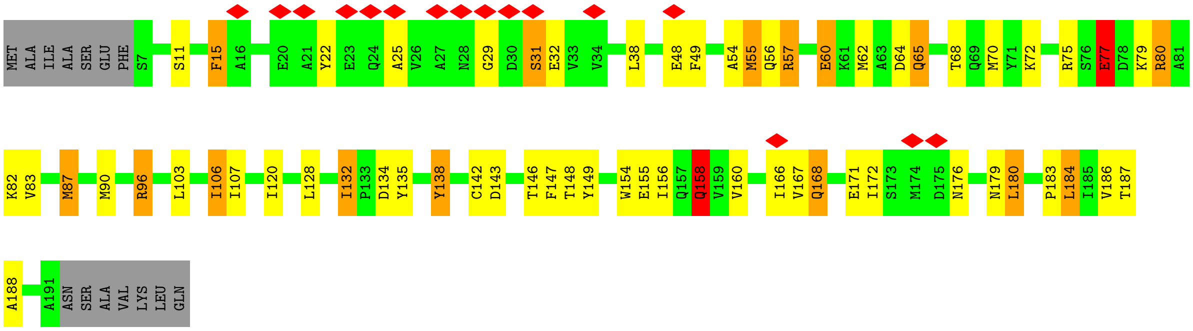
- Molecule 2: Non-structural protein 8

Chain B:



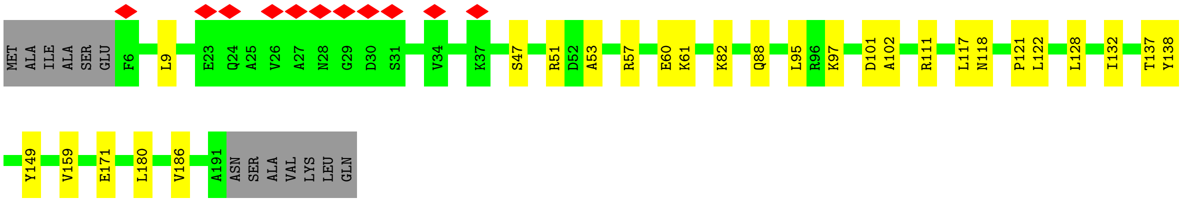
- Molecule 2: Non-structural protein 8

Chain D:



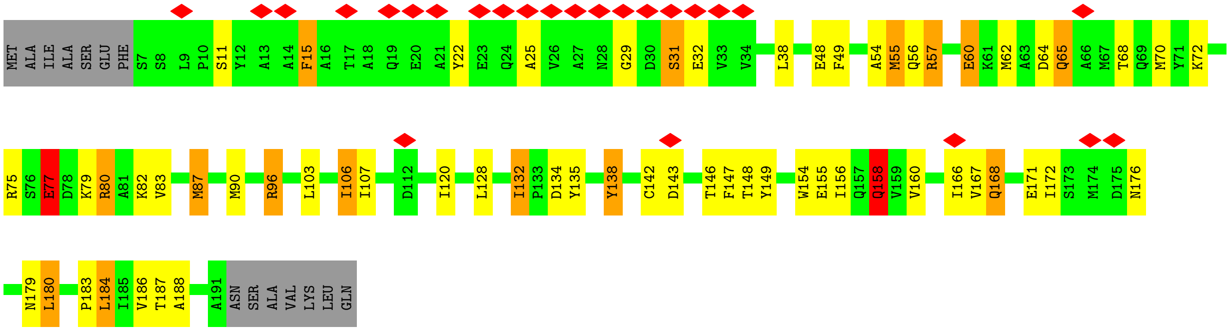
- Molecule 2: Non-structural protein 8

Chain H:



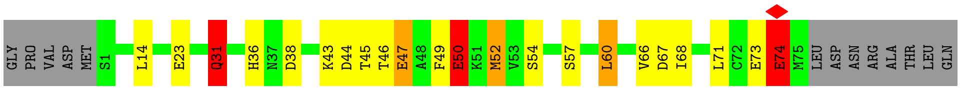
- Molecule 2: Non-structural protein 8

Chain J:



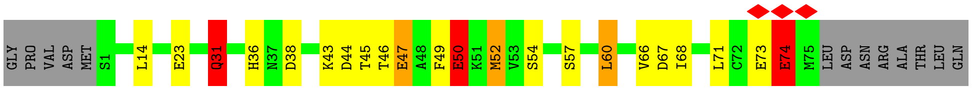
- Molecule 3: Non-structural protein 7

Chain C:

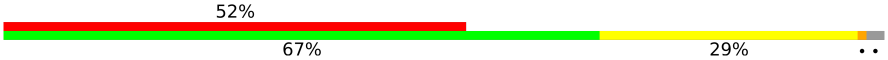



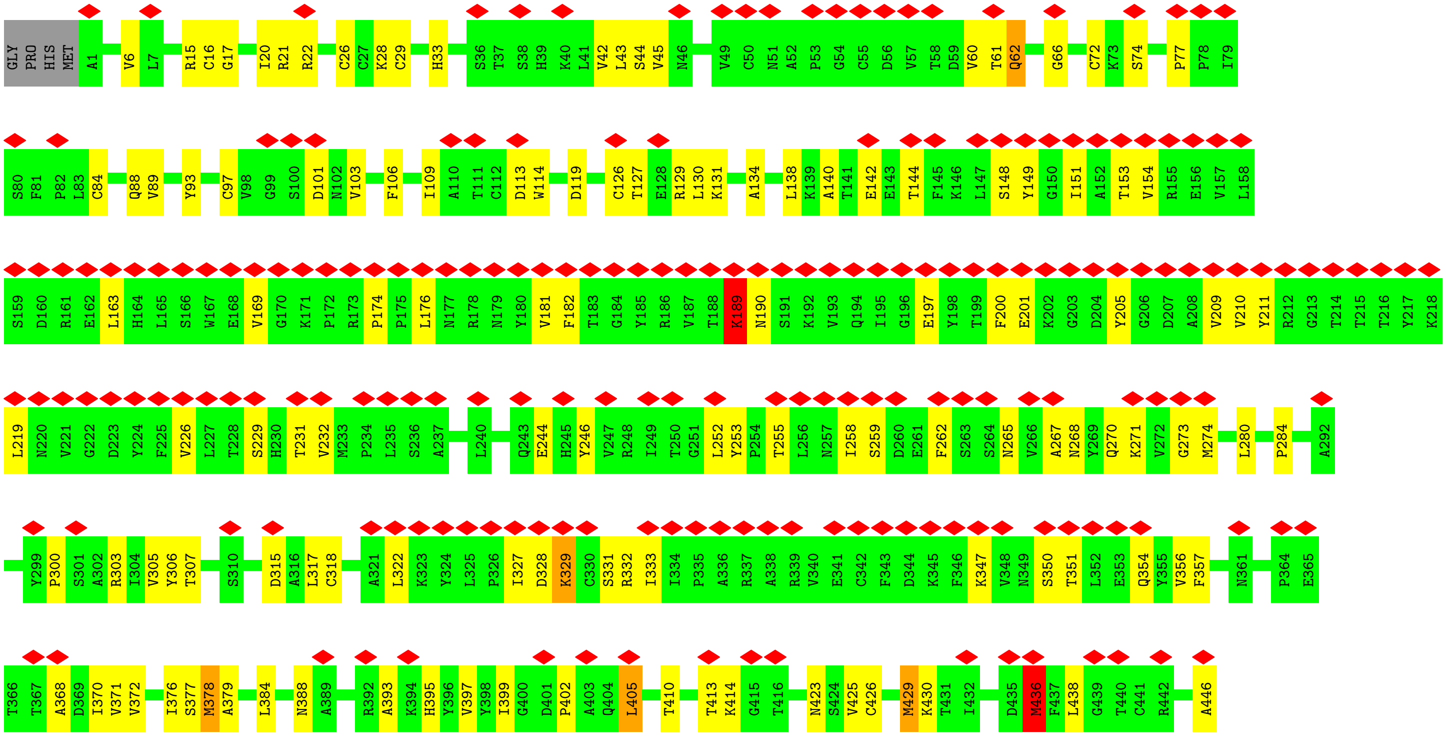
- Molecule 3: Non-structural protein 7

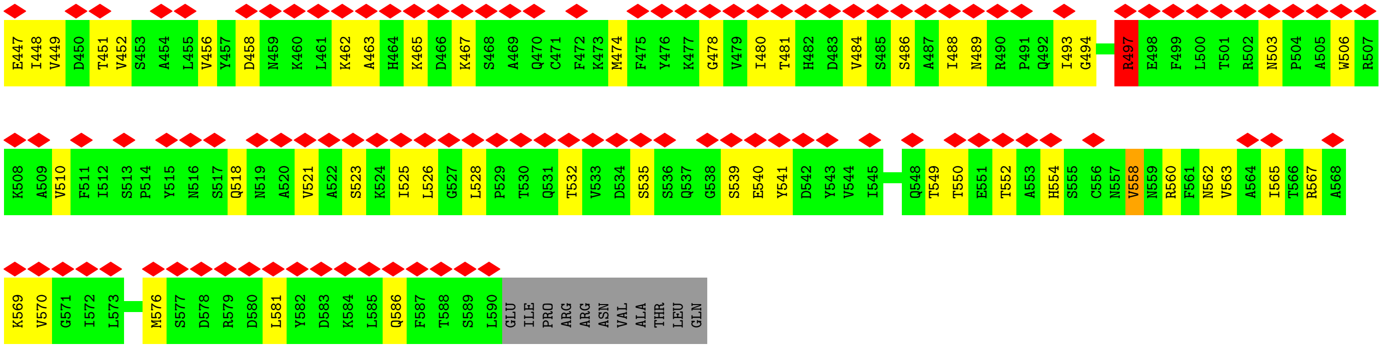
Chain I:

- Molecule 4: Helicase

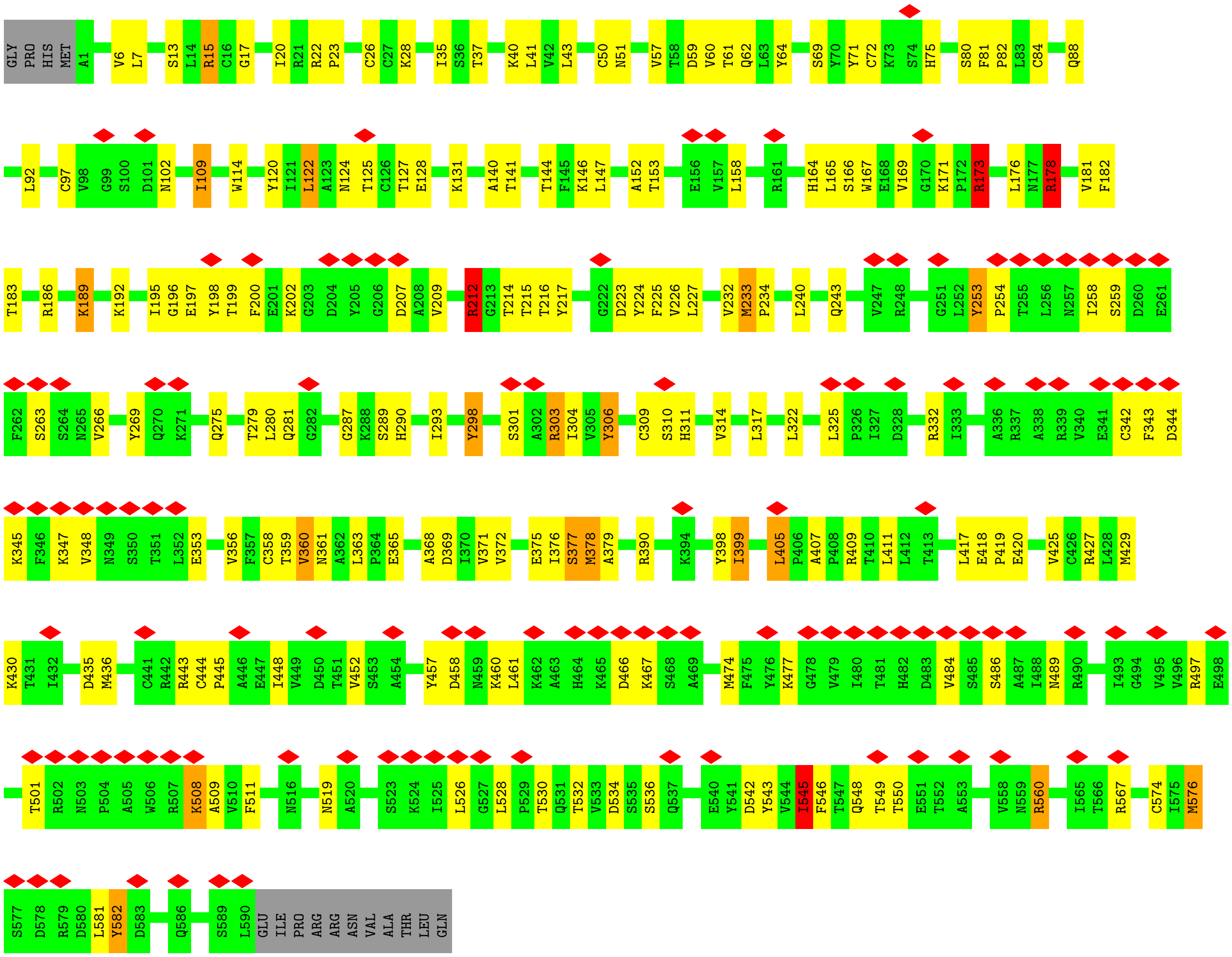
Chain E:






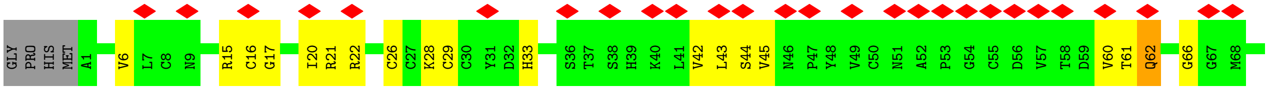
- Molecule 4: Helicase

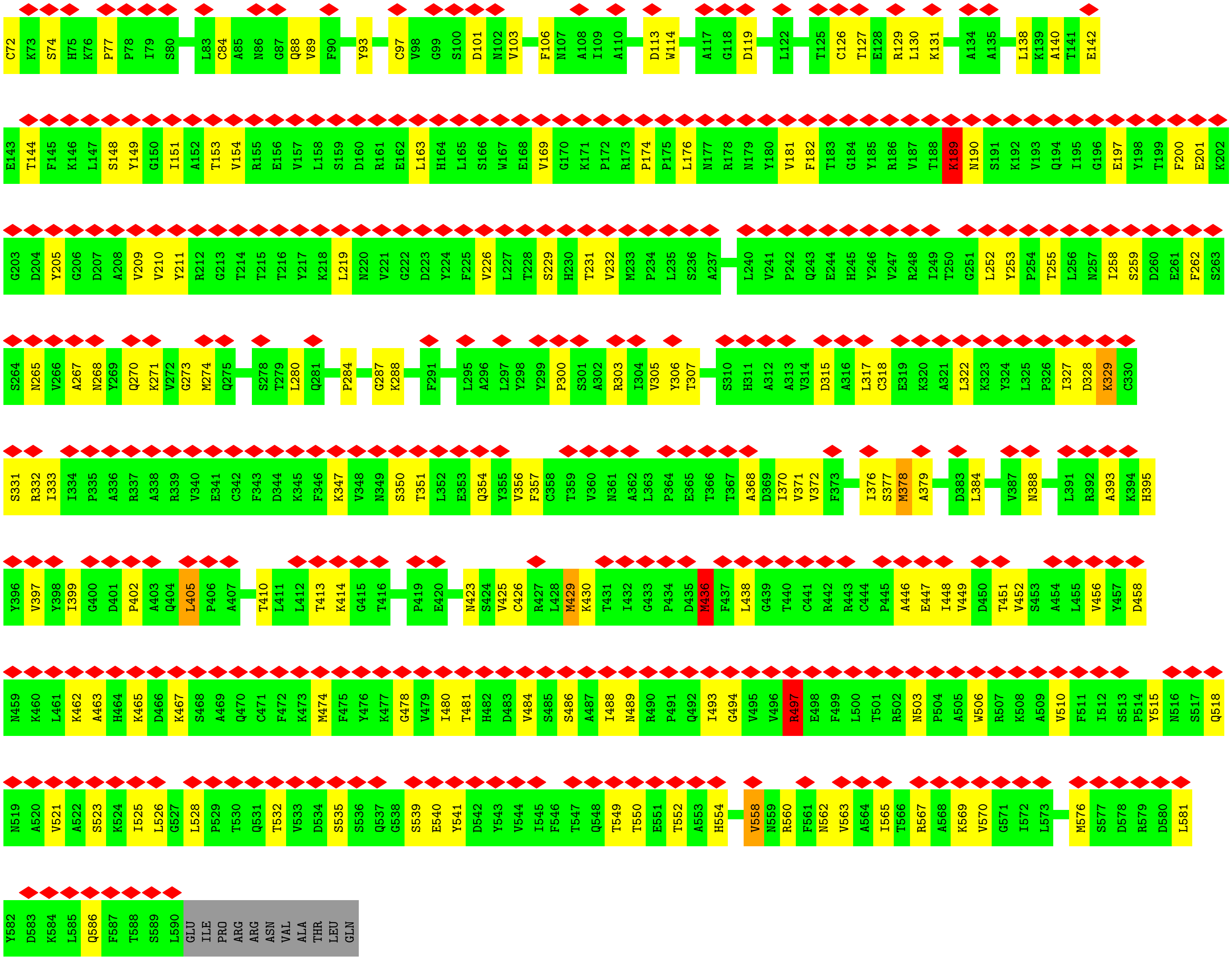
Chain F:



- Molecule 4: Helicase

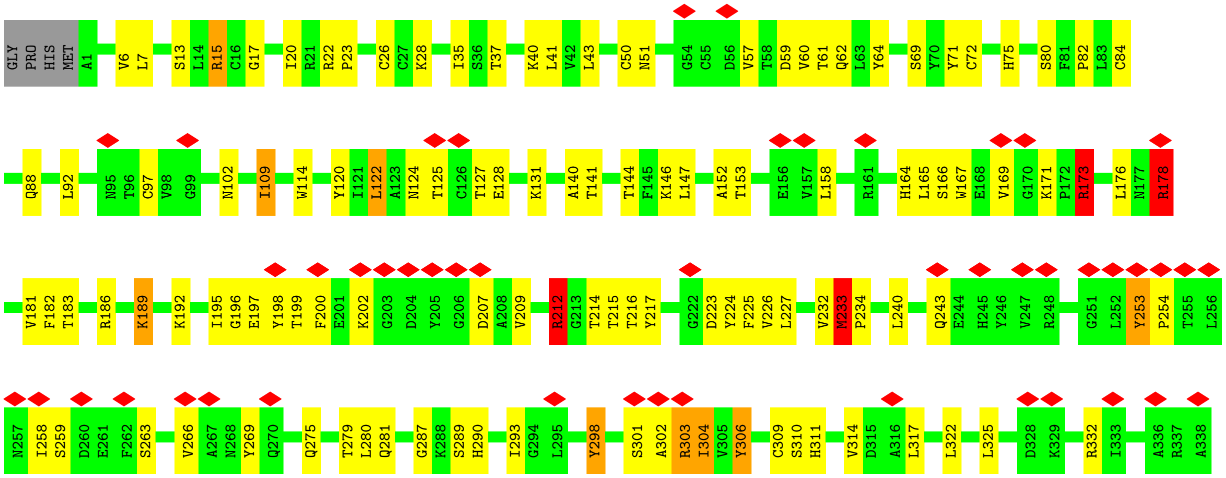
Chain K:

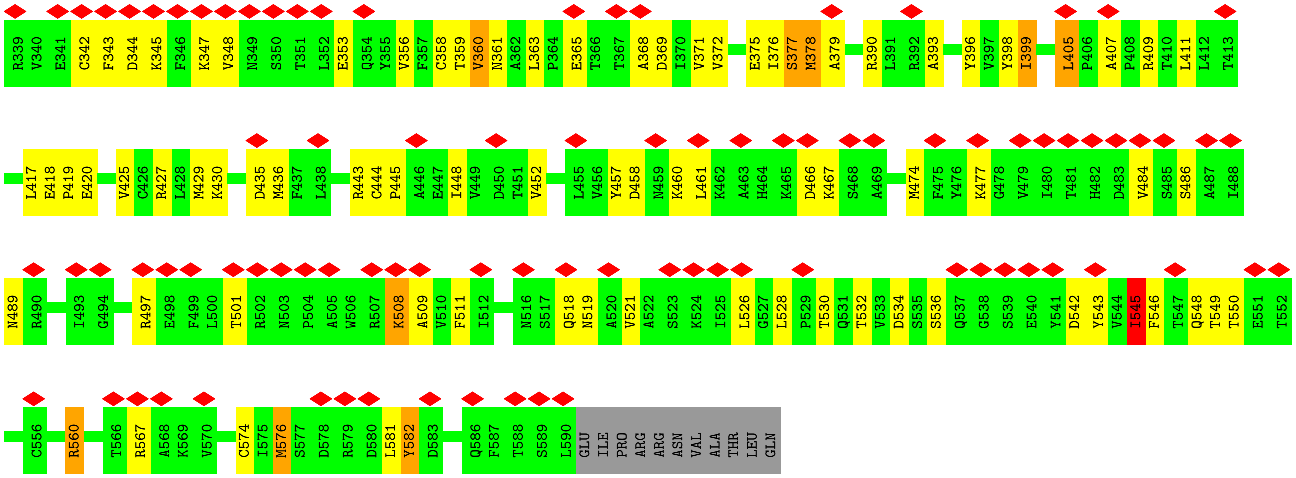




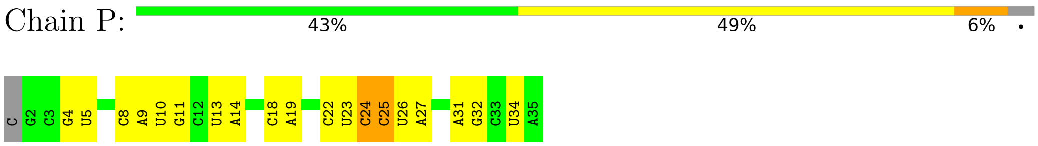
- Molecule 4: Helicase

Chain L:

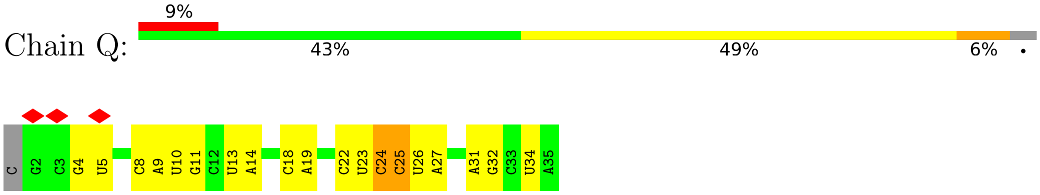




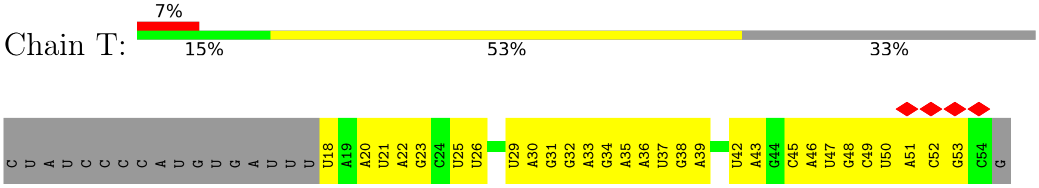
- Molecule 5: Product RNA



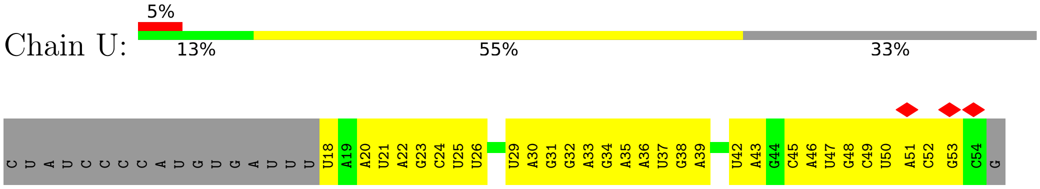
- Molecule 5: Product RNA



- Molecule 6: Template 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	35392	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 ($e^-/\text{Å}^2$)	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	2.600	Depositor
Minimum map value	-1.047	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, AF3, 1N7, ADP, 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	A	0.30	0/7659	0.57	8/10394 (0.1%)
1	G	0.30	0/7659	0.57	8/10394 (0.1%)
2	B	0.26	0/1427	0.50	0/1937
2	D	0.36	0/1434	0.85	5/1943 (0.3%)
2	H	0.26	0/1424	0.53	0/1933
2	J	0.37	0/1425	0.85	5/1932 (0.3%)
3	C	0.48	0/579	0.98	7/779 (0.9%)
3	I	0.48	0/579	0.98	7/779 (0.9%)
4	E	0.29	0/4605	0.61	7/6275 (0.1%)
4	F	0.31	0/4665	0.67	10/6351 (0.2%)
4	K	0.29	0/4605	0.61	7/6275 (0.1%)
4	L	0.31	0/4665	0.67	11/6351 (0.2%)
5	P	0.22	0/802	0.79	0/1246
5	Q	0.22	0/802	0.79	0/1246
6	T	0.23	0/882	0.80	0/1372
6	U	0.23	0/882	0.80	0/1372
All	All	0.30	0/44094	0.65	75/60579 (0.1%)

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	A	0	1
1	G	0	1
2	D	0	4
2	J	0	4
4	E	0	1
4	F	0	4
4	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	L	0	4
All	All	0	20

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	55	MET	CB-CG-SD	12.02	148.46	112.40
2	J	55	MET	CB-CG-SD	12.01	148.42	112.40
2	J	55	MET	CA-CB-CG	9.77	129.91	113.30
2	D	55	MET	CA-CB-CG	9.75	129.88	113.30
1	A	55	ARG	CG-CD-NE	8.20	129.02	111.80
1	G	55	ARG	CG-CD-NE	8.17	128.95	111.80
3	C	50	GLU	CA-CB-CG	7.87	130.72	113.40
3	I	50	GLU	CA-CB-CG	7.85	130.67	113.40
3	C	74	GLU	CA-CB-CG	7.81	130.59	113.40
3	I	74	GLU	CA-CB-CG	7.79	130.53	113.40
1	G	924	MET	CB-CG-SD	7.73	135.59	112.40
1	A	924	MET	CB-CG-SD	7.73	135.58	112.40
1	A	109	ASP	CB-CG-OD2	7.72	125.25	118.30
4	K	436	MET	CG-SD-CE	-7.67	87.94	100.20
1	G	109	ASP	CB-CG-OD2	7.66	125.19	118.30
4	E	436	MET	CG-SD-CE	-7.65	87.96	100.20
3	I	52	MET	CB-CG-SD	7.27	134.21	112.40
3	C	52	MET	CB-CG-SD	7.26	134.18	112.40
3	C	31	GLN	CA-CB-CG	7.08	128.97	113.40
3	I	31	GLN	CA-CB-CG	7.05	128.91	113.40
2	J	55	MET	CG-SD-CE	6.92	111.27	100.20
2	D	55	MET	CG-SD-CE	6.91	111.25	100.20
4	L	212	ARG	CG-CD-NE	6.68	125.83	111.80
4	F	212	ARG	CG-CD-NE	6.67	125.81	111.80
4	F	178	ARG	CB-CG-CD	6.66	128.91	111.60
4	L	178	ARG	CB-CG-CD	6.65	128.90	111.60
4	E	62	GLN	CA-CB-CG	6.44	127.56	113.40
4	K	62	GLN	CA-CB-CG	6.42	127.53	113.40
3	C	52	MET	CG-SD-CE	6.41	110.46	100.20
3	I	52	MET	CG-SD-CE	6.40	110.44	100.20
4	L	178	ARG	CG-CD-NE	-6.17	98.85	111.80
4	F	178	ARG	CG-CD-NE	-6.15	98.89	111.80
4	K	378	MET	CB-CG-SD	6.13	130.80	112.40
4	E	378	MET	CB-CG-SD	6.11	130.73	112.40
2	D	158	GLN	CA-CB-CG	6.05	126.72	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	158	GLN	CA-CB-CG	6.02	126.65	113.40
3	I	67	ASP	CB-CG-OD1	5.94	123.64	118.30
3	C	67	ASP	CB-CG-OD1	5.93	123.64	118.30
3	I	52	MET	CA-CB-CG	5.78	123.12	113.30
3	C	52	MET	CA-CB-CG	5.77	123.10	113.30
4	F	173	ARG	N-CA-CB	-5.70	100.35	110.60
4	L	173	ARG	N-CA-CB	-5.69	100.36	110.60
1	A	924	MET	CG-SD-CE	5.67	109.28	100.20
4	K	497	ARG	CG-CD-NE	5.67	123.72	111.80
1	G	924	MET	CG-SD-CE	5.67	109.27	100.20
4	E	497	ARG	CG-CD-NE	5.66	123.69	111.80
4	L	122	LEU	CA-CB-CG	5.66	128.31	115.30
4	F	122	LEU	CA-CB-CG	5.64	128.27	115.30
4	F	178	ARG	CD-NE-CZ	5.61	131.46	123.60
4	F	233	MET	CB-CG-SD	5.61	129.22	112.40
4	L	233	MET	CB-CG-SD	5.60	129.21	112.40
4	L	178	ARG	CD-NE-CZ	5.60	131.43	123.60
4	L	545	ILE	CG1-CB-CG2	-5.49	99.33	111.40
4	F	545	ILE	CG1-CB-CG2	-5.47	99.36	111.40
1	A	924	MET	CA-CB-CG	5.44	122.54	113.30
1	G	924	MET	CA-CB-CG	5.43	122.54	113.30
4	K	189	LYS	C-N-CA	5.41	135.23	121.70
4	E	189	LYS	C-N-CA	5.40	135.19	121.70
1	G	498	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	A	498	LEU	CB-CG-CD2	-5.34	101.91	111.00
1	G	55	ARG	CD-NE-CZ	5.23	130.92	123.60
2	D	77	GLU	CA-CB-CG	5.22	124.90	113.40
2	J	77	GLU	CA-CB-CG	5.22	124.89	113.40
4	L	233	MET	CA-CB-CG	5.21	122.16	113.30
1	A	55	ARG	CD-NE-CZ	5.21	130.89	123.60
4	F	233	MET	CA-CB-CG	5.20	122.14	113.30
4	E	497	ARG	CA-CB-CG	5.18	124.80	113.40
4	K	497	ARG	CA-CB-CG	5.18	124.80	113.40
4	F	560	ARG	CB-CG-CD	5.16	125.00	111.60
4	L	560	ARG	CB-CG-CD	5.14	124.97	111.60
4	K	378	MET	CG-SD-CE	5.12	108.39	100.20
4	E	378	MET	CG-SD-CE	5.11	108.38	100.20
1	A	718	LYS	CA-CB-CG	5.03	124.47	113.40
4	L	178	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	G	718	LYS	CA-CB-CG	5.01	124.43	113.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ARG	Sidechain
2	D	158	GLN	Peptide
2	D	168	GLN	Peptide
2	D	31	SER	Peptide
2	D	82	LYS	Peptide
4	E	189	LYS	Peptide
4	F	15	ARG	Sidechain
4	F	178	ARG	Sidechain
4	F	189	LYS	Peptide
4	F	581	LEU	Peptide
1	G	55	ARG	Sidechain
2	J	158	GLN	Peptide
2	J	168	GLN	Peptide
2	J	31	SER	Peptide
2	J	82	LYS	Peptide
4	K	189	LYS	Peptide
4	L	15	ARG	Sidechain
4	L	178	ARG	Sidechain
4	L	189	LYS	Peptide
4	L	581	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7470	0	7206	102	0
1	G	7470	0	7206	106	0
2	B	1408	0	1407	18	0
2	D	1415	0	1431	39	0
2	H	1405	0	1405	24	0
2	J	1406	0	1418	39	0
3	C	576	0	608	10	0
3	I	576	0	608	10	0
4	E	4507	0	4429	109	0
4	F	4563	0	4514	124	0
4	K	4507	0	4429	110	0
4	L	4563	0	4514	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	719	0	366	23	0
5	Q	719	0	366	23	0
6	T	789	0	398	33	0
6	U	789	0	398	34	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
7	G	2	0	0	0	0
7	K	3	0	0	0	0
7	L	3	0	0	0	0
8	A	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
9	A	27	0	12	1	0
9	E	27	0	12	0	0
9	F	27	0	12	3	0
9	G	27	0	12	1	0
9	K	27	0	12	1	0
9	L	27	0	12	3	0
10	E	4	0	0	0	0
10	F	4	0	0	1	0
10	K	4	0	0	0	0
10	L	4	0	0	1	0
11	E	36	0	52	1	0
11	K	36	0	52	1	0
All	All	43154	0	40879	892	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 11.

All (892) 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:L:253:TYR:HE2	4:L:301:SER:HG	1.20	0.89
4:L:50:CYS:SG	4:L:75:HIS:HE1	1.93	0.89
4:F:50:CYS:SG	4:F:75:HIS:HE1	1.93	0.88
4:F:253:TYR:HE2	4:F:301:SER:HG	1.24	0.86
4:E:494:GLY:HA2	4:E:497:ARG:HD2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:494:GLY:HA2	4:K:497:ARG:HD2	1.59	0.84
4:F:344:ASP:O	1:G:81:GLN:NE2	2.10	0.84
4:E:497:ARG:HH21	4:E:525:ILE:HD13	1.43	0.83
4:K:497:ARG:HH21	4:K:525:ILE:HD13	1.43	0.83
3:I:31:GLN:OE1	3:I:31:GLN:N	2.14	0.78
4:F:375:GLU:HG3	4:F:378:MET:HB2	1.67	0.77
3:C:31:GLN:OE1	3:C:31:GLN:N	2.14	0.77
4:L:375:GLU:HG3	4:L:378:MET:HB2	1.67	0.77
4:F:445:PRO:HB3	4:F:467:LYS:HA	1.65	0.77
4:L:445:PRO:HB3	4:L:467:LYS:HA	1.65	0.77
4:K:189:LYS:H	4:K:190:ASN:HB2	1.50	0.76
4:E:189:LYS:H	4:E:190:ASN:HB2	1.50	0.76
4:L:419:PRO:HB2	4:L:430:LYS:HD2	1.67	0.76
4:E:66:GLY:HA3	4:E:77:PRO:HG2	1.68	0.76
4:F:419:PRO:HB2	4:F:430:LYS:HD2	1.67	0.76
4:K:66:GLY:HA3	4:K:77:PRO:HG2	1.68	0.76
4:E:268:ASN:HA	4:E:436:MET:HE1	1.66	0.75
2:H:53:ALA:HB1	2:H:57:ARG:HH12	1.51	0.75
4:F:212:ARG:HH11	4:F:212:ARG:HG2	1.51	0.75
4:L:212:ARG:HG2	4:L:212:ARG:HH11	1.51	0.75
4:L:59:ASP:HB3	4:L:62:GLN:HE21	1.52	0.74
4:F:59:ASP:HB3	4:F:62:GLN:HE21	1.52	0.73
4:F:303:ARG:NH1	4:F:353:GLU:O	2.21	0.73
1:A:81:GLN:NE2	4:L:344:ASP:O	2.21	0.73
4:L:303:ARG:NH1	4:L:353:GLU:O	2.21	0.72
4:L:359:THR:HG22	4:L:361:ASN:H	1.53	0.72
4:F:359:THR:HG22	4:F:361:ASN:H	1.53	0.72
4:F:360:VAL:HA	4:F:363:LEU:HG	1.71	0.72
4:L:360:VAL:HA	4:L:363:LEU:HG	1.71	0.72
4:F:445:PRO:HD2	4:F:448:ILE:HD11	1.73	0.70
4:L:445:PRO:HD2	4:L:448:ILE:HD11	1.73	0.70
2:B:6:PHE:N	2:B:56:GLN:OE1	2.24	0.70
1:A:305:ARG:HH21	1:A:470:LEU:HB3	1.56	0.70
4:K:268:ASN:HA	4:K:436:MET:HE1	1.72	0.70
1:G:305:ARG:HH21	1:G:470:LEU:HB3	1.56	0.70
4:K:448:ILE:HD11	4:K:565:ILE:HB	1.74	0.70
4:E:448:ILE:HD11	4:E:565:ILE:HB	1.74	0.69
2:D:180:LEU:HD12	2:D:184:LEU:HD11	1.75	0.69
2:J:180:LEU:HD12	2:J:184:LEU:HD11	1.75	0.68
4:E:300:PRO:O	4:E:354:GLN:NE2	2.27	0.68
4:K:300:PRO:O	4:K:354:GLN:NE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASP:OD1	1:G:735:ARG:NH2	2.28	0.67
4:F:519:ASN:OD1	4:F:530:THR:OG1	2.13	0.67
4:F:212:ARG:NH1	4:F:212:ARG:O	2.27	0.67
4:L:212:ARG:O	4:L:212:ARG:NH1	2.27	0.67
1:A:291:ASP:OD1	1:A:735:ARG:NH2	2.28	0.67
4:L:519:ASN:OD1	4:L:530:THR:OG1	2.13	0.67
4:K:271:LYS:HD2	4:K:436:MET:HE3	1.77	0.66
4:K:488:ILE:HA	4:K:518:GLN:HB2	1.77	0.66
2:J:158:GLN:HE21	2:J:158:GLN:HA	1.61	0.66
2:D:158:GLN:HA	2:D:158:GLN:HE21	1.61	0.66
4:E:488:ILE:HA	4:E:518:GLN:HB2	1.76	0.66
1:A:516:TYR:OH	1:A:569:ARG:NH1	2.28	0.66
4:F:280:LEU:HB3	4:F:399:ILE:HG23	1.77	0.66
1:A:284:ASP:OD2	2:H:111:ARG:NH1	2.28	0.65
4:E:126:CYS:SG	4:E:127:THR:N	2.67	0.65
4:E:271:LYS:HD2	4:E:436:MET:HE3	1.77	0.65
1:G:715:ILE:HD12	1:G:775:LEU:HD21	1.78	0.65
4:L:280:LEU:HB3	4:L:399:ILE:HG23	1.77	0.65
1:A:715:ILE:HD12	1:A:775:LEU:HD21	1.78	0.65
1:G:516:TYR:OH	1:G:569:ARG:NH1	2.28	0.65
4:L:466:ASP:OD1	4:L:467:LYS:N	2.30	0.65
4:E:126:CYS:O	4:E:131:LYS:NZ	2.30	0.65
4:F:269:TYR:HD2	4:F:298:TYR:HD2	1.45	0.64
4:K:126:CYS:O	4:K:131:LYS:NZ	2.30	0.64
4:L:269:TYR:HD2	4:L:298:TYR:HD2	1.45	0.64
4:E:255:THR:HB	4:E:258:ILE:HG22	1.80	0.64
4:K:255:THR:HB	4:K:258:ILE:HG22	1.80	0.64
4:K:126:CYS:SG	4:K:127:THR:N	2.67	0.64
2:B:111:ARG:NH1	1:G:284:ASP:OD2	2.32	0.63
2:H:101:ASP:OD2	2:H:102:ALA:N	2.30	0.63
4:K:154:VAL:HG21	4:K:219:LEU:HD13	1.81	0.63
4:E:379:ALA:O	4:E:423:ASN:ND2	2.29	0.63
4:F:57:VAL:HG13	4:F:62:GLN:HE22	1.63	0.63
4:E:154:VAL:HG21	4:E:219:LEU:HD13	1.81	0.62
4:L:548:GLN:HB3	4:L:576:MET:HA	1.81	0.62
4:L:57:VAL:HG13	4:L:62:GLN:HE22	1.63	0.62
4:F:548:GLN:HB3	4:F:576:MET:HA	1.81	0.62
4:K:449:VAL:HG11	4:K:463:ALA:HB2	1.80	0.62
4:E:449:VAL:HG11	4:E:463:ALA:HB2	1.81	0.62
4:F:466:ASP:OD1	4:F:467:LYS:N	2.30	0.62
4:K:379:ALA:O	4:K:423:ASN:ND2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TYR:OH	1:A:664:SER:O	2.17	0.62
1:G:346:TYR:OH	1:G:664:SER:O	2.17	0.62
4:K:306:TYR:HD2	4:K:357:PHE:HE1	1.48	0.62
4:E:306:TYR:HD2	4:E:357:PHE:HE1	1.48	0.61
3:I:73:GLU:N	3:I:73:GLU:OE1	2.32	0.61
4:L:303:ARG:HG2	4:L:368:ALA:HA	1.81	0.61
4:F:303:ARG:HG2	4:F:368:ALA:HA	1.81	0.61
3:C:73:GLU:OE1	3:C:73:GLU:N	2.32	0.61
2:J:132:ILE:HG21	2:J:138:TYR:HB2	1.81	0.61
2:D:25:ALA:O	2:D:29:GLY:N	2.28	0.61
4:E:144:THR:HG22	4:E:229:SER:HA	1.83	0.61
4:F:311:HIS:HA	4:F:314:VAL:HG12	1.83	0.61
4:L:311:HIS:HA	4:L:314:VAL:HG12	1.83	0.61
4:L:546:PHE:HB3	4:L:574:CYS:HA	1.83	0.61
2:D:132:ILE:HG21	2:D:138:TYR:HB2	1.81	0.60
4:K:144:THR:HG22	4:K:229:SER:HA	1.83	0.60
4:F:546:PHE:HB3	4:F:574:CYS:HA	1.83	0.60
4:K:181:VAL:HG21	4:K:197:GLU:HG2	1.84	0.60
4:E:181:VAL:HG21	4:E:197:GLU:HG2	1.84	0.60
4:E:552:THR:HG23	4:E:554:HIS:H	1.65	0.60
4:K:552:THR:HG23	4:K:554:HIS:H	1.65	0.60
4:F:186:ARG:HG2	4:F:195:ILE:HD13	1.83	0.60
4:L:186:ARG:HG2	4:L:195:ILE:HD13	1.83	0.60
1:A:128:VAL:O	1:A:132:ARG:HB2	2.02	0.60
2:J:25:ALA:O	2:J:29:GLY:N	2.28	0.60
1:A:494:ILE:HD11	1:A:577:LYS:HE2	1.84	0.59
1:G:128:VAL:O	1:G:132:ARG:HB2	2.02	0.59
1:G:598:TRP:HA	1:G:601:MET:HE2	1.84	0.59
1:G:494:ILE:HD11	1:G:577:LYS:HE2	1.83	0.59
3:C:47:GLU:HA	3:C:50:GLU:OE2	2.03	0.59
3:I:47:GLU:HA	3:I:50:GLU:OE2	2.03	0.59
4:F:303:ARG:HB3	4:F:369:ASP:H	1.68	0.59
4:L:37:THR:O	4:L:40:LYS:NZ	2.34	0.59
4:F:37:THR:O	4:F:40:LYS:NZ	2.34	0.59
4:L:303:ARG:HB3	4:L:369:ASP:H	1.68	0.59
1:A:598:TRP:HA	1:A:601:MET:HE2	1.85	0.59
4:L:458:ASP:H	4:L:460:LYS:HE3	1.68	0.59
4:F:458:ASP:H	4:F:460:LYS:HE3	1.68	0.59
4:E:151:ILE:HA	4:E:226:VAL:HG22	1.85	0.59
4:K:151:ILE:HA	4:K:226:VAL:HG22	1.85	0.59
1:A:717:ASP:OD1	1:A:720:VAL:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:ARG:NH2	9:G:2003:ADP:O3B	2.31	0.59
1:A:340:PHE:CE1	2:B:95:LEU:HD11	2.37	0.58
4:E:15:ARG:HB2	4:E:43:LEU:HB2	1.85	0.58
4:K:15:ARG:HB2	4:K:43:LEU:HB2	1.85	0.58
4:L:158:LEU:HG	4:L:164:HIS:HD2	1.69	0.58
1:A:116:ARG:NH2	9:A:2003:ADP:O3B	2.31	0.58
4:F:158:LEU:HG	4:F:164:HIS:HD2	1.69	0.58
1:G:568:ASN:OD1	1:G:654:ARG:NH2	2.37	0.58
4:E:42:VAL:HB	4:E:60:VAL:HG21	1.85	0.58
6:T:52:C:H2’	6:T:53:G:C8	2.38	0.58
1:A:568:ASN:OD1	1:A:654:ARG:NH2	2.37	0.58
2:H:118:ASN:ND2	1:G:326:PHE:O	2.35	0.58
6:U:52:C:H2’	6:U:53:G:C8	2.38	0.58
4:K:42:VAL:HB	4:K:60:VAL:HG21	1.85	0.58
2:D:65:GLN:HA	2:D:65:GLN:OE1	2.02	0.58
1:G:628:ASN:HB3	1:G:663:LEU:HD21	1.85	0.58
1:A:628:ASN:HB3	1:A:663:LEU:HD21	1.85	0.57
1:G:572:HIS:HB3	1:G:576:LEU:HD13	1.86	0.57
2:J:65:GLN:OE1	2:J:65:GLN:HA	2.02	0.57
2:J:158:GLN:HB2	2:J:187:THR:HB	1.86	0.57
1:G:717:ASP:OD1	1:G:720:VAL:N	2.32	0.57
1:A:340:PHE:HE1	2:B:95:LEU:HD11	1.69	0.57
2:J:160:VAL:HA	2:J:167:VAL:HG22	1.85	0.57
2:D:158:GLN:HB2	2:D:187:THR:HB	1.86	0.57
1:A:572:HIS:HB3	1:A:576:LEU:HD13	1.86	0.57
4:F:181:VAL:HA	4:F:199:THR:HG22	1.85	0.57
4:L:181:VAL:HA	4:L:199:THR:HG22	1.85	0.57
4:L:200:PHE:HD2	4:L:209:VAL:HG11	1.69	0.57
1:G:408:GLN:NE2	6:U:18:U:O2	2.38	0.57
4:F:200:PHE:HD2	4:F:209:VAL:HG11	1.69	0.57
2:D:160:VAL:HA	2:D:167:VAL:HG22	1.85	0.57
1:A:462:THR:HB	1:A:627:PRO:HB3	1.87	0.57
4:L:178:ARG:O	4:L:199:THR:HG21	2.04	0.57
1:A:408:GLN:NE2	6:T:18:U:O2	2.38	0.56
1:G:462:THR:HB	1:G:627:PRO:HB3	1.87	0.56
4:K:539:SER:HB2	4:K:541:TYR:HE2	1.70	0.56
4:E:539:SER:HB2	4:E:541:TYR:HE2	1.70	0.56
4:F:178:ARG:O	4:F:199:THR:HG21	2.04	0.56
1:A:333:ILE:HG22	1:A:361:LEU:HD23	1.88	0.56
4:F:124:ASN:HA	4:F:131:LYS:HE2	1.88	0.56
4:L:124:ASN:HA	4:L:131:LYS:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:52:C:H2'	6:U:53:G:H8	1.70	0.56
4:E:305:VAL:HG23	4:E:356:VAL:HB	1.88	0.56
1:G:333:ILE:HG22	1:G:361:LEU:HD23	1.88	0.56
4:K:305:VAL:HG23	4:K:356:VAL:HB	1.88	0.56
6:T:52:C:H2'	6:T:53:G:H8	1.70	0.56
2:J:171:GLU:HB2	2:J:176:ASN:ND2	2.20	0.56
2:D:171:GLU:HB2	2:D:176:ASN:ND2	2.20	0.56
1:A:239:SER:OG	1:A:465:ASP:OD1	2.20	0.56
1:A:495:VAL:HG21	1:A:498:LEU:HD21	1.87	0.55
4:L:293:ILE:HD12	4:L:325:LEU:HG	1.89	0.55
1:A:819:LEU:HD11	1:A:826:TYR:HB3	1.88	0.55
1:G:495:VAL:HG21	1:G:498:LEU:HD21	1.87	0.55
1:G:819:LEU:HD11	1:G:826:TYR:HB3	1.88	0.55
4:E:376:ILE:HG21	4:E:425:VAL:HB	1.87	0.55
4:F:293:ILE:HD12	4:F:325:LEU:HG	1.88	0.55
6:T:50:U:H2'	6:T:51:A:H8	1.71	0.55
4:L:178:ARG:O	4:L:178:ARG:HG2	2.04	0.55
6:U:50:U:H2'	6:U:51:A:H8	1.71	0.55
1:A:726:ARG:HA	1:A:729:GLU:HG2	1.89	0.55
1:G:239:SER:OG	1:G:465:ASP:OD1	2.20	0.55
4:K:376:ILE:HG21	4:K:425:VAL:HB	1.87	0.55
4:K:518:GLN:HA	4:K:521:VAL:HG22	1.89	0.55
4:L:125:THR:HG22	4:L:427:ARG:HH22	1.72	0.55
4:E:518:GLN:HA	4:E:521:VAL:HG22	1.89	0.55
1:G:726:ARG:HA	1:G:729:GLU:HG2	1.89	0.55
4:F:178:ARG:O	4:F:178:ARG:HG2	2.04	0.55
4:F:240:LEU:HD21	4:F:425:VAL:HG22	1.89	0.55
4:F:489:ASN:HB2	4:F:549:THR:HG23	1.89	0.55
5:P:18:C:H2'	5:P:19:A:H8	1.72	0.55
4:L:489:ASN:HB2	4:L:549:THR:HG23	1.89	0.55
1:A:358:ASP:HB2	1:A:534:ASN:HD21	1.72	0.55
4:L:240:LEU:HD21	4:L:425:VAL:HG22	1.89	0.55
5:Q:18:C:H2'	5:Q:19:A:H8	1.72	0.55
4:E:61:THR:HA	4:E:84:CYS:HB2	1.89	0.55
4:E:270:GLN:O	4:E:273:GLY:N	2.39	0.55
4:F:125:THR:HG22	4:F:427:ARG:HH22	1.72	0.55
2:H:53:ALA:HB1	2:H:57:ARG:NH1	2.22	0.55
4:L:28:LYS:HE3	4:L:88:GLN:HE21	1.70	0.55
1:A:676:LYS:NZ	1:A:679:GLY:O	2.35	0.55
2:D:56:GLN:NE2	2:D:60:GLU:OE2	2.40	0.55
4:F:363:LEU:O	4:F:390:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:358:ASP:HB2	1:G:534:ASN:HD21	1.72	0.55
4:L:363:LEU:O	4:L:390:ARG:NH1	2.40	0.55
4:F:7:LEU:HD12	4:F:102:ASN:HB2	1.89	0.54
2:J:56:GLN:NE2	2:J:60:GLU:OE2	2.40	0.54
4:K:61:THR:HA	4:K:84:CYS:HB2	1.89	0.54
4:K:270:GLN:O	4:K:273:GLY:N	2.39	0.54
4:L:7:LEU:HD12	4:L:102:ASN:HB2	1.89	0.54
6:T:29:U:H2'	6:T:30:A:H8	1.72	0.54
1:G:676:LYS:NZ	1:G:679:GLY:O	2.35	0.54
4:F:28:LYS:HE3	4:F:88:GLN:HE21	1.70	0.54
6:U:29:U:H2'	6:U:30:A:H8	1.72	0.54
4:E:449:VAL:HA	4:E:452:VAL:HG12	1.89	0.54
4:F:233:MET:SD	4:F:234:PRO:HD2	2.47	0.54
4:L:233:MET:SD	4:L:234:PRO:HD2	2.47	0.54
1:A:326:PHE:O	2:B:118:ASN:ND2	2.41	0.54
2:B:21:ALA:HB1	2:B:38:LEU:HD11	1.90	0.54
4:E:493:ILE:HD11	4:E:518:GLN:HG3	1.90	0.54
4:F:281:GLN:HE22	4:F:457:TYR:HE2	1.55	0.54
4:K:26:CYS:HB3	4:K:29:CYS:HB2	1.89	0.54
4:K:493:ILE:HD11	4:K:518:GLN:HG3	1.90	0.54
4:L:141:THR:HA	4:L:144:THR:HG22	1.90	0.54
4:E:26:CYS:HB3	4:E:29:CYS:HB2	1.89	0.54
4:L:178:ARG:NH2	4:L:310:SER:OG	2.41	0.54
4:F:178:ARG:NH2	4:F:310:SER:OG	2.41	0.53
4:K:449:VAL:HA	4:K:452:VAL:HG12	1.89	0.53
4:L:281:GLN:HE22	4:L:457:TYR:HE2	1.55	0.53
4:F:141:THR:HA	4:F:144:THR:HG22	1.90	0.53
1:A:437:LEU:HD13	1:A:843:PHE:HE2	1.73	0.53
2:B:139:LYS:NZ	2:B:143:ASP:OD2	2.39	0.53
1:G:75:HIS:CG	1:G:76:THR:H	2.27	0.53
1:A:75:HIS:CG	1:A:76:THR:H	2.27	0.53
2:H:95:LEU:HD11	1:G:340:PHE:CE1	2.44	0.53
4:E:532:THR:HG23	4:E:535:SER:H	1.73	0.53
1:G:531:THR:HG21	1:G:567:THR:HG21	1.90	0.53
4:K:497:ARG:NH2	4:K:525:ILE:HD13	2.18	0.53
4:K:532:THR:HG23	4:K:535:SER:H	1.73	0.53
1:A:531:THR:HG21	1:A:567:THR:HG21	1.90	0.53
1:A:858:ARG:NH1	5:P:32:G:OP1	2.42	0.53
4:F:509:ALA:HB3	4:F:528:LEU:HD13	1.91	0.53
4:E:497:ARG:NH2	4:E:525:ILE:HD13	2.18	0.53
4:K:189:LYS:N	4:K:190:ASN:HB2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:17:GLY:HA2	4:L:22:ARG:HD3	1.91	0.53
4:L:509:ALA:HB3	4:L:528:LEU:HD13	1.91	0.53
4:E:280:LEU:HB3	4:E:399:ILE:HG22	1.91	0.53
1:G:437:LEU:HD13	1:G:843:PHE:HE2	1.73	0.53
1:G:858:ARG:NH1	5:Q:32:G:OP1	2.42	0.53
4:L:146:LYS:HG3	4:L:227:LEU:HD23	1.91	0.53
4:F:146:LYS:HG3	4:F:227:LEU:HD23	1.91	0.53
4:E:189:LYS:N	4:E:190:ASN:HB2	2.21	0.52
4:K:280:LEU:HB3	4:K:399:ILE:HG22	1.91	0.52
4:F:17:GLY:HA2	4:F:22:ARG:HD3	1.91	0.52
2:J:77:GLU:HA	2:J:80:ARG:HB2	1.91	0.52
1:A:691:ASN:HB3	1:A:759:SER:O	2.09	0.52
1:A:834:PRO:HG2	1:A:877:TYR:CD1	2.44	0.52
4:F:164:HIS:ND1	4:F:207:ASP:O	2.40	0.52
4:F:279:THR:H	4:F:435:ASP:HB2	1.74	0.52
4:L:279:THR:H	4:L:435:ASP:HB2	1.74	0.52
2:D:77:GLU:HA	2:D:80:ARG:HB2	1.91	0.52
4:F:309:CYS:HA	4:F:360:VAL:HG13	1.90	0.52
4:E:480:ILE:HD13	4:E:550:THR:HG22	1.92	0.52
4:F:17:GLY:N	4:F:41:LEU:O	2.40	0.52
4:F:197:GLU:O	4:F:212:ARG:NH2	2.26	0.52
1:G:105:ARG:NH1	1:G:108:GLY:O	2.43	0.52
4:K:480:ILE:HD13	4:K:550:THR:HG22	1.92	0.52
4:L:314:VAL:HA	4:L:317:LEU:HG	1.92	0.52
1:A:105:ARG:NH1	1:A:108:GLY:O	2.43	0.52
5:P:26:U:H2’	5:P:27:A:H8	1.75	0.52
1:G:691:ASN:HB3	1:G:759:SER:O	2.09	0.52
1:G:834:PRO:HG2	1:G:877:TYR:CD1	2.44	0.52
4:L:309:CYS:HA	4:L:360:VAL:HG13	1.90	0.52
5:Q:26:U:H2’	5:Q:27:A:H8	1.75	0.52
4:E:103:VAL:HA	4:E:106:PHE:HB3	1.91	0.52
4:L:167:TRP:CD2	4:L:173:ARG:HG2	2.44	0.52
4:F:183:THR:N	4:F:226:VAL:O	2.35	0.52
4:F:314:VAL:HA	4:F:317:LEU:HG	1.92	0.52
3:I:60:LEU:HD11	2:J:106:ILE:HG23	1.92	0.52
4:L:164:HIS:ND1	4:L:207:ASP:O	2.40	0.52
3:C:46:THR:O	3:C:49:PHE:N	2.43	0.51
5:P:8:C:H2’	5:P:9:A:H8	1.75	0.51
5:Q:8:C:H2’	5:Q:9:A:H8	1.75	0.51
1:G:892:HIS:NE2	1:G:910:ASP:OD2	2.42	0.51
3:I:46:THR:O	3:I:49:PHE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:103:VAL:HA	4:K:106:PHE:HB3	1.91	0.51
1:A:892:HIS:NE2	1:A:910:ASP:OD2	2.42	0.51
3:C:60:LEU:HD11	2:D:106:ILE:HG23	1.92	0.51
4:K:447:GLU:O	4:K:451:THR:HG23	2.11	0.51
4:E:331:SER:HB3	4:E:356:VAL:HA	1.91	0.51
4:E:447:GLU:O	4:E:451:THR:HG23	2.11	0.51
4:F:167:TRP:CD2	4:F:173:ARG:HG2	2.44	0.51
4:F:176:LEU:HD13	4:F:200:PHE:HB2	1.92	0.51
4:K:331:SER:HB3	4:K:356:VAL:HA	1.91	0.51
4:L:17:GLY:N	4:L:41:LEU:O	2.40	0.51
6:T:42:U:H2'	6:T:43:A:H8	1.75	0.51
1:G:468:GLN:HA	1:G:731:LEU:HD22	1.91	0.51
4:L:376:ILE:HD11	4:L:398:TYR:HB3	1.92	0.51
6:U:42:U:H2'	6:U:43:A:H8	1.75	0.51
6:T:34:G:H2'	6:T:35:A:H8	1.75	0.51
4:L:183:THR:N	4:L:226:VAL:O	2.35	0.51
4:F:376:ILE:HD11	4:F:398:TYR:HB3	1.92	0.51
4:K:328:ASP:OD1	4:K:329:LYS:N	2.43	0.51
4:L:197:GLU:O	4:L:212:ARG:NH2	2.26	0.51
6:U:25:U:H2'	6:U:26:U:H6	1.76	0.51
6:U:34:G:H2'	6:U:35:A:H8	1.75	0.51
1:A:267:LYS:HE2	1:A:267:LYS:HA	1.92	0.51
1:A:468:GLN:HA	1:A:731:LEU:HD22	1.91	0.51
4:L:72:CYS:H	4:L:75:HIS:CE1	2.29	0.51
4:L:176:LEU:HD13	4:L:200:PHE:HB2	1.92	0.51
6:U:29:U:H2'	6:U:30:A:C8	2.45	0.51
4:E:306:TYR:CD2	4:E:357:PHE:HE1	2.28	0.51
4:F:72:CYS:H	4:F:75:HIS:CE1	2.29	0.51
6:T:25:U:H2'	6:T:26:U:H6	1.76	0.51
2:J:138:TYR:CD1	2:J:142:CYS:HB2	2.45	0.51
4:L:254:PRO:HB3	4:L:298:TYR:HE1	1.76	0.51
2:D:65:GLN:HE21	6:T:29:U:H4'	1.76	0.50
2:D:138:TYR:CD1	2:D:142:CYS:HB2	2.45	0.50
6:T:29:U:H2'	6:T:30:A:C8	2.45	0.50
6:U:50:U:H2'	6:U:51:A:C8	2.46	0.50
2:D:120:ILE:HA	2:D:128:LEU:HD13	1.94	0.50
2:J:65:GLN:HE21	6:U:29:U:H4'	1.76	0.50
2:J:120:ILE:HA	2:J:128:LEU:HD13	1.94	0.50
1:A:875:GLN:NE2	1:A:879:ASP:OD1	2.44	0.50
4:F:254:PRO:HB3	4:F:298:TYR:HE1	1.76	0.50
1:G:915:TYR:O	1:G:921:TYR:OH	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:VAL:HG11	4:L:23:PRO:HB2	1.93	0.50
4:E:328:ASP:OD1	4:E:329:LYS:N	2.43	0.50
4:F:6:VAL:HG11	4:F:23:PRO:HB2	1.93	0.50
1:G:267:LYS:HE2	1:G:267:LYS:HA	1.92	0.50
4:L:152:ALA:O	4:L:225:PHE:N	2.45	0.50
4:K:306:TYR:CD2	4:K:357:PHE:HE1	2.28	0.50
4:K:402:PRO:HG2	4:K:430:LYS:HE3	1.93	0.50
4:L:377:SER:O	4:L:407:ALA:N	2.44	0.50
4:F:420:GLU:HB2	4:F:427:ARG:HG3	1.94	0.50
4:F:152:ALA:O	4:F:225:PHE:N	2.45	0.50
4:F:443:ARG:HH12	4:F:567:ARG:HH21	1.60	0.50
4:L:114:TRP:HB2	4:L:411:LEU:HD23	1.94	0.50
4:L:420:GLU:HB2	4:L:427:ARG:HG3	1.94	0.50
4:L:443:ARG:HH12	4:L:567:ARG:HH21	1.60	0.50
4:E:402:PRO:HG2	4:E:430:LYS:HE3	1.93	0.50
4:F:377:SER:O	4:F:407:ALA:N	2.44	0.50
5:P:18:C:H2'	5:P:19:A:C8	2.46	0.50
4:K:347:LYS:HG2	4:K:350:SER:HB2	1.93	0.50
4:E:446:ALA:HB3	4:E:467:LYS:HG2	1.92	0.50
4:F:186:ARG:NH1	4:F:223:ASP:OD2	2.43	0.50
2:H:47:SER:O	2:H:51:ARG:HG2	2.12	0.50
6:T:35:A:H2'	6:T:36:A:H8	1.77	0.50
1:G:614:LEU:HB2	1:G:802:GLU:HB3	1.93	0.50
6:U:35:A:H2'	6:U:36:A:H8	1.77	0.50
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.47	0.49
1:G:875:GLN:NE2	1:G:879:ASP:OD1	2.43	0.49
5:Q:18:C:H2'	5:Q:19:A:C8	2.46	0.49
1:A:847:ILE:HG22	2:D:79:LYS:HG3	1.93	0.49
1:A:851:ASP:OD2	2:D:75:ARG:NH2	2.40	0.49
4:F:114:TRP:HB2	4:F:411:LEU:HD23	1.94	0.49
6:T:50:U:H2'	6:T:51:A:C8	2.46	0.49
1:G:847:ILE:HG22	2:J:79:LYS:HG3	1.93	0.49
4:K:446:ALA:HB3	4:K:467:LYS:HG2	1.92	0.49
1:A:614:LEU:HB2	1:A:802:GLU:HB3	1.93	0.49
1:A:915:TYR:O	1:A:921:TYR:OH	2.24	0.49
2:H:88:GLN:HG2	1:G:371:LEU:HD11	1.94	0.49
6:T:47:U:H2'	6:T:48:G:H8	1.77	0.49
3:I:14:LEU:HD22	3:I:36:HIS:CG	2.47	0.49
5:Q:24:C:H2'	5:Q:25:C:H6	1.76	0.49
6:U:47:U:H2'	6:U:48:G:H8	1.77	0.49
1:A:576:LEU:HD21	1:A:686:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:347:LYS:HG2	4:E:350:SER:HB2	1.93	0.49
2:D:142:CYS:HG	2:D:147:PHE:HD1	1.59	0.49
4:F:199:THR:HG23	4:F:212:ARG:HE	1.78	0.49
1:G:576:LEU:HD21	1:G:686:THR:HG22	1.94	0.49
1:G:851:ASP:OD2	2:J:75:ARG:NH2	2.39	0.49
4:L:186:ARG:NH1	4:L:223:ASP:OD2	2.43	0.49
4:E:451:THR:HG22	4:E:586:GLN:H	1.78	0.49
5:P:24:C:H2'	5:P:25:C:H6	1.76	0.49
4:K:140:ALA:O	4:K:144:THR:HG23	2.13	0.49
4:K:451:THR:HG22	4:K:586:GLN:H	1.78	0.49
4:E:140:ALA:O	4:E:144:THR:HG23	2.13	0.49
2:J:54:ALA:O	2:J:57:ARG:HB2	2.13	0.49
4:L:199:THR:HG23	4:L:212:ARG:HE	1.78	0.49
4:L:243:GLN:NE2	4:L:275:GLN:OE1	2.39	0.49
4:E:558:VAL:HG13	4:E:581:LEU:HD21	1.95	0.49
4:F:345:LYS:HD3	1:G:77:PHE:HZ	1.78	0.49
1:G:378:PRO:HD2	1:G:537:PRO:HB2	1.94	0.49
4:K:510:VAL:HG11	4:K:541:TYR:HE1	1.78	0.49
1:A:378:PRO:HD2	1:A:537:PRO:HB2	1.94	0.48
4:E:510:VAL:HG11	4:E:541:TYR:HE1	1.78	0.48
2:D:54:ALA:O	2:D:57:ARG:HB2	2.13	0.48
4:K:558:VAL:HG13	4:K:581:LEU:HD21	1.95	0.48
4:E:456:VAL:HG21	4:E:562:ASN:ND2	2.28	0.48
4:K:306:TYR:HB3	4:K:317:LEU:HD21	1.95	0.48
4:L:508:LYS:HZ1	4:L:542:ASP:H	1.62	0.48
4:E:306:TYR:HB3	4:E:317:LEU:HD21	1.95	0.48
1:A:531:THR:O	1:A:657:ASN:ND2	2.46	0.48
4:E:465:LYS:NZ	4:E:569:LYS:O	2.47	0.48
4:K:465:LYS:NZ	4:K:569:LYS:O	2.47	0.48
4:F:322:LEU:HD11	4:F:343:PHE:CZ	2.49	0.48
4:K:456:VAL:HG21	4:K:562:ASN:ND2	2.28	0.48
4:L:322:LEU:HD11	4:L:343:PHE:CZ	2.49	0.48
4:F:532:THR:HG23	4:F:534:ASP:H	1.78	0.48
1:G:836:ARG:NH2	5:Q:34:U:OP2	2.47	0.48
1:G:531:THR:O	1:G:657:ASN:ND2	2.46	0.48
4:K:119:ASP:N	4:K:119:ASP:OD1	2.46	0.48
4:K:489:ASN:HB2	4:K:549:THR:HG23	1.96	0.48
4:L:532:THR:HG23	4:L:534:ASP:H	1.77	0.48
4:E:489:ASN:HB2	4:E:549:THR:HG23	1.96	0.47
4:F:444:CYS:HB3	4:F:448:ILE:HG13	1.95	0.47
1:G:726:ARG:NH2	1:G:744:GLU:OE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:305:VAL:HG12	4:K:371:VAL:HG12	1.96	0.47
1:A:34:ALA:HA	1:A:47:LYS:HA	1.96	0.47
1:A:382:ALA:HB3	2:B:117:LEU:HD11	1.95	0.47
1:A:836:ARG:NH2	5:P:34:U:OP2	2.47	0.47
4:L:444:CYS:HB3	4:L:448:ILE:HG13	1.95	0.47
2:D:138:TYR:CE2	2:D:172:ILE:HG21	2.49	0.47
4:E:268:ASN:HA	4:E:436:MET:CE	2.42	0.47
4:E:405:LEU:HD21	4:E:560:ARG:HA	1.97	0.47
2:J:158:GLN:HB2	2:J:187:THR:CB	2.45	0.47
4:K:268:ASN:HA	4:K:436:MET:CE	2.42	0.47
4:K:372:VAL:HA	4:K:397:VAL:HB	1.95	0.47
4:L:61:THR:HA	4:L:84:CYS:HB3	1.96	0.47
5:Q:13:U:H2'	5:Q:14:A:H8	1.78	0.47
2:D:158:GLN:HB2	2:D:187:THR:CB	2.45	0.47
4:E:119:ASP:OD1	4:E:119:ASP:N	2.46	0.47
4:E:305:VAL:HG12	4:E:371:VAL:HG12	1.96	0.47
5:P:13:U:H2'	5:P:14:A:H8	1.78	0.47
1:G:116:ARG:HG2	1:G:217:TYR:HB2	1.96	0.47
4:K:405:LEU:HD21	4:K:560:ARG:HA	1.97	0.47
4:F:61:THR:HA	4:F:84:CYS:HB3	1.96	0.47
4:F:243:GLN:NE2	4:F:275:GLN:OE1	2.39	0.47
2:H:117:LEU:HD11	1:G:382:ALA:HB3	1.97	0.47
2:J:138:TYR:CE2	2:J:172:ILE:HG21	2.49	0.47
4:K:113:ASP:OD1	4:K:113:ASP:N	2.42	0.47
4:K:267:ALA:HA	4:K:270:GLN:OE1	2.14	0.47
4:K:322:LEU:HD12	4:K:327:ILE:HD12	1.96	0.47
4:L:64:TYR:CE2	4:L:82:PRO:HG3	2.50	0.47
1:A:739:THR:O	1:A:743:ASN:ND2	2.47	0.47
4:E:113:ASP:OD1	4:E:113:ASP:N	2.42	0.47
4:E:322:LEU:HD12	4:E:327:ILE:HD12	1.95	0.47
1:A:116:ARG:HG2	1:A:217:TYR:HB2	1.96	0.47
1:A:330:VAL:HG11	2:B:117:LEU:HD13	1.95	0.47
1:A:726:ARG:NH2	1:A:744:GLU:OE2	2.41	0.47
2:D:134:ASP:OD1	2:D:135:TYR:N	2.48	0.47
2:D:172:ILE:HG13	2:D:180:LEU:HD11	1.96	0.47
4:E:267:ALA:HA	4:E:270:GLN:OE1	2.14	0.47
4:E:372:VAL:HA	4:E:397:VAL:HB	1.95	0.47
4:F:64:TYR:CE2	4:F:82:PRO:HG3	2.50	0.47
4:F:332:ARG:NH1	4:F:342:CYS:SG	2.87	0.47
4:F:508:LYS:HZ1	4:F:542:ASP:H	1.63	0.47
2:H:171:GLU:HG2	2:H:180:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:25:C:H2'	5:P:26:U:H6	1.80	0.47
1:G:34:ALA:HA	1:G:47:LYS:HA	1.97	0.47
1:G:545:LYS:HB2	1:G:555:ARG:HG2	1.95	0.47
1:G:739:THR:O	1:G:743:ASN:ND2	2.47	0.47
2:J:134:ASP:OD1	2:J:135:TYR:N	2.48	0.47
4:L:332:ARG:NH1	4:L:342:CYS:SG	2.87	0.47
4:L:511:PHE:HB3	4:L:530:THR:HA	1.96	0.47
5:Q:25:C:H2'	5:Q:26:U:H6	1.80	0.47
1:A:545:LYS:HB2	1:A:555:ARG:HG2	1.95	0.47
4:E:368:ALA:HB3	4:E:393:ALA:HB2	1.95	0.47
4:F:511:PHE:HB3	4:F:530:THR:HA	1.96	0.47
2:J:172:ILE:HG13	2:J:180:LEU:HD11	1.96	0.47
4:K:284:PRO:HB2	4:K:567:ARG:HH22	1.79	0.47
1:A:695:ASN:HD22	1:A:757:ILE:HG23	1.80	0.47
2:H:117:LEU:HD13	1:G:330:VAL:HG11	1.96	0.47
1:G:100:ASP:HB3	1:G:115:SER:HB3	1.96	0.47
4:K:368:ALA:HB3	4:K:393:ALA:HB2	1.95	0.47
1:A:100:ASP:HB3	1:A:115:SER:HB3	1.96	0.47
4:F:376:ILE:O	4:F:379:ALA:N	2.47	0.47
2:H:95:LEU:HD11	1:G:340:PHE:HE1	1.80	0.47
1:G:200:GLY:HA3	1:G:227:PRO:HA	1.97	0.47
4:L:376:ILE:O	4:L:379:ALA:N	2.47	0.47
1:A:200:GLY:HA3	1:A:227:PRO:HA	1.98	0.46
2:D:103:LEU:O	2:D:107:ILE:HG12	2.15	0.46
4:E:6:VAL:O	4:E:129:ARG:HG2	2.15	0.46
4:E:252:LEU:HD22	4:E:370:ILE:HD11	1.97	0.46
4:E:284:PRO:HB2	4:E:567:ARG:HH22	1.79	0.46
4:E:413:THR:HG23	4:E:414:LYS:HG3	1.97	0.46
1:G:695:ASN:HD22	1:G:757:ILE:HG23	1.80	0.46
4:F:266:VAL:HG13	4:F:298:TYR:HE2	1.80	0.46
2:J:103:LEU:O	2:J:107:ILE:HG12	2.15	0.46
2:J:147:PHE:N	2:J:154:TRP:O	2.48	0.46
4:K:413:THR:HG23	4:K:414:LYS:HG3	1.97	0.46
6:U:35:A:H2'	6:U:36:A:C8	2.50	0.46
2:D:147:PHE:N	2:D:154:TRP:O	2.48	0.46
6:T:35:A:H2'	6:T:36:A:C8	2.51	0.46
4:K:252:LEU:HD22	4:K:370:ILE:HD11	1.97	0.46
4:L:197:GLU:O	4:L:214:THR:OG1	2.33	0.46
4:E:510:VAL:HG11	4:E:541:TYR:CE1	2.50	0.46
4:K:6:VAL:O	4:K:129:ARG:HG2	2.15	0.46
4:K:510:VAL:HG11	4:K:541:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:192:LYS:HD2	4:L:224:TYR:OH	2.16	0.46
4:F:197:GLU:O	4:F:214:THR:OG1	2.34	0.46
2:H:121:PRO:HB2	1:G:387:LEU:HD13	1.97	0.46
4:L:443:ARG:HH11	4:L:567:ARG:HA	1.81	0.46
4:E:273:GLY:O	4:E:395:HIS:NE2	2.48	0.46
4:F:420:GLU:HB2	4:F:427:ARG:HA	1.97	0.46
4:F:443:ARG:HH11	4:F:567:ARG:HA	1.81	0.46
5:P:24:C:H2'	5:P:25:C:C6	2.50	0.46
4:L:266:VAL:HG13	4:L:298:TYR:HE2	1.80	0.46
5:Q:24:C:H2'	5:Q:25:C:C6	2.50	0.46
4:F:17:GLY:HA3	4:F:41:LEU:HG	1.97	0.46
4:F:195:ILE:HB	4:F:217:TYR:HD2	1.81	0.46
5:P:26:U:H2'	5:P:27:A:C8	2.50	0.46
2:J:68:THR:O	2:J:72:LYS:HG2	2.15	0.46
4:L:182:PHE:HB3	4:L:225:PHE:HB3	1.98	0.46
1:A:242:MET:HG2	1:A:463:MET:HG2	1.98	0.46
4:F:182:PHE:HB3	4:F:225:PHE:HB3	1.98	0.46
4:K:384:LEU:O	4:K:388:ASN:ND2	2.26	0.46
4:F:192:LYS:HD2	4:F:224:TYR:OH	2.16	0.46
5:P:31:A:H2'	5:P:32:G:H8	1.81	0.46
4:L:51:ASN:HB3	4:L:69:SER:HB3	1.98	0.46
4:L:195:ILE:HB	4:L:217:TYR:HD2	1.81	0.46
2:D:68:THR:O	2:D:72:LYS:HG2	2.15	0.46
5:P:8:C:H2'	5:P:9:A:C8	2.51	0.46
1:G:242:MET:HG2	1:G:463:MET:HG2	1.98	0.46
4:K:273:GLY:O	4:K:395:HIS:NE2	2.48	0.46
5:Q:8:C:H2'	5:Q:9:A:C8	2.51	0.46
4:F:51:ASN:HB3	4:F:69:SER:HB3	1.99	0.45
4:F:165:LEU:HD23	4:F:209:VAL:HG21	1.98	0.45
4:L:165:LEU:HD23	4:L:209:VAL:HG21	1.98	0.45
4:L:420:GLU:HB2	4:L:427:ARG:HA	1.97	0.45
1:A:304:ASP:OD2	1:A:640:ARG:NE	2.49	0.45
4:E:142:GLU:OE2	4:E:410:THR:OG1	2.34	0.45
1:G:80:TYR:HA	1:G:114:ILE:HD11	1.99	0.45
4:L:17:GLY:HA3	4:L:41:LEU:HG	1.98	0.45
5:Q:26:U:H2'	5:Q:27:A:C8	2.50	0.45
5:Q:31:A:H2'	5:Q:32:G:H8	1.81	0.45
1:A:80:TYR:HA	1:A:114:ILE:HD11	1.99	0.45
2:D:15:PHE:HD1	2:D:15:PHE:O	1.99	0.45
4:F:358:CYS:SG	4:F:359:THR:N	2.90	0.45
4:K:503:ASN:HB3	4:K:506:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:15:ARG:O	4:E:43:LEU:N	2.44	0.45
2:H:128:LEU:HD11	2:H:149:TYR:HD2	1.81	0.45
1:G:755:MET:HG2	1:G:764:VAL:HG22	1.98	0.45
4:L:358:CYS:SG	4:L:359:THR:N	2.90	0.45
1:A:149:TYR:HE2	1:A:212:LEU:HD13	1.82	0.45
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.98	0.45
3:C:57:SER:HA	3:C:60:LEU:HB2	1.98	0.45
4:E:114:TRP:CD1	4:E:138:LEU:HD13	2.52	0.45
2:H:61:LYS:HE2	6:U:32:G:OP1	2.17	0.45
1:G:202:VAL:N	1:G:223:ILE:O	2.41	0.45
2:J:15:PHE:O	2:J:15:PHE:HD1	1.99	0.45
4:E:503:ASN:HB3	4:E:506:TRP:CD1	2.51	0.45
4:F:266:VAL:HG13	4:F:298:TYR:CE2	2.51	0.45
1:G:151:CYS:HA	1:G:177:ASN:HD22	1.81	0.45
4:K:142:GLU:OE2	4:K:410:THR:OG1	2.34	0.45
4:K:332:ARG:NH1	4:K:333:ILE:O	2.49	0.45
2:D:143:ASP:O	2:D:146:THR:OG1	2.33	0.45
4:E:130:LEU:HD23	4:E:130:LEU:HA	1.85	0.45
4:F:420:GLU:HB3	4:F:430:LYS:HD3	1.98	0.45
5:P:10:U:H2'	5:P:11:G:H8	1.81	0.45
3:I:57:SER:HA	3:I:60:LEU:HB2	1.98	0.45
4:K:114:TRP:CD1	4:K:138:LEU:HD13	2.52	0.45
4:L:13:SER:HB3	4:L:92:LEU:HD12	1.99	0.45
4:L:178:ARG:NH1	4:L:310:SER:OG	2.50	0.45
1:A:642:HIS:HB3	1:A:646:CYS:HB2	1.99	0.45
4:E:332:ARG:NH1	4:E:333:ILE:O	2.49	0.45
4:E:384:LEU:O	4:E:388:ASN:ND2	2.26	0.45
4:F:377:SER:HB3	4:F:405:LEU:O	2.16	0.45
2:H:57:ARG:O	2:H:60:GLU:HG3	2.17	0.45
1:G:149:TYR:HE2	1:G:212:LEU:HD13	1.82	0.45
1:G:642:HIS:HB3	1:G:646:CYS:HB2	1.99	0.45
4:K:163:LEU:HB2	4:K:211:TYR:CD1	2.52	0.45
4:F:13:SER:HB3	4:F:92:LEU:HD12	1.99	0.45
2:J:11:SER:HB2	2:J:49:PHE:HD1	1.82	0.45
4:L:266:VAL:HG13	4:L:298:TYR:CE2	2.51	0.45
4:L:420:GLU:HB3	4:L:430:LYS:HD3	1.98	0.45
5:Q:10:U:H2'	5:Q:11:G:H8	1.81	0.45
6:U:45:C:H2'	6:U:46:A:H8	1.80	0.45
1:A:151:CYS:HA	1:A:177:ASN:HD22	1.81	0.45
1:A:202:VAL:N	1:A:223:ILE:O	2.41	0.45
1:A:825:ASP:OD1	1:A:825:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:163:LEU:HB2	4:E:211:TYR:CD1	2.52	0.45
4:E:200:PHE:HB3	4:E:209:VAL:HG21	1.98	0.45
6:T:45:C:H2'	6:T:46:A:H8	1.80	0.45
1:G:55:ARG:NH1	1:G:55:ARG:HB2	2.32	0.45
4:K:332:ARG:HA	4:K:357:PHE:HB2	1.99	0.45
4:L:289:SER:O	4:L:293:ILE:HG12	2.17	0.45
2:D:11:SER:HB2	2:D:49:PHE:HD1	1.82	0.44
4:E:332:ARG:HA	4:E:357:PHE:HB2	1.99	0.44
4:F:178:ARG:NH1	4:F:310:SER:OG	2.50	0.44
4:F:289:SER:O	4:F:293:ILE:HG12	2.17	0.44
6:T:32:G:H2'	6:T:33:A:H8	1.81	0.44
4:L:377:SER:HB3	4:L:405:LEU:O	2.16	0.44
1:A:18:ARG:NH2	1:A:60:ASP:O	2.50	0.44
1:A:55:ARG:NH1	1:A:55:ARG:HB2	2.33	0.44
1:A:503:GLY:O	1:A:507:ASN:ND2	2.49	0.44
1:G:18:ARG:NH2	1:G:60:ASP:O	2.50	0.44
2:J:83:VAL:O	2:J:87:MET:N	2.42	0.44
4:K:200:PHE:HB3	4:K:209:VAL:HG21	1.98	0.44
4:L:198:TYR:HB2	4:L:225:PHE:CE2	2.53	0.44
4:F:198:TYR:HB2	4:F:225:PHE:CE2	2.53	0.44
1:G:30:VAL:HG22	1:G:51:THR:HG22	2.00	0.44
2:J:143:ASP:O	2:J:146:THR:OG1	2.33	0.44
1:A:885:LEU:HD12	1:A:885:LEU:HA	1.82	0.44
1:A:30:VAL:HG22	1:A:51:THR:HG22	2.00	0.44
6:T:47:U:H2'	6:T:48:G:C8	2.52	0.44
6:T:49:C:H2'	6:T:50:U:H6	1.82	0.44
1:G:601:MET:HE2	1:G:601:MET:HB2	1.85	0.44
1:G:902:MET:HG3	4:K:93:TYR:CZ	2.53	0.44
4:L:140:ALA:HB2	4:L:232:VAL:HG11	2.00	0.44
6:U:47:U:H2'	6:U:48:G:C8	2.52	0.44
4:K:15:ARG:O	4:K:43:LEU:N	2.44	0.44
4:L:71:TYR:HB3	4:L:75:HIS:HD1	1.83	0.44
6:U:32:G:H2'	6:U:33:A:H8	1.81	0.44
1:A:736:ASP:OD1	1:A:736:ASP:N	2.43	0.44
1:A:902:MET:HG3	4:E:93:TYR:CZ	2.53	0.44
2:B:159:VAL:HG22	2:B:186:VAL:HG12	1.99	0.44
4:F:140:ALA:HB2	4:F:232:VAL:HG11	2.00	0.44
1:G:54:CYS:SG	1:G:74:ARG:NH2	2.91	0.44
1:G:55:ARG:HB2	1:G:55:ARG:HH11	1.82	0.44
4:K:21:ARG:NH2	4:K:232:VAL:O	2.51	0.44
1:A:54:CYS:SG	1:A:74:ARG:NH2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LEU:HD11	4:F:81:PHE:HD1	1.83	0.44
4:F:71:TYR:HB3	4:F:75:HIS:HD1	1.83	0.44
6:T:31:G:H2'	6:T:32:G:H8	1.82	0.44
1:G:503:GLY:O	1:G:507:ASN:ND2	2.49	0.44
6:U:49:C:H2'	6:U:50:U:H6	1.82	0.44
2:D:158:GLN:HA	2:D:158:GLN:NE2	2.31	0.44
4:F:26:CYS:HB2	4:F:97:CYS:SG	2.58	0.44
4:F:287:GLY:HA3	9:F:1003:ADP:H8	1.83	0.44
2:H:128:LEU:HD12	1:G:387:LEU:HD23	2.00	0.44
6:T:38:G:H2'	6:T:39:A:H8	1.83	0.44
4:K:462:LYS:HD3	4:K:462:LYS:HA	1.82	0.44
6:U:31:G:H2'	6:U:32:G:H8	1.82	0.44
6:U:34:G:H2'	6:U:35:A:C8	2.52	0.44
4:E:21:ARG:NH2	4:E:232:VAL:O	2.51	0.43
4:E:258:ILE:HG13	4:E:259:SER:N	2.33	0.43
4:F:158:LEU:HG	4:F:164:HIS:CD2	2.51	0.43
6:T:34:G:H2'	6:T:35:A:C8	2.52	0.43
6:T:37:U:H2'	6:T:38:G:H8	1.83	0.43
6:T:42:U:H2'	6:T:43:A:C8	2.53	0.43
2:J:142:CYS:HG	2:J:147:PHE:HD1	1.64	0.43
4:L:26:CYS:HB2	4:L:97:CYS:SG	2.58	0.43
4:L:254:PRO:HB3	4:L:298:TYR:CE1	2.53	0.43
4:L:287:GLY:HA3	9:L:1003:ADP:H8	1.83	0.43
6:U:32:G:H2'	6:U:33:A:C8	2.53	0.43
4:E:462:LYS:HD3	4:E:462:LYS:HA	1.82	0.43
4:F:254:PRO:HB3	4:F:298:TYR:CE1	2.53	0.43
6:T:36:A:H2'	6:T:37:U:C6	2.53	0.43
5:Q:4:G:H2'	5:Q:5:U:C6	2.53	0.43
6:U:36:A:H2'	6:U:37:U:C6	2.53	0.43
1:A:699:ALA:O	1:A:703:ASN:ND2	2.47	0.43
4:F:344:ASP:HA	4:F:348:VAL:HG21	1.99	0.43
4:K:258:ILE:HG13	4:K:259:SER:N	2.33	0.43
6:U:37:U:H2'	6:U:38:G:H8	1.82	0.43
6:U:38:G:H2'	6:U:39:A:H8	1.83	0.43
6:U:42:U:H2'	6:U:43:A:C8	2.53	0.43
1:A:55:ARG:HB2	1:A:55:ARG:HH11	1.82	0.43
1:A:107:ASP:OD1	1:A:108:GLY:N	2.40	0.43
5:P:4:G:H2'	5:P:5:U:C6	2.53	0.43
6:T:32:G:H2'	6:T:33:A:C8	2.53	0.43
4:L:344:ASP:HA	4:L:348:VAL:HG21	1.99	0.43
4:L:484:VAL:HG13	4:L:486:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:536:SER:HB3	4:L:567:ARG:HH11	1.83	0.43
1:A:77:PHE:HZ	4:L:345:LYS:HD3	1.82	0.43
2:D:83:VAL:O	2:D:87:MET:N	2.42	0.43
4:E:84:CYS:SG	4:E:89:VAL:HG22	2.58	0.43
2:H:82:LYS:HE3	2:H:82:LYS:HB2	1.78	0.43
5:P:22:C:H2'	5:P:23:U:H6	1.84	0.43
2:J:158:GLN:HA	2:J:158:GLN:NE2	2.31	0.43
4:K:130:LEU:HD23	4:K:130:LEU:HA	1.85	0.43
4:K:176:LEU:HD13	4:K:201:GLU:HB3	2.00	0.43
5:Q:22:C:H2'	5:Q:23:U:H6	1.84	0.43
5:Q:23:U:H2'	5:Q:24:C:C6	2.54	0.43
1:A:59:LYS:HB3	1:A:65:LEU:HD22	2.01	0.43
4:E:176:LEU:HD13	4:E:201:GLU:HB3	2.00	0.43
4:F:536:SER:HB3	4:F:567:ARG:HH11	1.84	0.43
2:H:132:ILE:HG21	2:H:138:TYR:HB2	2.01	0.43
6:T:36:A:H2'	6:T:37:U:H6	1.83	0.43
1:G:59:LYS:HB3	1:G:65:LEU:HD22	2.01	0.43
1:G:615:MET:HB2	1:G:766:PHE:CE1	2.53	0.43
4:K:494:GLY:O	4:K:497:ARG:HB2	2.18	0.43
4:L:158:LEU:HG	4:L:164:HIS:CD2	2.51	0.43
4:E:478:GLY:O	4:E:489:ASN:ND2	2.48	0.43
4:F:484:VAL:HG13	4:F:486:SER:H	1.83	0.43
5:P:23:U:H2'	5:P:24:C:C6	2.54	0.43
1:G:824:ASP:OD1	1:G:824:ASP:N	2.52	0.43
4:K:84:CYS:SG	4:K:89:VAL:HG22	2.58	0.43
6:U:36:A:H2'	6:U:37:U:H6	1.83	0.43
1:A:615:MET:HB2	1:A:766:PHE:CE1	2.53	0.43
1:A:804:ASP:OD2	1:A:807:LYS:NZ	2.52	0.43
1:G:107:ASP:OD1	1:G:108:GLY:N	2.40	0.43
4:K:478:GLY:O	4:K:489:ASN:ND2	2.48	0.43
1:A:824:ASP:OD1	1:A:824:ASP:N	2.52	0.43
4:E:494:GLY:O	4:E:497:ARG:HB2	2.18	0.43
1:G:736:ASP:OD1	1:G:736:ASP:N	2.43	0.43
4:L:290:HIS:ND1	9:L:1003:ADP:N7	2.67	0.43
6:U:25:U:H2'	6:U:26:U:C6	2.53	0.43
2:B:12:TYR:HB2	2:B:49:PHE:CE1	2.53	0.43
4:E:259:SER:HB2	4:E:262:PHE:HD2	1.84	0.43
4:F:526:LEU:HD13	4:F:528:LEU:HD12	2.01	0.43
1:G:804:ASP:OD2	1:G:807:LYS:NZ	2.52	0.43
4:K:426:CYS:HA	4:K:429:MET:HG2	2.00	0.43
4:K:515:TYR:HH	4:K:550:THR:HG1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:526:LEU:HD13	4:L:528:LEU:HD12	2.01	0.43
4:F:15:ARG:HB2	4:F:43:LEU:HB2	2.01	0.42
4:F:253:TYR:HA	4:F:254:PRO:HD3	1.89	0.42
6:T:25:U:H2'	6:T:26:U:C6	2.53	0.42
1:G:676:LYS:NZ	1:G:678:GLY:O	2.49	0.42
4:L:109:ILE:HD13	4:L:109:ILE:HA	1.84	0.42
1:A:503:GLY:HA3	1:A:561:SER:HA	2.01	0.42
1:A:583:ARG:HA	1:A:583:ARG:HD3	1.89	0.42
4:E:16:CYS:SG	4:E:33:HIS:CD2	3.13	0.42
4:E:148:SER:OG	4:E:149:TYR:N	2.51	0.42
2:J:31:SER:HB3	2:J:32:GLU:HB2	2.01	0.42
4:K:16:CYS:SG	4:K:33:HIS:CD2	3.12	0.42
4:K:259:SER:HB2	4:K:262:PHE:HD2	1.84	0.42
4:L:15:ARG:HB2	4:L:43:LEU:HB2	2.01	0.42
4:L:253:TYR:HA	4:L:254:PRO:HD3	1.89	0.42
4:L:258:ILE:HG23	4:L:259:SER:H	1.84	0.42
1:A:518:SER:HB2	2:B:80:ARG:HG3	2.01	0.42
2:D:31:SER:HB3	2:D:32:GLU:HB2	2.01	0.42
2:D:183:PRO:HD3	4:E:253:TYR:CD2	2.54	0.42
4:F:258:ILE:HG23	4:F:259:SER:H	1.84	0.42
2:H:9:LEU:HD23	2:H:9:LEU:HA	1.86	0.42
5:P:25:C:H2'	5:P:26:U:C6	2.54	0.42
1:G:503:GLY:HA3	1:G:561:SER:HA	2.01	0.42
1:G:636:LEU:HD21	1:G:655:LEU:HD22	2.00	0.42
3:I:54:SER:O	3:I:57:SER:OG	2.26	0.42
2:J:106:ILE:HG22	2:J:107:ILE:HG23	1.99	0.42
4:K:148:SER:OG	4:K:149:TYR:N	2.51	0.42
1:A:636:LEU:HD21	1:A:655:LEU:HD22	2.00	0.42
4:F:186:ARG:HD3	4:F:223:ASP:OD1	2.20	0.42
4:F:290:HIS:ND1	9:F:1003:ADP:N7	2.67	0.42
4:F:582:TYR:HD1	4:F:582:TYR:HA	1.63	0.42
1:G:699:ALA:O	1:G:703:ASN:ND2	2.47	0.42
2:J:183:PRO:HD3	4:K:253:TYR:CD2	2.54	0.42
4:K:265:ASN:O	4:K:268:ASN:HB2	2.20	0.42
4:L:411:LEU:HD12	4:L:411:LEU:HA	1.90	0.42
4:E:72:CYS:SG	4:E:74:SER:OG	2.69	0.42
4:E:426:CYS:HA	4:E:429:MET:HG2	2.00	0.42
4:F:407:ALA:HB3	4:F:409:ARG:CZ	2.50	0.42
1:G:885:LEU:HD12	1:G:885:LEU:HA	1.82	0.42
4:K:72:CYS:SG	4:K:74:SER:OG	2.69	0.42
4:L:215:THR:HG21	4:L:217:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:LYS:NZ	1:A:678:GLY:O	2.49	0.42
2:D:106:ILE:HG22	2:D:107:ILE:HG23	1.99	0.42
4:E:265:ASN:O	4:E:268:ASN:HB2	2.20	0.42
4:E:526:LEU:HD12	4:E:528:LEU:H	1.85	0.42
4:K:526:LEU:HD12	4:K:528:LEU:H	1.85	0.42
4:F:195:ILE:HG13	4:F:196:GLY:N	2.34	0.42
4:F:215:THR:HG21	4:F:217:TYR:CE2	2.55	0.42
9:F:1003:ADP:O1B	10:F:1005:AF3:F1	2.28	0.42
4:K:288:LYS:HE2	4:K:288:LYS:HB2	1.88	0.42
4:L:186:ARG:HD3	4:L:223:ASP:OD1	2.20	0.42
9:L:1003:ADP:O2B	10:L:1005:AF3:F1	2.28	0.42
4:E:28:LYS:HG3	4:E:97:CYS:SG	2.60	0.42
4:L:195:ILE:HG13	4:L:196:GLY:N	2.34	0.42
4:L:407:ALA:HB3	4:L:409:ARG:CZ	2.50	0.42
2:B:132:ILE:HG21	2:B:138:TYR:HB2	2.02	0.42
2:B:132:ILE:HD13	2:B:138:TYR:HD1	1.83	0.42
4:E:271:LYS:HA	4:E:274:MET:SD	2.60	0.42
1:G:583:ARG:HA	1:G:583:ARG:HD3	1.89	0.42
4:K:28:LYS:HG3	4:K:97:CYS:SG	2.60	0.42
4:K:271:LYS:HA	4:K:274:MET:SD	2.60	0.42
5:Q:10:U:H2’	5:Q:11:G:C8	2.55	0.42
5:Q:23:U:H2’	5:Q:24:C:H6	1.84	0.42
6:U:20:A:H2’	6:U:21:U:C6	2.55	0.42
5:P:10:U:H2’	5:P:11:G:C8	2.55	0.42
1:A:488:ILE:HD11	1:A:573:GLN:HB3	2.01	0.41
1:A:851:ASP:HB3	1:A:854:LEU:HD12	2.02	0.41
4:E:244:GLU:OE2	4:E:246:TYR:OH	2.35	0.41
11:E:707:1N7:H14	11:E:707:1N7:H29	1.77	0.41
5:P:23:U:H2’	5:P:24:C:H6	1.85	0.41
1:G:493:VAL:HG21	1:G:570:GLN:HG2	2.01	0.41
1:G:851:ASP:HB3	1:G:854:LEU:HD12	2.02	0.41
4:L:358:CYS:SG	4:L:363:LEU:HD23	2.59	0.41
1:A:493:VAL:HG21	1:A:570:GLN:HG2	2.01	0.41
6:T:20:A:H2’	6:T:21:U:C6	2.55	0.41
1:G:33:ARG:HG3	1:G:50:LYS:HD3	2.02	0.41
1:G:488:ILE:HD11	1:G:573:GLN:HB3	2.01	0.41
4:K:540:GLU:HB2	4:K:569:LYS:HE3	2.01	0.41
5:Q:25:C:H2’	5:Q:26:U:C6	2.54	0.41
1:A:33:ARG:HG3	1:A:50:LYS:HD3	2.02	0.41
1:A:409:THR:OG1	3:C:23:GLU:OE2	2.34	0.41
1:A:523:ASP:OD1	1:A:523:ASP:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:44:SER:OG	4:E:45:VAL:N	2.53	0.41
4:F:358:CYS:SG	4:F:363:LEU:HD23	2.59	0.41
5:P:13:U:H2'	5:P:14:A:C8	2.55	0.41
5:Q:22:C:H2'	5:Q:23:U:C6	2.55	0.41
1:A:206:THR:OG1	1:A:209:ASN:ND2	2.54	0.41
2:B:48:GLU:HA	2:B:51:ARG:HH12	1.86	0.41
2:D:147:PHE:CE2	2:D:149:TYR:HB2	2.55	0.41
4:E:174:PRO:HG2	4:E:182:PHE:CZ	2.55	0.41
4:E:201:GLU:HG3	4:E:210:VAL:HG23	2.02	0.41
2:H:159:VAL:HG22	2:H:186:VAL:HG12	2.02	0.41
5:P:22:C:H2'	5:P:23:U:C6	2.55	0.41
1:G:206:THR:OG1	1:G:209:ASN:ND2	2.54	0.41
1:G:409:THR:OG1	3:I:23:GLU:OE2	2.34	0.41
4:K:201:GLU:HG3	4:K:210:VAL:HG23	2.03	0.41
4:K:205:TYR:OH	4:L:365:GLU:O	2.37	0.41
11:K:707:1N7:H14	11:K:707:1N7:H29	1.77	0.41
4:E:17:GLY:O	4:E:22:ARG:NH1	2.53	0.41
4:F:109:ILE:HD13	4:F:109:ILE:HA	1.84	0.41
4:F:153:THR:HA	4:F:224:TYR:HA	2.03	0.41
4:K:17:GLY:O	4:K:22:ARG:NH1	2.53	0.41
4:K:174:PRO:HG2	4:K:182:PHE:CZ	2.55	0.41
4:L:511:PHE:HA	4:L:545:ILE:HG23	2.03	0.41
5:Q:13:U:H2'	5:Q:14:A:C8	2.55	0.41
2:D:22:TYR:HB2	2:D:38:LEU:HG	2.01	0.41
2:D:154:TRP:HB3	2:D:188:ALA:HB1	2.03	0.41
4:E:540:GLU:HB2	4:E:569:LYS:HE3	2.01	0.41
4:F:511:PHE:HA	4:F:545:ILE:HG23	2.03	0.41
4:L:582:TYR:HD1	4:L:582:TYR:HA	1.63	0.41
1:A:647:SER:OG	1:A:648:LEU:N	2.54	0.41
4:E:205:TYR:OH	4:F:365:GLU:O	2.37	0.41
2:H:118:ASN:O	2:H:122:LEU:HD23	2.21	0.41
1:G:647:SER:OG	1:G:648:LEU:N	2.54	0.41
1:G:695:ASN:HD21	1:G:762:ALA:HB2	1.86	0.41
4:K:44:SER:OG	4:K:45:VAL:N	2.53	0.41
4:L:153:THR:HA	4:L:224:TYR:HA	2.03	0.41
4:E:305:VAL:CG1	4:E:371:VAL:HG12	2.51	0.41
1:G:304:ASP:OD2	1:G:640:ARG:NE	2.49	0.41
1:G:538:THR:OG1	1:G:661:GLN:HG2	2.21	0.41
2:J:22:TYR:HB2	2:J:38:LEU:HG	2.01	0.41
2:J:154:TRP:HB3	2:J:188:ALA:HB1	2.03	0.41
4:K:189:LYS:HB3	4:K:190:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD12	1:A:174:VAL:HB	2.03	0.41
1:A:538:THR:OG1	1:A:661:GLN:HG2	2.21	0.41
1:A:695:ASN:HD21	1:A:762:ALA:HB2	1.86	0.41
2:B:15:PHE:HE1	2:B:46:LYS:HB2	1.86	0.41
3:C:54:SER:O	3:C:57:SER:OG	2.27	0.41
2:D:96:ARG:O	2:D:96:ARG:HD3	2.21	0.41
2:D:147:PHE:HB2	2:D:156:ILE:HD11	2.03	0.41
4:E:189:LYS:HB3	4:E:190:ASN:ND2	2.35	0.41
4:E:315:ASP:O	4:E:318:CYS:HB2	2.21	0.41
4:E:489:ASN:O	4:E:493:ILE:HG13	2.21	0.41
4:F:306:TYR:N	4:F:356:VAL:O	2.48	0.41
5:P:31:A:H2’	5:P:32:G:C8	2.55	0.41
1:G:171:ILE:HD12	1:G:174:VAL:HB	2.03	0.41
1:G:523:ASP:OD1	1:G:523:ASP:N	2.45	0.41
1:G:708:LEU:HD23	1:G:708:LEU:HA	1.91	0.41
2:J:147:PHE:HB2	2:J:156:ILE:HD11	2.03	0.41
2:J:147:PHE:CE2	2:J:149:TYR:HB2	2.55	0.41
4:K:305:VAL:CG1	4:K:371:VAL:HG12	2.51	0.41
4:K:315:ASP:O	4:K:318:CYS:HB2	2.21	0.41
5:Q:31:A:H2’	5:Q:32:G:C8	2.55	0.41
6:U:30:A:H2’	6:U:31:G:H8	1.86	0.41
3:C:73:GLU:HG2	3:C:74:GLU:N	2.36	0.41
6:T:30:A:H2’	6:T:31:G:H8	1.86	0.41
3:I:73:GLU:HG2	3:I:74:GLU:N	2.36	0.41
2:J:96:ARG:O	2:J:96:ARG:HD3	2.21	0.41
4:K:28:LYS:HG2	4:K:88:GLN:HG3	2.03	0.41
4:K:489:ASN:O	4:K:493:ILE:HG13	2.21	0.41
4:E:28:LYS:HG2	4:E:88:GLN:HG3	2.03	0.40
4:E:163:LEU:HB3	4:E:209:VAL:HG13	2.03	0.40
2:H:132:ILE:HG23	2:H:137:THR:HB	2.03	0.40
6:T:22:A:H2’	6:T:23:G:H8	1.86	0.40
4:K:163:LEU:HB3	4:K:209:VAL:HG13	2.03	0.40
4:L:120:TYR:HB2	4:L:417:LEU:HD21	2.04	0.40
4:L:306:TYR:N	4:L:356:VAL:O	2.47	0.40
6:U:22:A:H2’	6:U:23:G:H8	1.87	0.40
6:U:37:U:H2’	6:U:38:G:C8	2.55	0.40
1:A:658:GLU:O	1:A:662:VAL:HB	2.21	0.40
1:A:667:VAL:HG23	1:A:676:LYS:HB2	2.04	0.40
1:A:731:LEU:HD23	1:A:731:LEU:HA	1.91	0.40
1:A:900:LEU:HD13	1:A:906:MET:HB2	2.04	0.40
4:F:372:VAL:HG13	4:F:399:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:LYS:HE3	2:H:97:LYS:HB2	1.81	0.40
1:G:667:VAL:HG23	1:G:676:LYS:HB2	2.04	0.40
4:L:393:ALA:HB3	4:L:396:TYR:CE1	2.56	0.40
6:U:37:U:C2	6:U:38:G:C8	3.09	0.40
4:F:120:TYR:HB2	4:F:417:LEU:HD21	2.04	0.40
6:T:31:G:H2'	6:T:32:G:C8	2.56	0.40
6:T:37:U:H2'	6:T:38:G:C8	2.55	0.40
6:T:37:U:C2	6:T:38:G:C8	3.09	0.40
1:G:436:GLU:OE1	1:G:438:LYS:NZ	2.54	0.40
1:G:900:LEU:HD13	1:G:906:MET:HB2	2.04	0.40
2:J:83:VAL:O	2:J:87:MET:HB3	2.21	0.40
4:L:302:ALA:O	4:L:304:ILE:HD13	2.21	0.40
4:L:508:LYS:HE3	4:L:543:TYR:HB2	2.02	0.40
4:F:508:LYS:HE3	4:F:543:TYR:HB2	2.02	0.40
1:G:81:GLN:O	1:G:85:THR:HG23	2.22	0.40
1:A:436:GLU:OE1	1:A:438:LYS:NZ	2.54	0.40
2:B:134:ASP:OD1	2:B:134:ASP:N	2.55	0.40
2:D:171:GLU:HB2	2:D:176:ASN:HD21	1.86	0.40
4:E:109:ILE:HD13	4:E:134:ALA:HB2	2.03	0.40
1:G:186:LEU:O	1:G:190:VAL:HG23	2.21	0.40
1:G:658:GLU:O	1:G:662:VAL:HB	2.21	0.40
4:K:287:GLY:N	9:K:704:ADP:O1B	2.49	0.40
4:L:114:TRP:CD1	4:L:141:THR:HG21	2.56	0.40
4:L:372:VAL:HG13	4:L:399:ILE:HD11	2.04	0.40
4:L:518:GLN:HA	4:L:521:VAL:HG22	2.03	0.40
6:U:23:G:H2'	6:U:24:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	886 (96%)	39 (4%)	0	100	100
1	G	925/932 (99%)	885 (96%)	40 (4%)	0	100	100
2	B	184/199 (92%)	179 (97%)	5 (3%)	0	100	100
2	D	183/199 (92%)	177 (97%)	6 (3%)	0	100	100
2	H	184/199 (92%)	180 (98%)	4 (2%)	0	100	100
2	J	183/199 (92%)	177 (97%)	6 (3%)	0	100	100
3	C	73/88 (83%)	69 (94%)	4 (6%)	0	100	100
3	I	73/88 (83%)	69 (94%)	4 (6%)	0	100	100
4	E	588/605 (97%)	540 (92%)	48 (8%)	0	100	100
4	F	588/605 (97%)	530 (90%)	58 (10%)	0	100	100
4	K	588/605 (97%)	540 (92%)	48 (8%)	0	100	100
4	L	588/605 (97%)	529 (90%)	59 (10%)	0	100	100
All	All	5082/5256 (97%)	4761 (94%)	321 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	776 (95%)	43 (5%)	22	56
1	G	819/823 (100%)	776 (95%)	43 (5%)	22	56
2	B	149/168 (89%)	149 (100%)	0	100	100
2	D	152/168 (90%)	126 (83%)	26 (17%)	2	9
2	H	148/168 (88%)	148 (100%)	0	100	100
2	J	150/168 (89%)	124 (83%)	26 (17%)	2	9
3	C	70/81 (86%)	57 (81%)	13 (19%)	1	7
3	I	70/81 (86%)	57 (81%)	13 (19%)	1	7
4	E	494/526 (94%)	467 (94%)	27 (6%)	21	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	505/526 (96%)	459 (91%)	46 (9%)	9	34
4	K	494/526 (94%)	467 (94%)	27 (6%)	21	55
4	L	505/526 (96%)	458 (91%)	47 (9%)	9	33
All	All	4375/4584 (95%)	4064 (93%)	311 (7%)	18	45

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	12	CYS
1	A	22	CYS
1	A	55	ARG
1	A	61	GLU
1	A	62	ASP
1	A	63	ASP
1	A	65	LEU
1	A	77	PHE
1	A	78	SER
1	A	83	GLU
1	A	109	ASP
1	A	116	ARG
1	A	132	ARG
1	A	226	THR
1	A	231	VAL
1	A	302	LEU
1	A	346	TYR
1	A	359	VAL
1	A	431	GLU
1	A	438	LYS
1	A	545	LYS
1	A	555	ARG
1	A	602	LEU
1	A	608	ASP
1	A	610	GLU
1	A	643	THR
1	A	666	MET
1	A	680	THR
1	A	681	SER
1	A	718	LYS
1	A	758	LEU
1	A	775	LEU

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Mol	Chain	Res	Type
1	A	796	GLU
1	A	847	ILE
1	A	854	LEU
1	A	877	TYR
1	A	902	MET
1	A	906	MET
1	A	911	ASN
1	A	913	SER
1	A	917	GLU
1	A	924	MET
3	C	31	GLN
3	C	38	ASP
3	C	43	LYS
3	C	44	ASP
3	C	45	THR
3	C	47	GLU
3	C	50	GLU
3	C	52	MET
3	C	60	LEU
3	C	66	VAL
3	C	68	ILE
3	C	71	LEU
3	C	74	GLU
2	D	15	PHE
2	D	48	GLU
2	D	55	MET
2	D	57	ARG
2	D	60	GLU
2	D	62	MET
2	D	64	ASP
2	D	65	GLN
2	D	70	MET
2	D	77	GLU
2	D	80	ARG
2	D	87	MET
2	D	90	MET
2	D	96	ARG
2	D	106	ILE
2	D	132	ILE
2	D	138	TYR
2	D	148	THR
2	D	155	GLU

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Mol	Chain	Res	Type
2	D	158	GLN
2	D	166	ILE
2	D	168	GLN
2	D	179	ASN
2	D	180	LEU
2	D	184	LEU
2	D	186	VAL
4	E	20	ILE
4	E	62	GLN
4	E	101	ASP
4	E	153	THR
4	E	169	VAL
4	E	231	THR
4	E	303	ARG
4	E	307	THR
4	E	329	LYS
4	E	351	THR
4	E	377	SER
4	E	378	MET
4	E	405	LEU
4	E	429	MET
4	E	436	MET
4	E	438	LEU
4	E	458	ASP
4	E	474	MET
4	E	481	THR
4	E	484	VAL
4	E	486	SER
4	E	497	ARG
4	E	523	SER
4	E	558	VAL
4	E	563	VAL
4	E	570	VAL
4	E	576	MET
4	F	20	ILE
4	F	35	ILE
4	F	60	VAL
4	F	80	SER
4	F	109	ILE
4	F	122	LEU
4	F	127	THR
4	F	128	GLU

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Mol	Chain	Res	Type
4	F	147	LEU
4	F	166	SER
4	F	169	VAL
4	F	171	LYS
4	F	173	ARG
4	F	178	ARG
4	F	189	LYS
4	F	202	LYS
4	F	212	ARG
4	F	216	THR
4	F	253	TYR
4	F	263	SER
4	F	298	TYR
4	F	303	ARG
4	F	304	ILE
4	F	306	TYR
4	F	347	LYS
4	F	360	VAL
4	F	371	VAL
4	F	377	SER
4	F	378	MET
4	F	399	ILE
4	F	405	LEU
4	F	418	GLU
4	F	429	MET
4	F	436	MET
4	F	452	VAL
4	F	461	LEU
4	F	474	MET
4	F	477	LYS
4	F	497	ARG
4	F	501	THR
4	F	508	LYS
4	F	545	ILE
4	F	550	THR
4	F	560	ARG
4	F	576	MET
4	F	582	TYR
1	G	8	LEU
1	G	12	CYS
1	G	22	CYS
1	G	55	ARG

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Mol	Chain	Res	Type
1	G	61	GLU
1	G	62	ASP
1	G	63	ASP
1	G	65	LEU
1	G	77	PHE
1	G	78	SER
1	G	83	GLU
1	G	109	ASP
1	G	116	ARG
1	G	132	ARG
1	G	226	THR
1	G	231	VAL
1	G	302	LEU
1	G	346	TYR
1	G	359	VAL
1	G	431	GLU
1	G	438	LYS
1	G	545	LYS
1	G	555	ARG
1	G	602	LEU
1	G	608	ASP
1	G	610	GLU
1	G	643	THR
1	G	666	MET
1	G	680	THR
1	G	681	SER
1	G	718	LYS
1	G	758	LEU
1	G	775	LEU
1	G	796	GLU
1	G	847	ILE
1	G	854	LEU
1	G	877	TYR
1	G	902	MET
1	G	906	MET
1	G	911	ASN
1	G	913	SER
1	G	917	GLU
1	G	924	MET
3	I	31	GLN
3	I	38	ASP
3	I	43	LYS

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Mol	Chain	Res	Type
3	I	44	ASP
3	I	45	THR
3	I	47	GLU
3	I	50	GLU
3	I	52	MET
3	I	60	LEU
3	I	66	VAL
3	I	68	ILE
3	I	71	LEU
3	I	74	GLU
2	J	15	PHE
2	J	48	GLU
2	J	55	MET
2	J	57	ARG
2	J	60	GLU
2	J	62	MET
2	J	64	ASP
2	J	65	GLN
2	J	70	MET
2	J	77	GLU
2	J	80	ARG
2	J	87	MET
2	J	90	MET
2	J	96	ARG
2	J	106	ILE
2	J	132	ILE
2	J	138	TYR
2	J	148	THR
2	J	155	GLU
2	J	158	GLN
2	J	166	ILE
2	J	168	GLN
2	J	179	ASN
2	J	180	LEU
2	J	184	LEU
2	J	186	VAL
4	K	20	ILE
4	K	62	GLN
4	K	101	ASP
4	K	153	THR
4	K	169	VAL
4	K	231	THR

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Mol	Chain	Res	Type
4	K	303	ARG
4	K	307	THR
4	K	329	LYS
4	K	351	THR
4	K	377	SER
4	K	378	MET
4	K	405	LEU
4	K	429	MET
4	K	436	MET
4	K	438	LEU
4	K	458	ASP
4	K	474	MET
4	K	481	THR
4	K	484	VAL
4	K	486	SER
4	K	497	ARG
4	K	523	SER
4	K	558	VAL
4	K	563	VAL
4	K	570	VAL
4	K	576	MET
4	L	20	ILE
4	L	35	ILE
4	L	60	VAL
4	L	80	SER
4	L	109	ILE
4	L	122	LEU
4	L	127	THR
4	L	128	GLU
4	L	147	LEU
4	L	166	SER
4	L	169	VAL
4	L	171	LYS
4	L	173	ARG
4	L	178	ARG
4	L	189	LYS
4	L	202	LYS
4	L	212	ARG
4	L	216	THR
4	L	233	MET
4	L	253	TYR
4	L	263	SER

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Mol	Chain	Res	Type
4	L	298	TYR
4	L	303	ARG
4	L	304	ILE
4	L	306	TYR
4	L	347	LYS
4	L	360	VAL
4	L	371	VAL
4	L	377	SER
4	L	378	MET
4	L	399	ILE
4	L	405	LEU
4	L	418	GLU
4	L	429	MET
4	L	436	MET
4	L	452	VAL
4	L	461	LEU
4	L	474	MET
4	L	477	LYS
4	L	497	ARG
4	L	501	THR
4	L	508	LYS
4	L	545	ILE
4	L	550	THR
4	L	560	ARG
4	L	576	MET
4	L	582	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	ASN
1	A	752	HIS
2	D	158	GLN
4	E	190	ASN
4	F	62	GLN
4	F	88	GLN
4	F	281	GLN
1	G	534	ASN
1	G	752	HIS
2	J	158	GLN
4	K	190	ASN
4	L	62	GLN

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Mol	Chain	Res	Type
4	L	88	GLN
4	L	281	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	33/35 (94%)	1 (3%)	1 (3%)
5	Q	33/35 (94%)	1 (3%)	1 (3%)
6	T	36/55 (65%)	0	0
6	U	36/55 (65%)	0	0
All	All	138/180 (76%)	2 (1%)	2 (1%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	25	C
5	Q	25	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	P	24	C
5	Q	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 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
10	AF3	K	706	-	0,3,3	-	-	-		
10	AF3	E	706	-	0,3,3	-	-	-		
9	ADP	F	1003	8	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	L	1003	8	24,29,29	0.96	1 (4%)	29,45,45	1.42	4 (13%)
9	ADP	G	2003	8	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
9	ADP	A	2003	8	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
10	AF3	L	1005	-	0,3,3	-	-	-		
11	1N7	E	707	-	39,39,46	2.82	22 (56%)	61,61,72	2.77	32 (52%)
10	AF3	F	1005	-	0,3,3	-	-	-		
9	ADP	E	704	8	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
9	ADP	K	704	8	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
11	1N7	K	707	-	39,39,46	2.81	22 (56%)	61,61,72	2.77	32 (52%)

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	F	1003	8	-	2/12/32/32	0/3/3/3
9	ADP	L	1003	8	-	2/12/32/32	0/3/3/3
9	ADP	G	2003	8	-	2/12/32/32	0/3/3/3
9	ADP	A	2003	8	-	2/12/32/32	0/3/3/3
11	1N7	E	707	-	-	6/17/82/92	0/4/4/4
9	ADP	E	704	8	-	1/12/32/32	0/3/3/3
9	ADP	K	704	8	-	3/12/32/32	0/3/3/3
11	1N7	K	707	-	-	6/17/82/92	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	707	1N7	C18-C17	6.12	1.63	1.53
11	E	707	1N7	C18-C17	6.09	1.63	1.53
11	K	707	1N7	C23-C24	5.14	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	707	1N7	C23-C24	5.09	1.61	1.51
11	E	707	1N7	C24-N1	4.93	1.44	1.33
11	K	707	1N7	C24-N1	4.91	1.44	1.33
11	K	707	1N7	C2-C19	4.69	1.64	1.56
11	E	707	1N7	C2-C19	4.66	1.64	1.56
11	K	707	1N7	C16-C17	4.21	1.60	1.52
11	E	707	1N7	C16-C17	4.19	1.60	1.52
11	E	707	1N7	C3-C19	4.18	1.60	1.53
11	K	707	1N7	C3-C19	4.15	1.60	1.53
11	E	707	1N7	C14-C13	3.73	1.58	1.51
11	E	707	1N7	C20-C9	3.72	1.60	1.54
11	K	707	1N7	C20-C9	3.71	1.60	1.54
11	K	707	1N7	C14-C13	3.70	1.58	1.51
11	E	707	1N7	C28-N2	3.64	1.60	1.50
11	K	707	1N7	C28-N2	3.60	1.60	1.50
11	E	707	1N7	C5-C4	3.55	1.60	1.54
11	K	707	1N7	C5-C4	3.51	1.60	1.54
11	E	707	1N7	C14-C15	3.31	1.59	1.53
11	K	707	1N7	C14-C15	3.30	1.59	1.53
11	K	707	1N7	C1-C2	3.18	1.59	1.54
11	E	707	1N7	C2-C15	3.18	1.60	1.55
11	K	707	1N7	C2-C15	3.13	1.60	1.55
11	E	707	1N7	C1-C2	3.12	1.59	1.54
11	E	707	1N7	C25-N1	3.05	1.53	1.46
11	K	707	1N7	C25-N1	3.00	1.53	1.46
11	E	707	1N7	C29-N2	2.93	1.58	1.50
11	K	707	1N7	C29-N2	2.90	1.58	1.50
11	E	707	1N7	C16-C15	2.90	1.58	1.53
11	K	707	1N7	C16-C15	2.89	1.58	1.53
11	K	707	1N7	C18-C6	2.88	1.59	1.53
11	E	707	1N7	C18-C6	2.87	1.59	1.53
11	E	707	1N7	C18-C19	2.75	1.59	1.53
11	K	707	1N7	C18-C19	2.74	1.59	1.53
11	K	707	1N7	C3-C4	2.59	1.57	1.53
11	E	707	1N7	C3-C4	2.53	1.57	1.53
9	F	1003	ADP	C5-C4	2.51	1.47	1.40
9	E	704	ADP	C5-C4	2.50	1.47	1.40
9	K	704	ADP	C5-C4	2.50	1.47	1.40
9	L	1003	ADP	C5-C4	2.49	1.47	1.40
9	G	2003	ADP	C5-C4	2.48	1.47	1.40
9	A	2003	ADP	C5-C4	2.47	1.47	1.40
11	E	707	1N7	C5-C6	2.46	1.59	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	707	1N7	C5-C6	2.44	1.59	1.55
11	E	707	1N7	C12-C13	2.31	1.57	1.51
11	K	707	1N7	C12-C13	2.30	1.57	1.51
11	E	707	1N7	C22-C23	2.04	1.59	1.52
11	K	707	1N7	C22-C23	2.02	1.59	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	707	1N7	C9-C5-C4	-6.91	111.36	117.67
11	E	707	1N7	C9-C5-C4	-6.86	111.41	117.67
11	K	707	1N7	C1-C2-C15	5.81	116.36	107.77
11	E	707	1N7	C1-C2-C15	5.81	116.36	107.77
11	E	707	1N7	C6-C18-C17	5.74	119.42	111.81
11	K	707	1N7	C6-C18-C17	5.73	119.41	111.81
11	K	707	1N7	C23-C24-N1	5.11	125.02	116.42
11	E	707	1N7	C23-C24-N1	5.08	124.98	116.42
11	E	707	1N7	C8-C9-C5	-5.02	98.63	103.55
11	K	707	1N7	C8-C9-C5	-5.00	98.65	103.55
11	E	707	1N7	C2-C19-C18	4.71	116.88	111.82
11	K	707	1N7	C2-C19-C18	4.67	116.83	111.82
11	E	707	1N7	C5-C9-C20	-4.53	114.08	119.50
11	K	707	1N7	C5-C9-C20	-4.51	114.12	119.50
11	K	707	1N7	C11-C2-C1	-4.39	101.19	108.26
11	E	707	1N7	C11-C2-C1	-4.36	101.24	108.26
11	K	707	1N7	C6-C5-C4	4.30	111.41	107.40
11	E	707	1N7	C6-C5-C4	4.29	111.39	107.40
11	E	707	1N7	C3-C19-C2	-4.00	109.60	113.73
11	K	707	1N7	C3-C19-C2	-3.99	109.61	113.73
9	K	704	ADP	PA-O3A-PB	-3.57	120.59	132.83
9	E	704	ADP	PA-O3A-PB	-3.56	120.60	132.83
11	K	707	1N7	C14-C15-C2	3.53	116.41	112.66
11	E	707	1N7	C14-C15-C2	3.52	116.40	112.66
9	A	2003	ADP	PA-O3A-PB	-3.51	120.80	132.83
9	G	2003	ADP	PA-O3A-PB	-3.51	120.80	132.83
11	E	707	1N7	C27-C26-C25	3.45	117.69	111.04
9	E	704	ADP	C3'-C2'-C1'	3.44	106.16	100.98
11	K	707	1N7	C27-C26-C25	3.44	117.68	111.04
9	K	704	ADP	C3'-C2'-C1'	3.40	106.10	100.98
11	E	707	1N7	C12-C1-C2	3.28	118.41	112.78
11	K	707	1N7	C12-C1-C2	3.27	118.39	112.78
11	E	707	1N7	C7-C6-C5	-3.21	100.41	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1003	ADP	C3'-C2'-C1'	3.19	105.79	100.98
11	K	707	1N7	C7-C6-C5	-3.19	100.43	103.55
9	L	1003	ADP	C3'-C2'-C1'	3.18	105.76	100.98
9	G	2003	ADP	N3-C2-N1	-3.17	123.73	128.68
9	E	704	ADP	N3-C2-N1	-3.16	123.75	128.68
9	F	1003	ADP	N3-C2-N1	-3.15	123.75	128.68
11	E	707	1N7	C29-N2-C28	-3.15	100.87	108.97
11	E	707	1N7	C8-C9-C20	3.15	117.02	112.15
9	A	2003	ADP	N3-C2-N1	-3.14	123.77	128.68
9	K	704	ADP	N3-C2-N1	-3.14	123.77	128.68
11	K	707	1N7	C29-N2-C28	-3.14	100.91	108.97
9	L	1003	ADP	N3-C2-N1	-3.13	123.79	128.68
11	K	707	1N7	C8-C9-C20	3.13	116.99	112.15
11	K	707	1N7	C11-C2-C19	-3.13	106.87	111.18
11	E	707	1N7	C11-C2-C19	-3.11	106.90	111.18
9	G	2003	ADP	C3'-C2'-C1'	3.10	105.64	100.98
9	A	2003	ADP	C3'-C2'-C1'	3.09	105.63	100.98
11	K	707	1N7	O1-C24-C23	-3.07	116.40	122.02
11	E	707	1N7	O1-C24-C23	-3.05	116.44	122.02
11	E	707	1N7	C3-C4-C5	-3.01	108.16	111.24
11	K	707	1N7	C3-C4-C5	-3.00	108.16	111.24
11	K	707	1N7	C1-C12-C13	2.98	114.29	110.47
11	E	707	1N7	C1-C12-C13	2.97	114.28	110.47
11	K	707	1N7	C19-C2-C15	2.81	112.52	108.58
9	L	1003	ADP	PA-O3A-PB	-2.79	123.24	132.83
9	F	1003	ADP	PA-O3A-PB	-2.78	123.27	132.83
11	E	707	1N7	C19-C2-C15	2.77	112.47	108.58
9	F	1003	ADP	C4-C5-N7	-2.69	106.59	109.40
11	E	707	1N7	C30-N2-C28	-2.65	102.16	108.97
11	E	707	1N7	C16-C15-C2	-2.65	109.85	112.66
11	K	707	1N7	C30-N2-C28	-2.65	102.17	108.97
11	K	707	1N7	C16-C15-C2	-2.64	109.86	112.66
9	E	704	ADP	C4-C5-N7	-2.62	106.67	109.40
9	L	1003	ADP	C4-C5-N7	-2.62	106.67	109.40
9	A	2003	ADP	C4-C5-N7	-2.61	106.68	109.40
9	K	704	ADP	C4-C5-N7	-2.56	106.73	109.40
9	G	2003	ADP	C4-C5-N7	-2.55	106.74	109.40
11	E	707	1N7	C10-C5-C9	-2.53	107.26	111.21
11	K	707	1N7	C10-C5-C9	-2.52	107.27	111.21
11	K	707	1N7	C25-N1-C24	2.45	127.39	122.84
11	E	707	1N7	C7-C8-C9	2.45	109.98	105.13
11	E	707	1N7	C19-C3-C4	2.45	117.53	114.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	707	1N7	C25-N1-C24	2.43	127.35	122.84
11	K	707	1N7	C7-C8-C9	2.42	109.92	105.13
11	K	707	1N7	C19-C3-C4	2.41	117.49	114.30
11	K	707	1N7	C22-C23-C24	2.35	118.29	113.04
11	K	707	1N7	O1-C24-N1	-2.35	118.57	123.01
11	E	707	1N7	O1-C24-N1	-2.35	118.58	123.01
11	E	707	1N7	C22-C23-C24	2.34	118.25	113.04
11	K	707	1N7	C10-C5-C4	2.33	111.44	109.07
11	E	707	1N7	C10-C5-C4	2.31	111.42	109.07
11	E	707	1N7	C15-C14-C13	2.21	116.01	112.76
11	K	707	1N7	C15-C14-C13	2.20	116.00	112.76
11	K	707	1N7	C23-C22-C20	2.06	118.28	114.52
11	E	707	1N7	C23-C22-C20	2.05	118.27	114.52

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2003	ADP	C5'-O5'-PA-O2A
9	A	2003	ADP	C5'-O5'-PA-O3A
9	G	2003	ADP	C5'-O5'-PA-O3A
11	E	707	1N7	C21-C20-C9-C5
11	K	707	1N7	C21-C20-C9-C5
11	E	707	1N7	C21-C20-C22-C23
11	K	707	1N7	C21-C20-C22-C23
11	E	707	1N7	C22-C20-C9-C5
11	K	707	1N7	C22-C20-C9-C5
9	F	1003	ADP	O4'-C4'-C5'-O5'
9	F	1003	ADP	C3'-C4'-C5'-O5'
9	L	1003	ADP	O4'-C4'-C5'-O5'
9	L	1003	ADP	C3'-C4'-C5'-O5'
11	E	707	1N7	C21-C20-C9-C8
11	K	707	1N7	C21-C20-C9-C8
11	E	707	1N7	C22-C20-C9-C8
11	K	707	1N7	C22-C20-C9-C8
9	K	704	ADP	PA-O3A-PB-O1B
11	E	707	1N7	C9-C20-C22-C23
11	K	707	1N7	C9-C20-C22-C23
9	G	2003	ADP	C5'-O5'-PA-O1A
9	E	704	ADP	O4'-C4'-C5'-O5'
9	K	704	ADP	O4'-C4'-C5'-O5'
9	K	704	ADP	C5'-O5'-PA-O1A

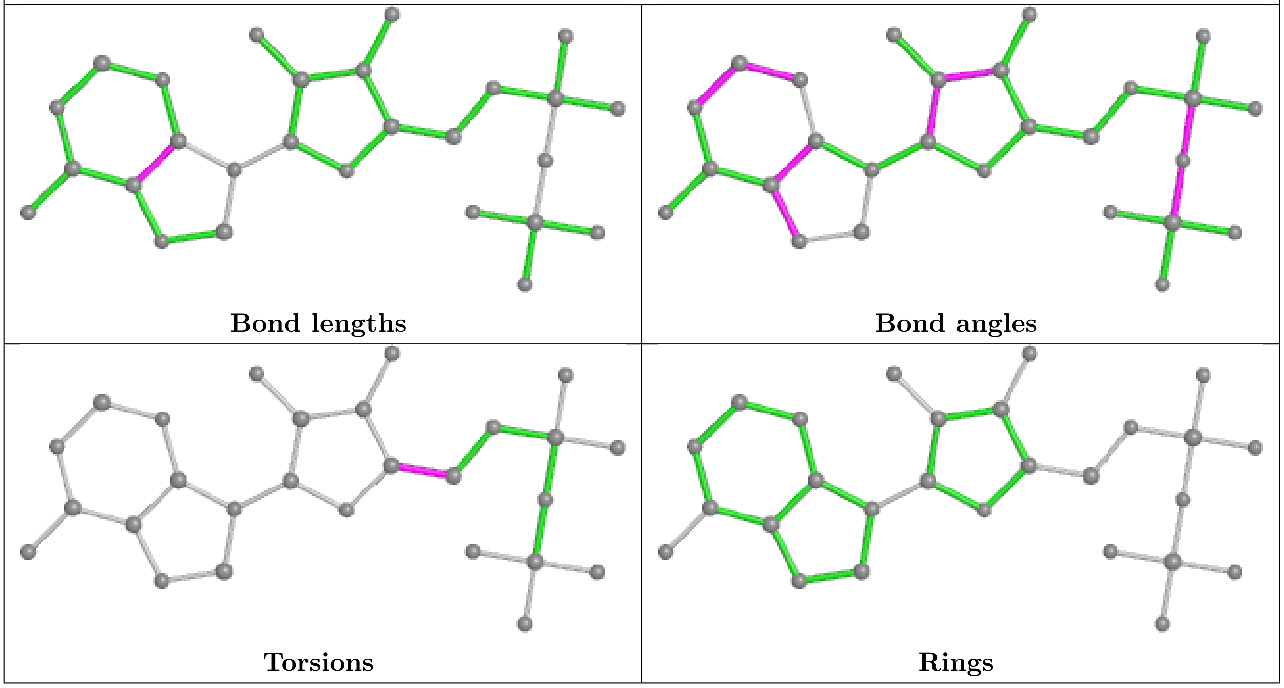
There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1003	ADP	3	0
9	L	1003	ADP	3	0
9	G	2003	ADP	1	0
9	A	2003	ADP	1	0
10	L	1005	AF3	1	0
11	E	707	1N7	1	0
10	F	1005	AF3	1	0
9	K	704	ADP	1	0
11	K	707	1N7	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 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 ADP F 1003



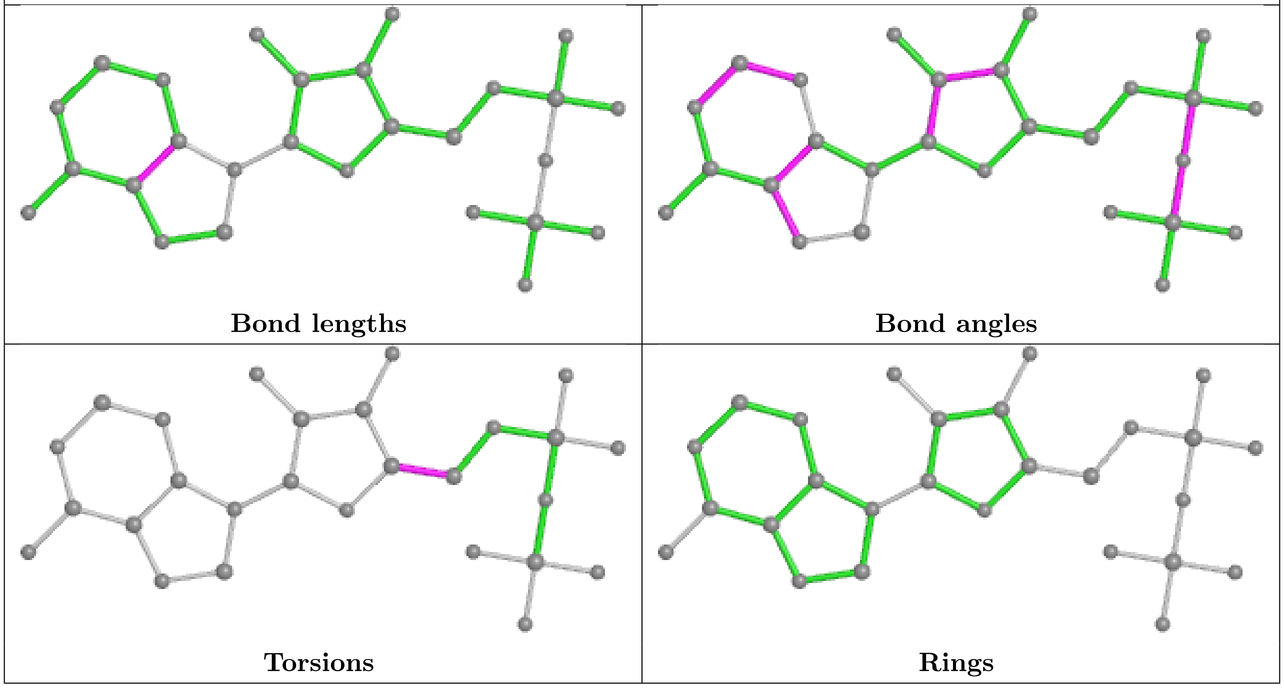
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP L 1003



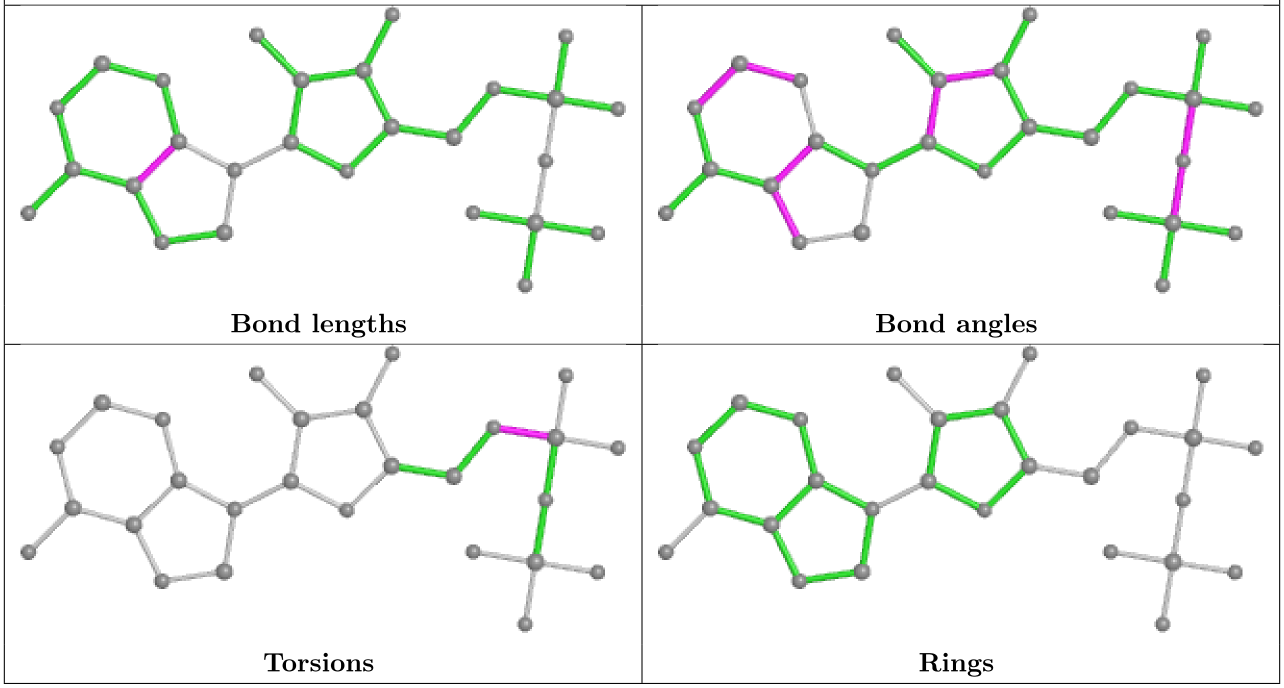
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 2003



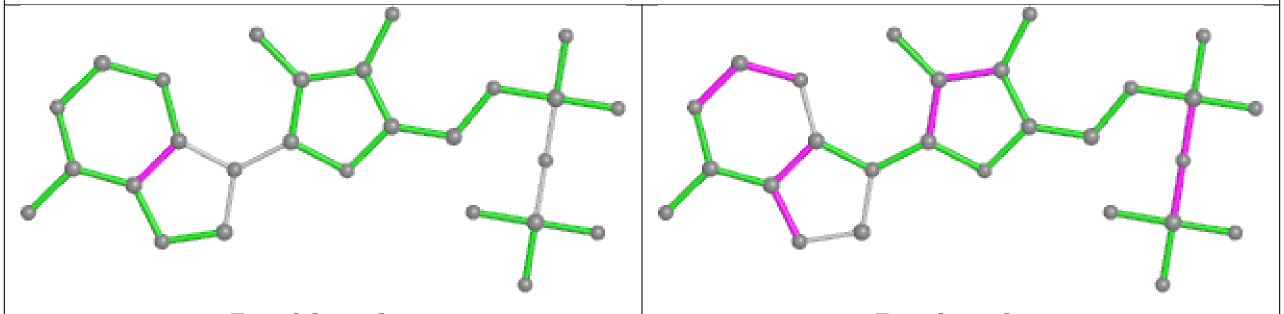
Bond lengths

Bond angles

Torsions

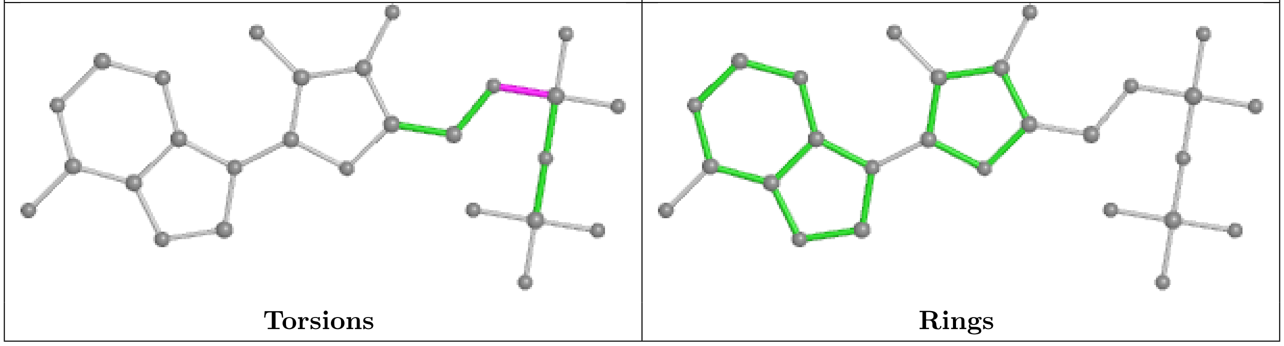
Rings

Ligand ADP A 2003



Bond lengths

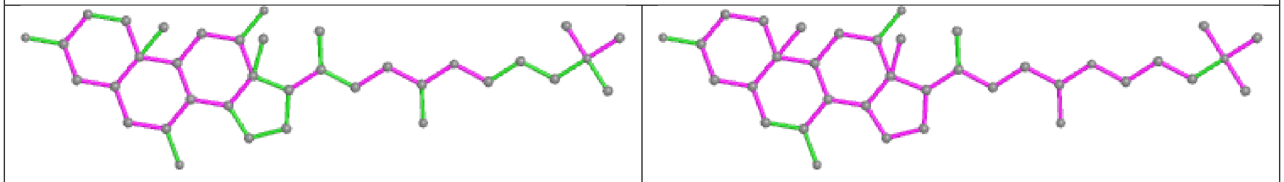
Bond angles



Torsions

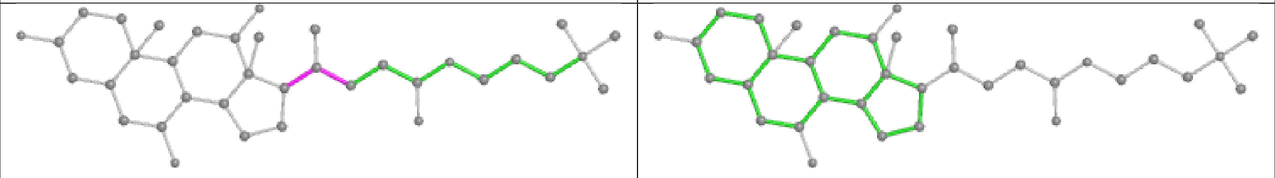
Rings

Ligand 1N7 E 707



Bond lengths

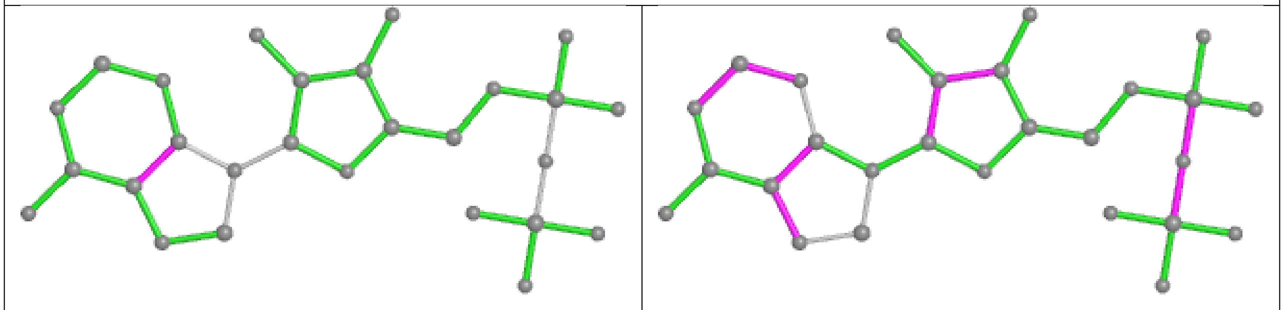
Bond angles



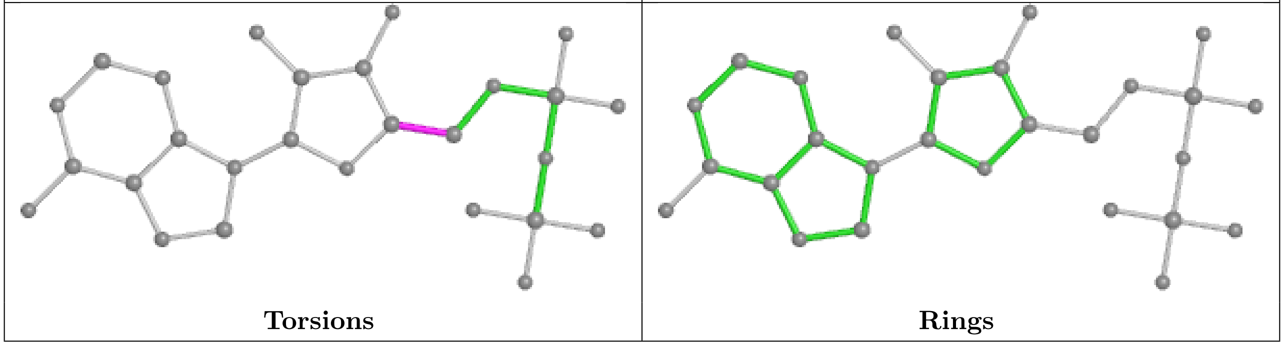
Torsions

Rings

Ligand ADP E 704

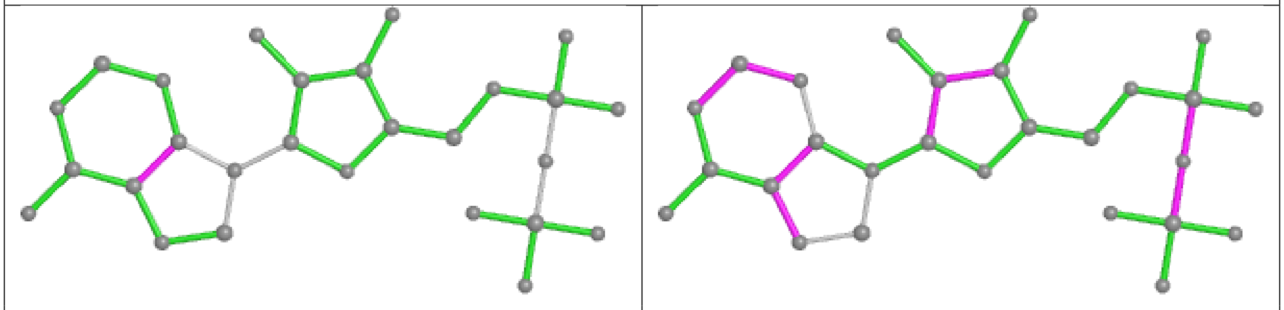


Bond lengths **Bond angles**

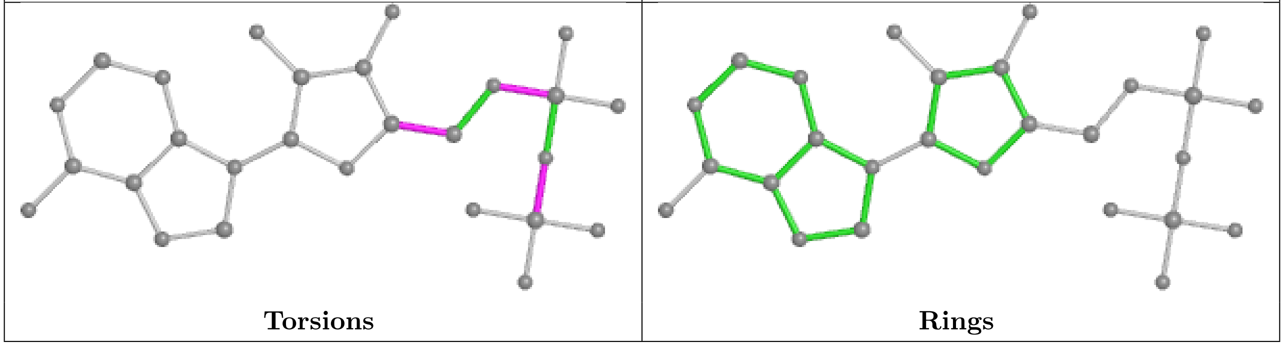


Torsions **Rings**

Ligand ADP K 704

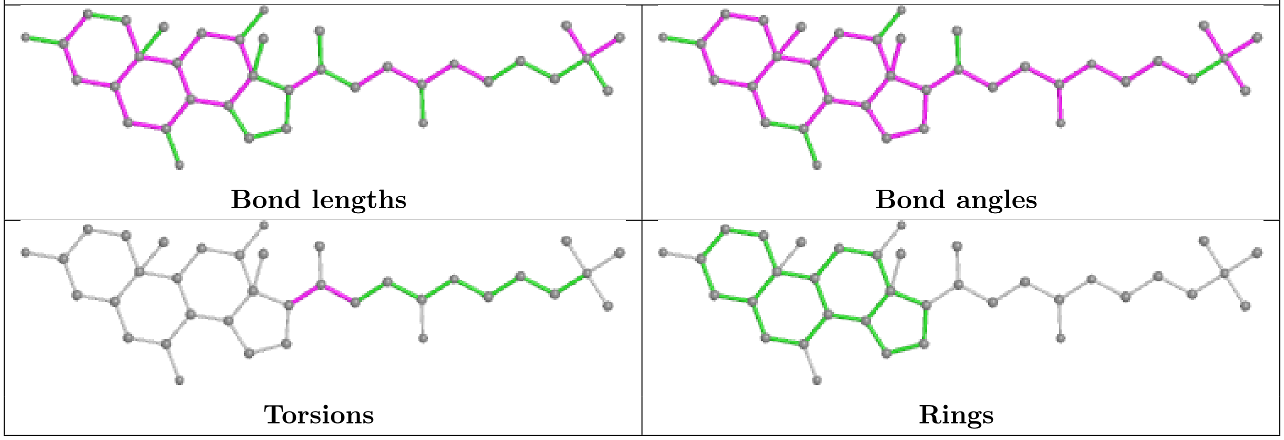


Bond lengths **Bond angles**



Torsions **Rings**

Ligand 1N7 K 707



Bond lengths

Bond angles

Torsions

Rings

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.

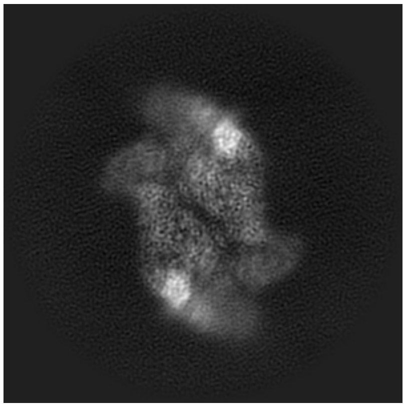
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-24432. These allow visual inspection of the internal detail of the map and identification of artifacts.

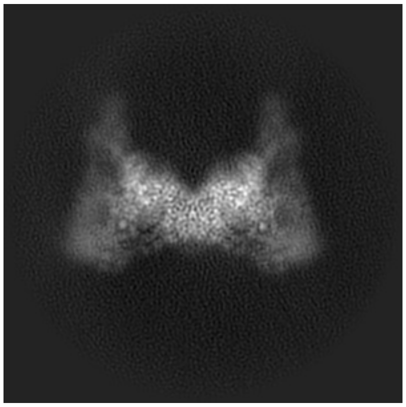
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

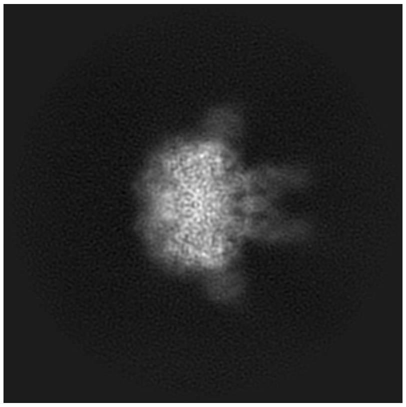
6.1.1 Primary map



X



Y

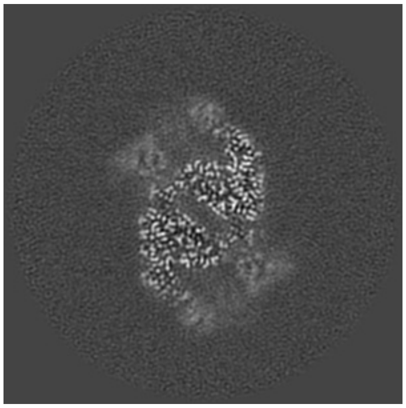


Z

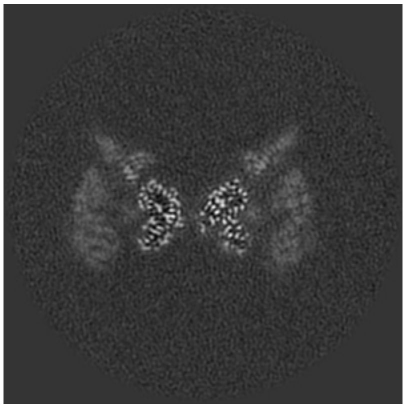
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

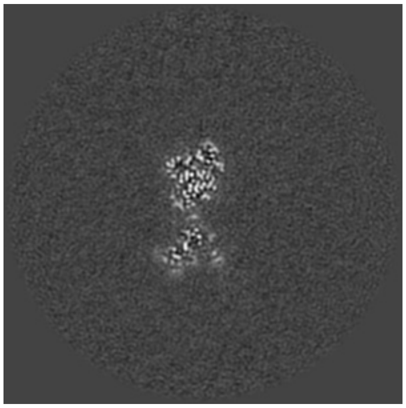
6.2.1 Primary map



X Index: 160



Y Index: 160

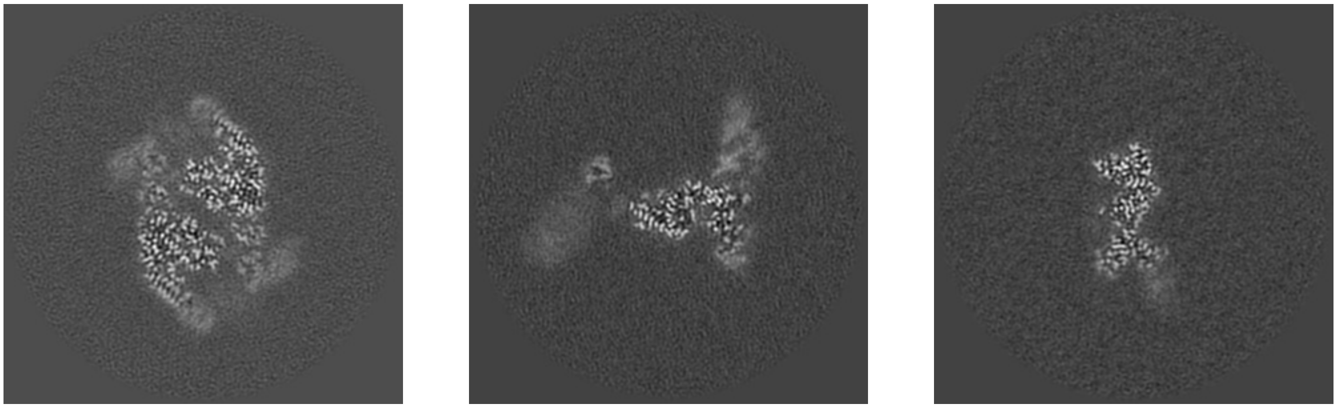


Z Index: 160

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

6.3 Largest variance slices

6.3.1 Primary map

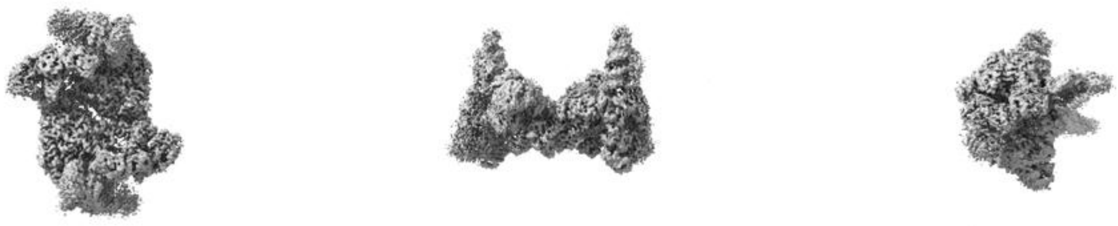


X Index: 164 Y Index: 182 Z Index: 169

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

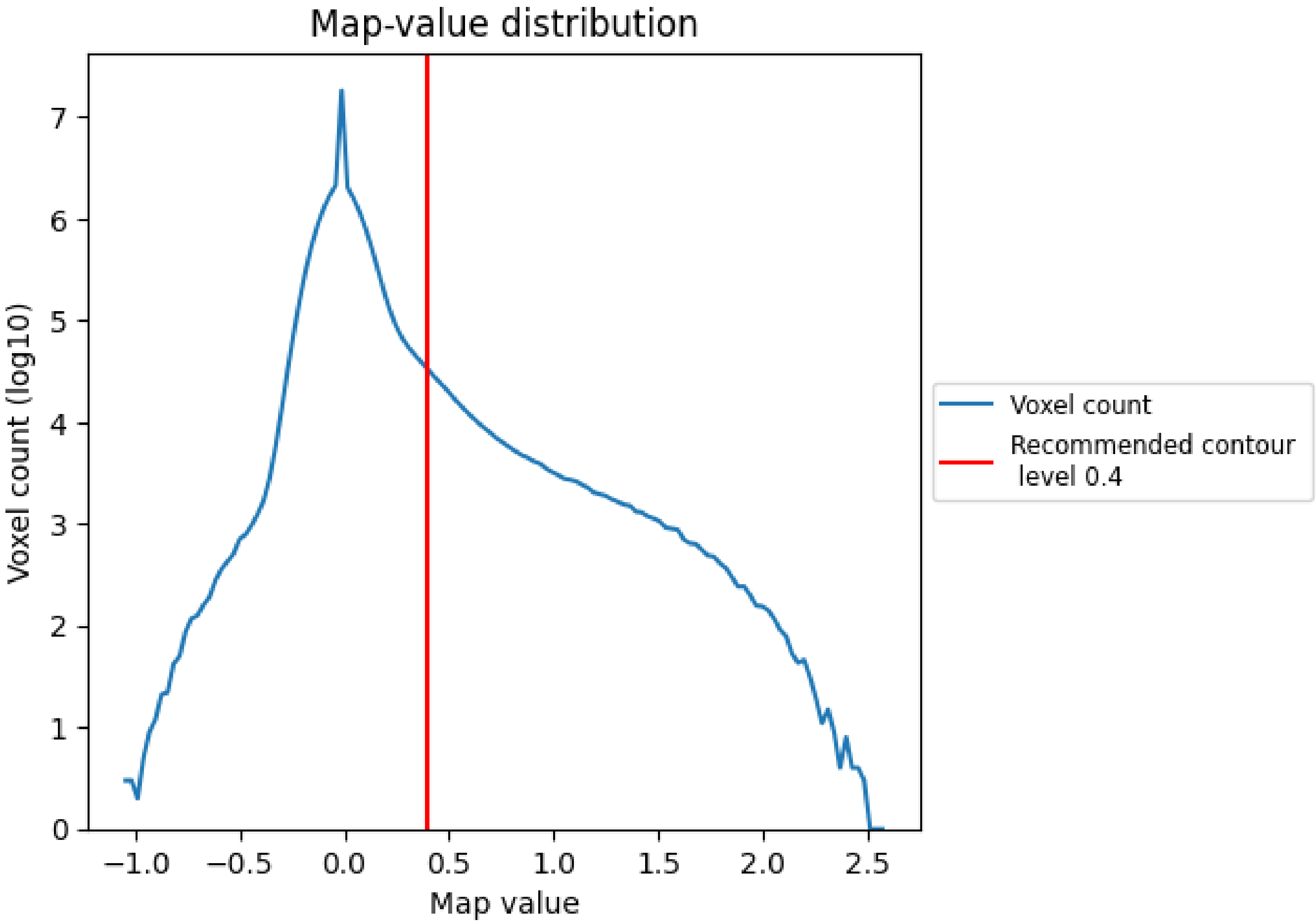
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

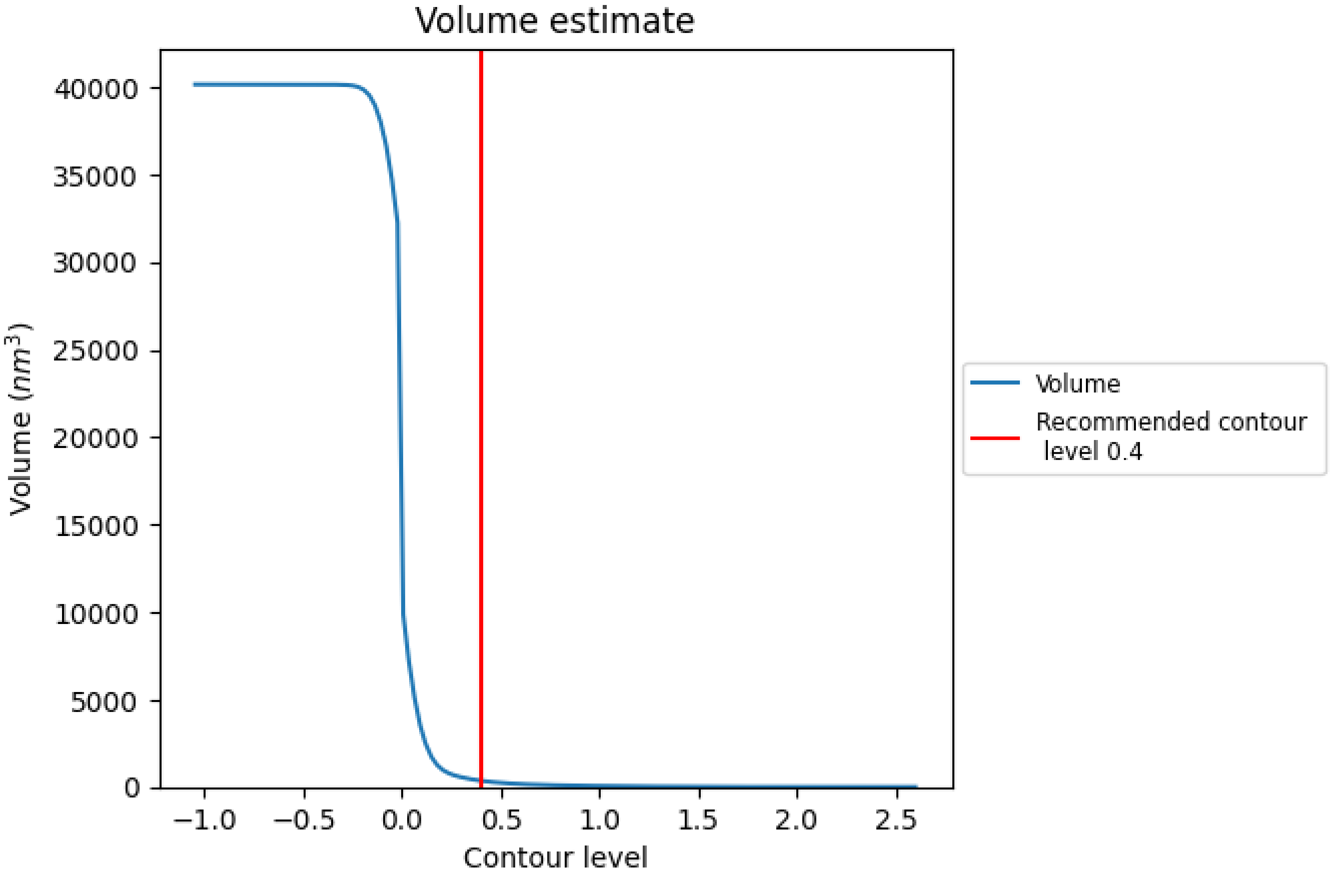
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

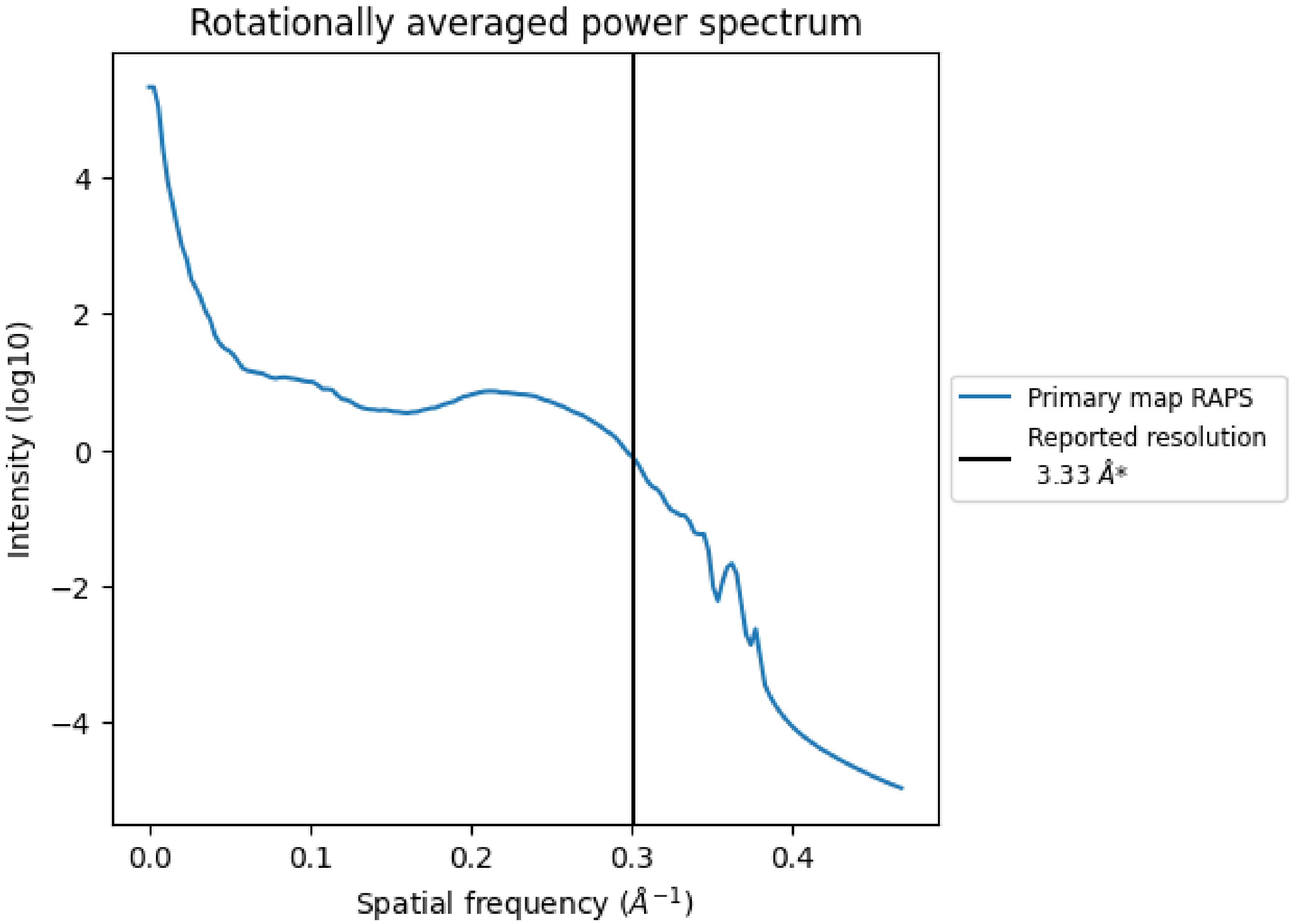
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 355 nm^3; this corresponds to an approximate mass of 320 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 ⓘ

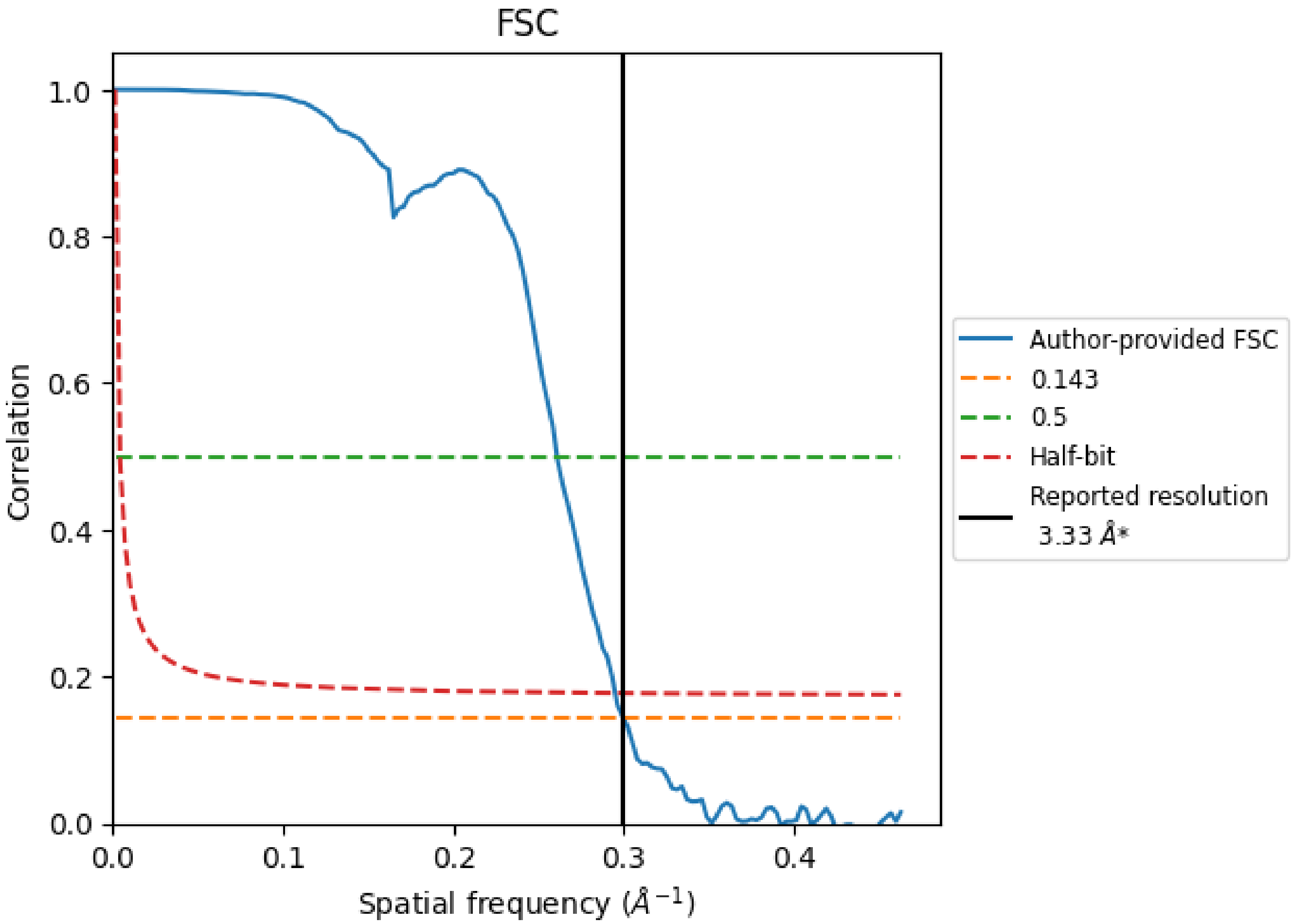


*Reported resolution corresponds to spatial frequency of 0.300 $\AA^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.300 $\AA^{-1}$

8.2 Resolution estimates ⓘ

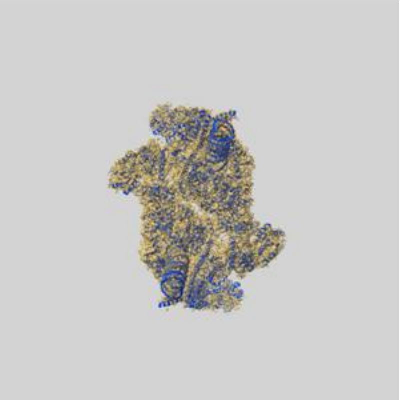
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.83	3.39
Unmasked-calculated*	-	-	-

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

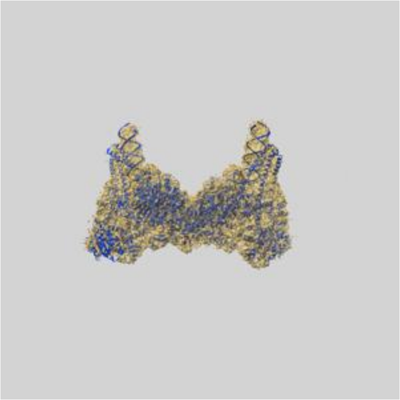
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-24432 and PDB model 7RE3. Per-residue inclusion information can be found in section 3 on page 10.

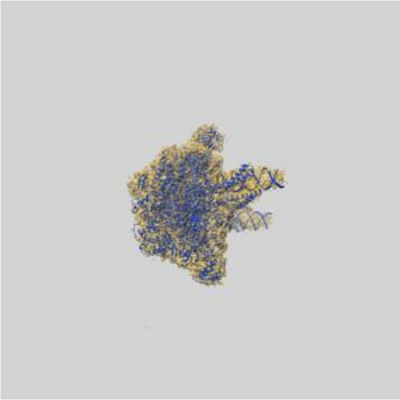
9.1 Map-model overlay ⓘ



X



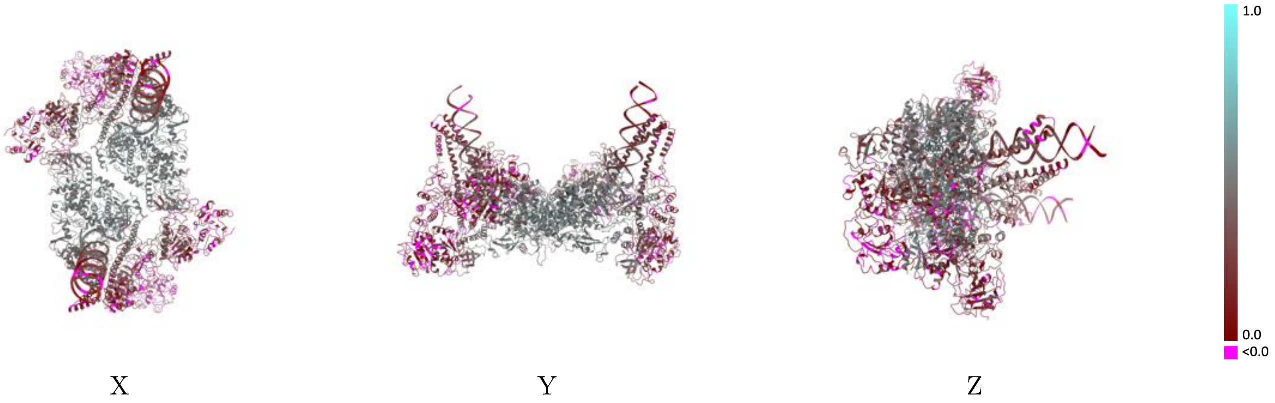
Y



Z

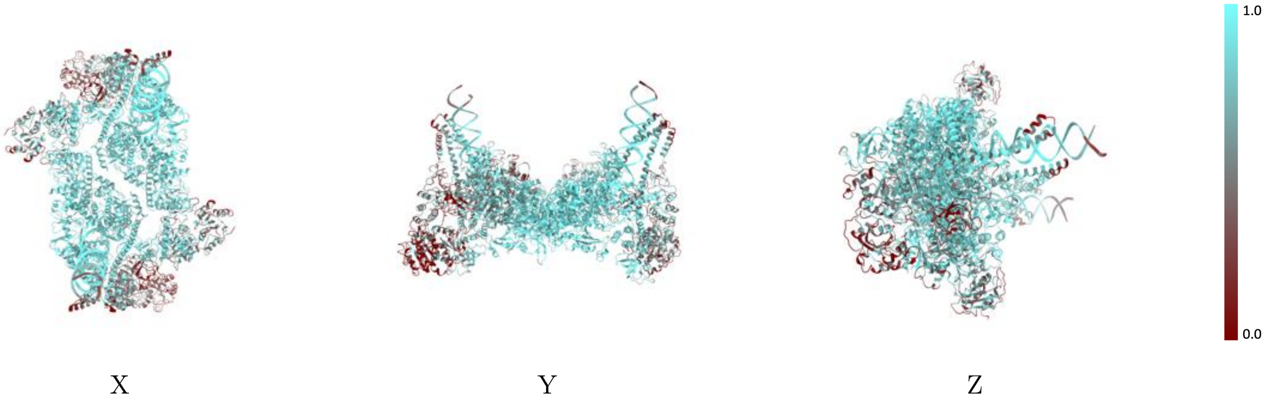
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



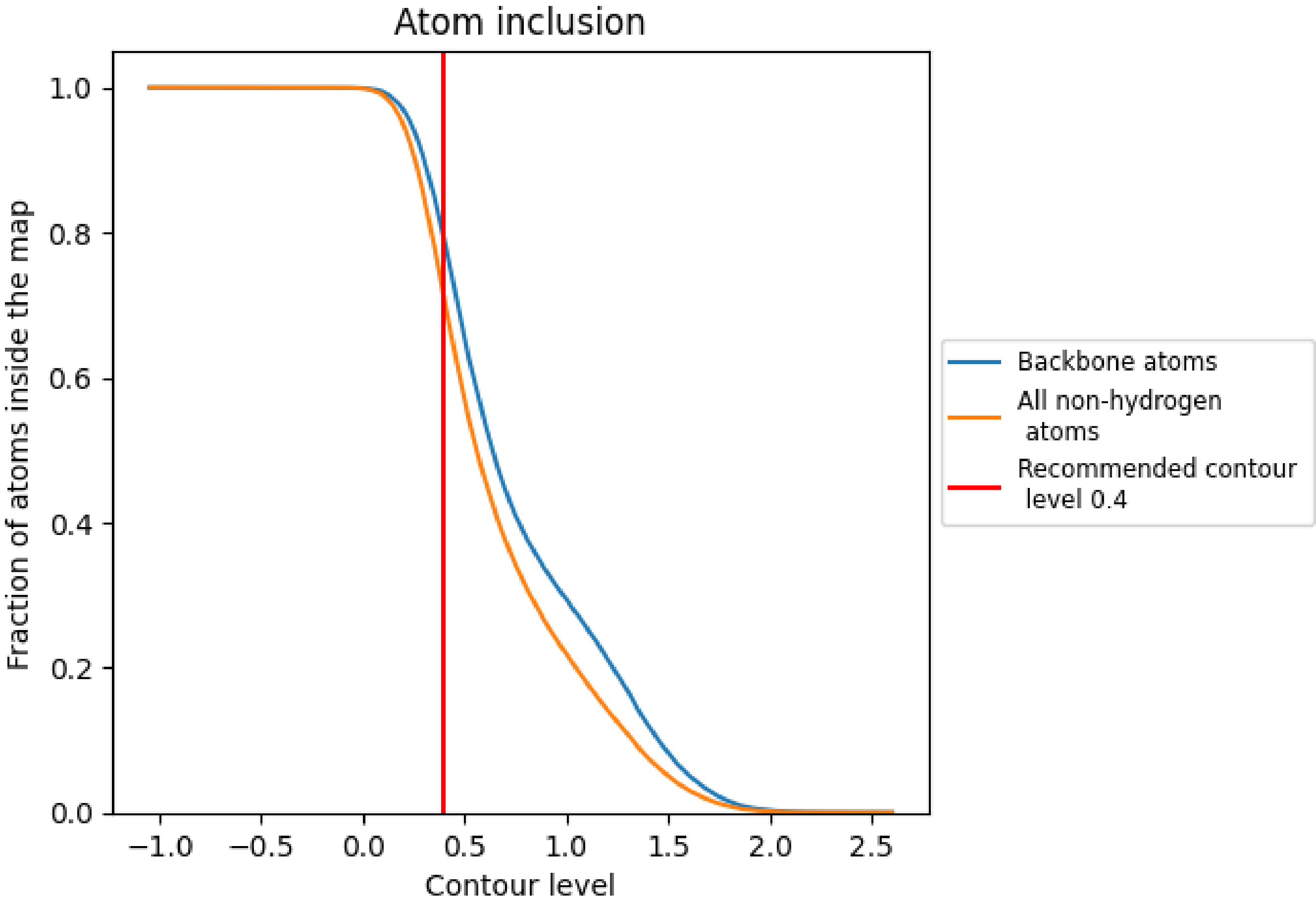
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7083	0.3210
A	0.9340	0.5010
B	0.8456	0.4150
C	0.8551	0.4290
D	0.7559	0.3160
E	0.3924	0.1360
F	0.6550	0.2260
G	0.9024	0.4880
H	0.8040	0.4060
I	0.7801	0.3900
J	0.6883	0.2750
K	0.2801	0.1090
L	0.6124	0.2080
P	0.9082	0.2960
Q	0.8428	0.2550
T	0.8568	0.2820
U	0.8226	0.3010