Full wwPDB EM Validation Report ⓘ

May 25, 2024 – 01:44 PM EDT

PDB ID	:	7RE0
EMDB ID	:	EMD-24429
Title	:	SARS-CoV-2 replication-transcription complex bound to nsp13 helicase - nsp13(2)-RTC - swiveled class
Authors	:	Chen, J.; Malone, B.; Campbell, E.A.; Darst, S.A.
Deposited on	:	2021-07-12
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

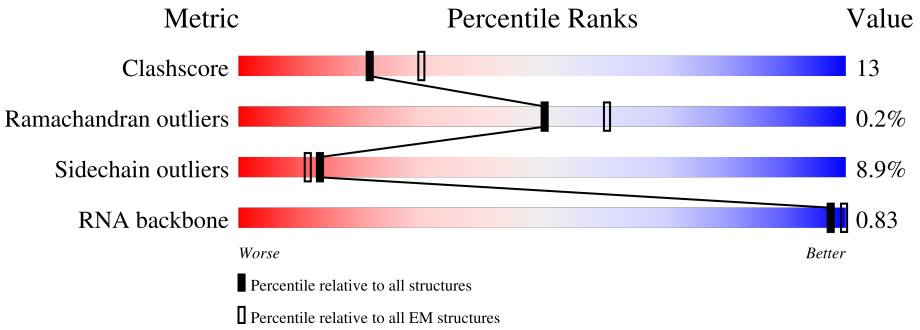
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 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	84% 15% ••
2	B	199	81% 10% •• 7%
2	D	199	69% 23% • 7%
3	C	88	73% 11% • 15%
4	E	605	64% 28% 5% •
4	F	605	60% 31% 6% •
5	P	35	43% 49% 6% •

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Mol	Chain	Length	Quality of chain
6	T	55	29% 38% 33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21577 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
1	A	927	Total	C	N	O	S	0	0
			7470	4770	1253	1393	54		

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

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

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
3	C	75	Total	C	N	O	S	0	0
			576	362	94	113	7		

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
4	E	590	Total 4550	C 2890	N 771	O 855	S 34	0	0
4	F	590	Total 4550	C 2890	N 771	O 855	S 34	0	0

There are 8 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

- Molecule 5 is a RNA chain called Product RNA.

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

- Molecule 6 is a RNA chain called Template RNA.

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

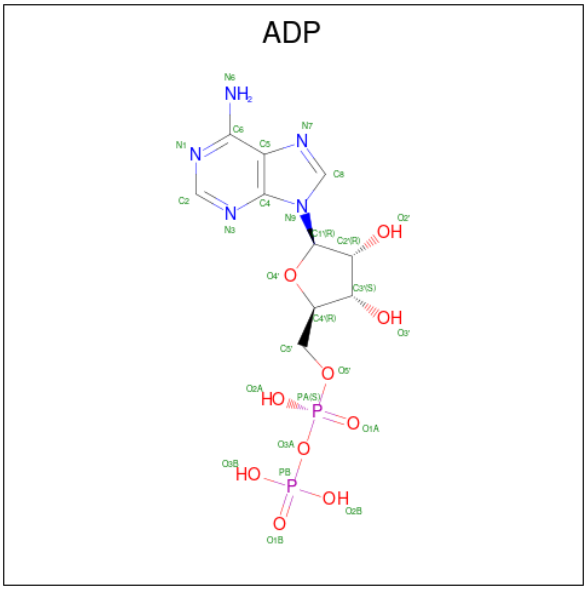
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

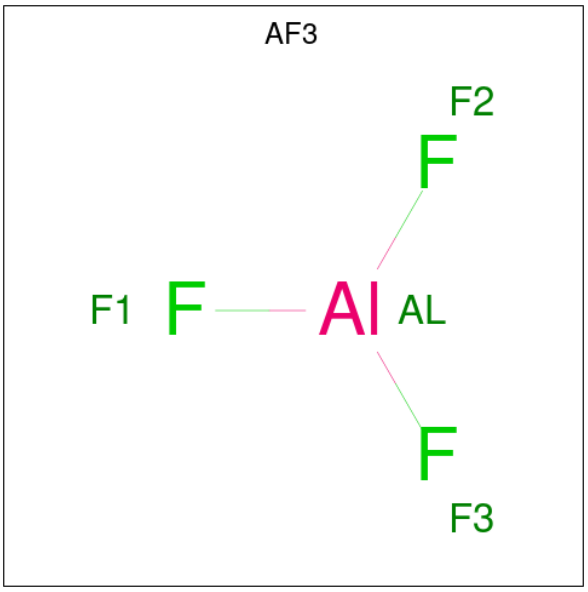
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Mg 1 1	0
8	E	1	Total Mg 1 1	0
8	F	1	Total Mg 1 1	0

- 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
9	A	1	Total C N O P 27 10 5 10 2	0
9	E	1	Total C N O P 27 10 5 10 2	0
9	F	1	Total C N O P 27 10 5 10 2	0

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



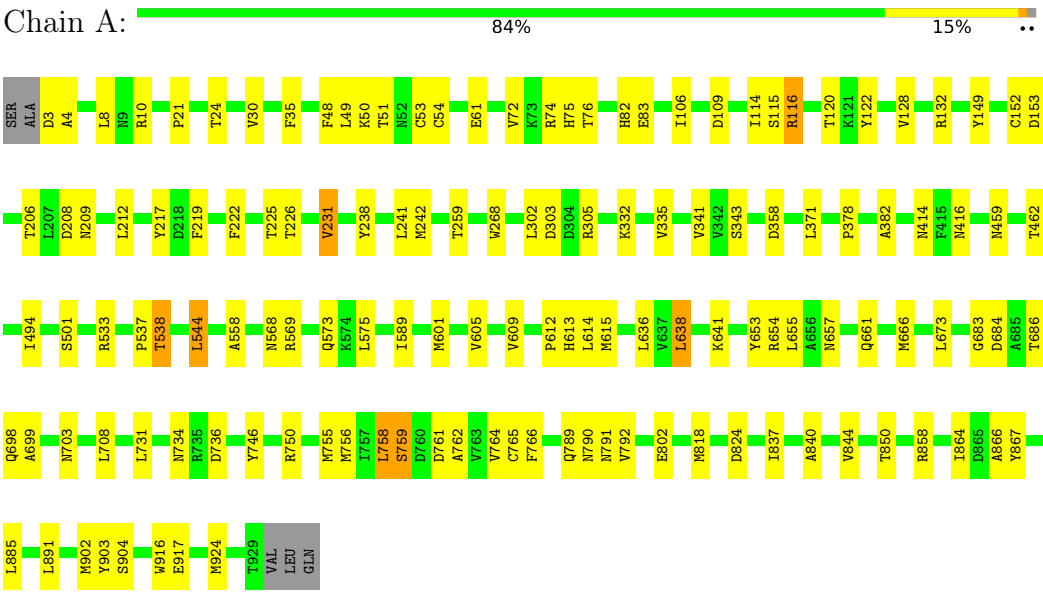
Mol	Chain	Residues	Atoms			AltConf
10	E	1	Total	Al	F	0
			4	1	3	
10	F	1	Total	Al	F	0
			4	1	3	

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.

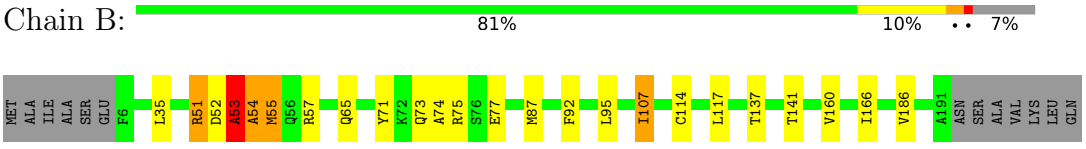
• Molecule 1: RNA-directed RNA polymerase

Chain A:



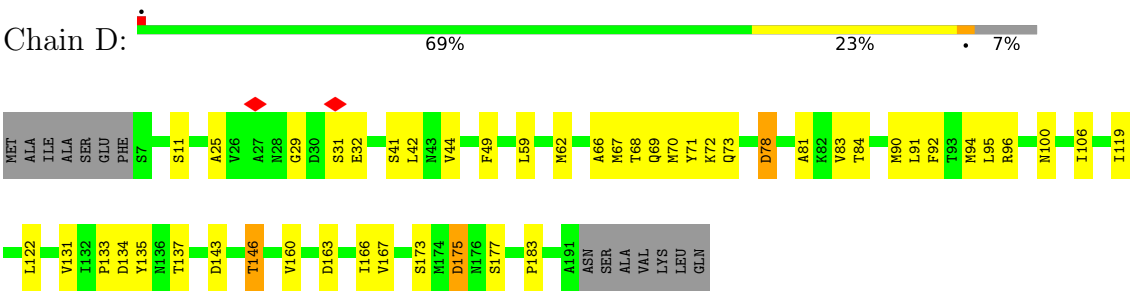
• Molecule 2: Non-structural protein 8

Chain B:



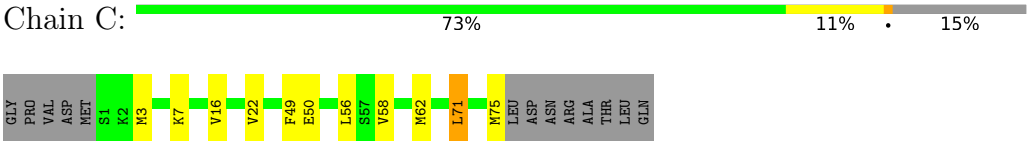
• Molecule 2: Non-structural protein 8

Chain D:



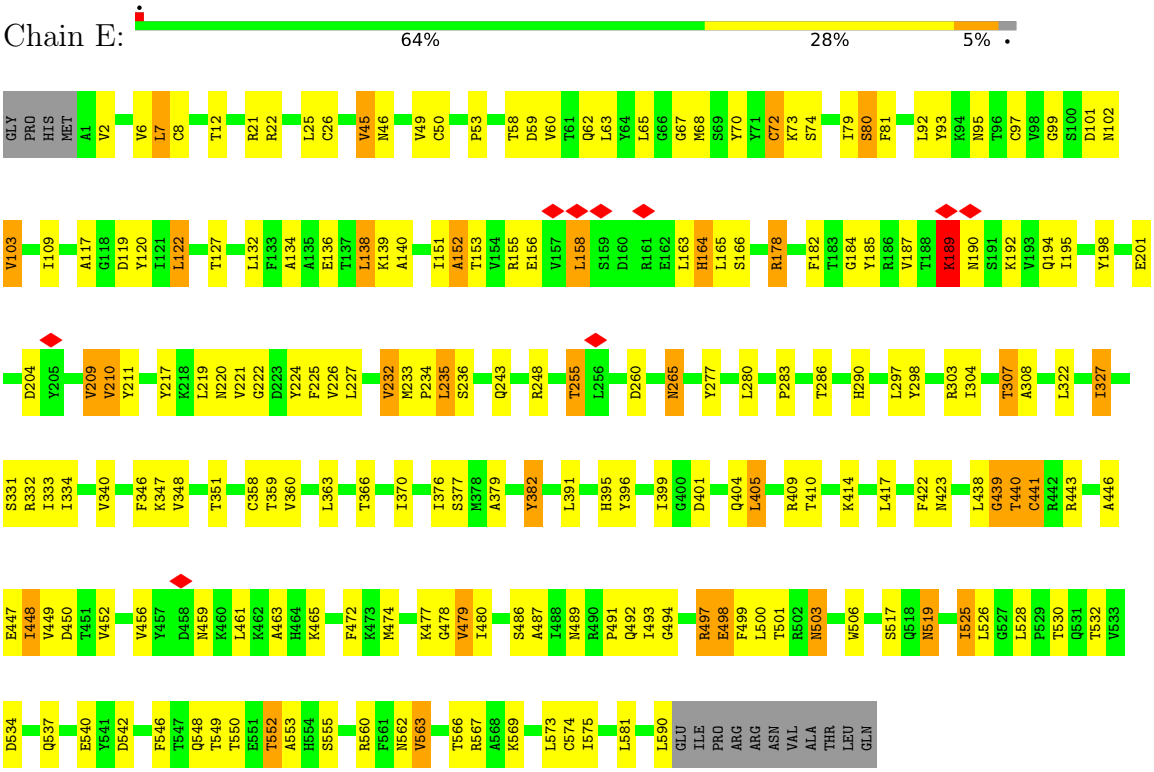
• Molecule 3: Non-structural protein 7

Chain C:



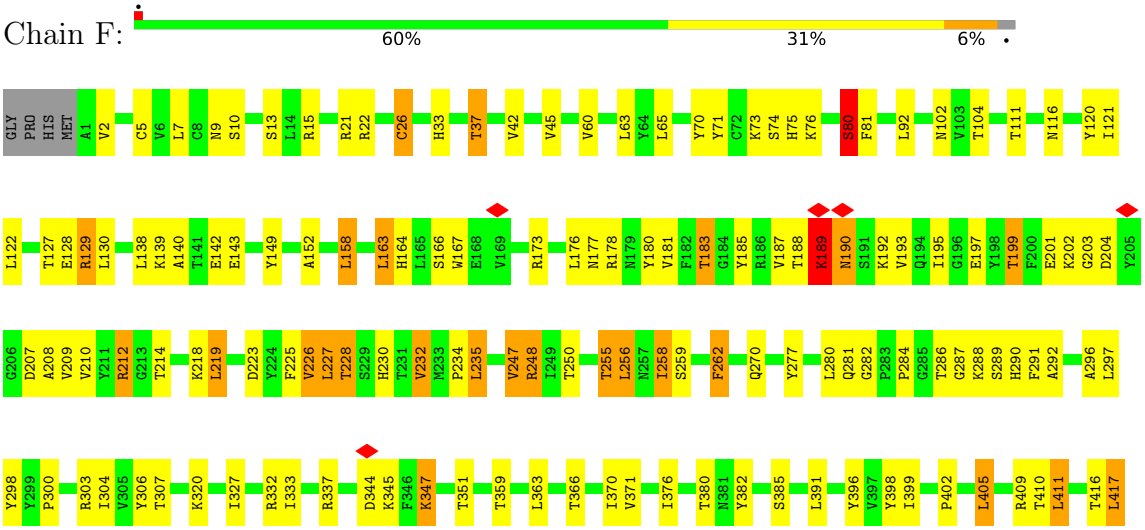
• Molecule 4: Helicase

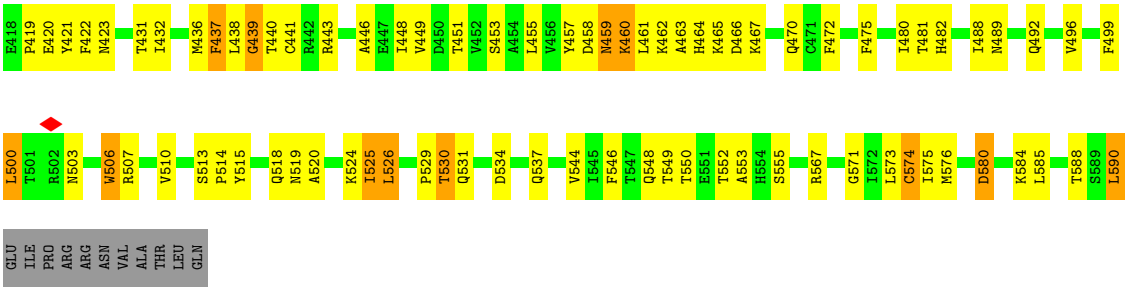
Chain E:



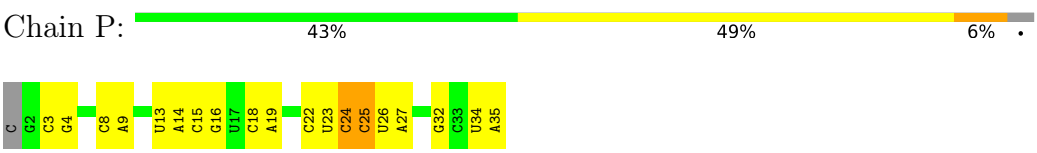
• Molecule 4: Helicase

Chain F:

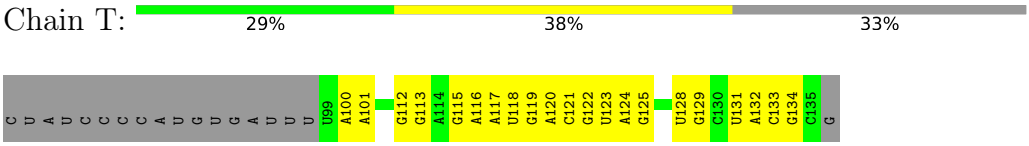




• Molecule 5: Product RNA



• Molecule 6: Template RNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54830	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 ($e^-/Å^2$)	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	36.550	Depositor
Minimum map value	-15.855	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.077	Depositor
Recommended contour level	3.5	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, ZN, ADP

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	0.45	0/10394
2	B	0.59	1/1426 (0.1%)	0.97	2/1934 (0.1%)
2	D	0.32	0/1434	0.48	0/1943
3	C	0.40	0/579	0.47	0/779
4	E	0.36	0/4651	0.55	4/6333 (0.1%)
4	F	0.38	1/4651 (0.0%)	0.57	7/6333 (0.1%)
5	P	0.33	0/802	0.81	0/1246
6	T	0.35	0/882	0.82	0/1372
All	All	0.38	2/22084 (0.0%)	0.58	13/30334 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	1
4	E	0	3
4	F	0	3
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	ALA	C-N	19.70	1.79	1.34
4	F	234	PRO	C-N	12.40	1.62	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	53	ALA	O-C-N	-37.28	63.04	122.70
4	F	234	PRO	O-C-N	-10.32	106.18	122.70
2	B	53	ALA	CA-C-N	8.40	135.68	117.20
4	E	152	ALA	N-CA-CB	-7.64	99.41	110.10
4	F	234	PRO	C-N-CA	7.22	139.75	121.70
4	F	439	GLY	N-CA-C	7.07	130.76	113.10
4	E	439	GLY	N-CA-C	6.83	130.17	113.10
4	F	189	LYS	C-N-CA	6.34	137.55	121.70
4	F	234	PRO	CA-C-N	5.93	130.25	117.20
4	F	80	SER	CB-CA-C	5.48	120.52	110.10
4	E	189	LYS	C-N-CA	5.48	135.40	121.70
4	E	440	THR	C-N-CA	-5.40	108.21	121.70
4	F	219	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	GLU	Peptide
2	D	31	SER	Peptide
4	E	189	LYS	Peptide
4	E	461	LEU	Peptide
4	E	80	SER	Peptide
4	F	189	LYS	Peptide
4	F	190	ASN	Peptide
4	F	80	SER	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	105	0
2	B	1408	0	1403	29	0
2	D	1415	0	1430	46	0
3	C	576	0	608	17	0
4	E	4550	0	4494	207	0
4	F	4550	0	4495	173	0
5	P	719	0	366	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	789	0	398	24	0
7	A	2	0	0	0	0
7	E	3	0	0	0	0
7	F	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
9	A	27	0	12	0	0
9	E	27	0	12	0	0
9	F	27	0	12	4	0
10	E	4	0	0	1	0
10	F	4	0	0	1	0
All	All	21577	0	20436	545	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 13.

All (545) 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:F:149:TYR:CB	4:F:227:LEU:HD21	1.35	1.51
2:D:73:GLN:NE2	4:E:45:VAL:CG2	1.67	1.50
3:C:3:MET:CE	3:C:7:LYS:HE3	1.38	1.50
4:E:139:LYS:NZ	4:E:382:TYR:CD2	1.78	1.41
4:E:136:GLU:CG	4:E:235:LEU:HD21	1.48	1.41
4:E:136:GLU:HG3	4:E:235:LEU:CD2	1.54	1.37
2:D:73:GLN:NE2	4:E:45:VAL:HG22	1.11	1.37
2:B:53:ALA:C	2:B:54:ALA:N	1.79	1.33
4:F:437:PHE:HZ	4:F:460:LYS:CB	1.42	1.31
2:B:53:ALA:O	2:B:54:ALA:N	1.65	1.30
1:A:902:MET:HG3	4:E:93:TYR:CE1	1.65	1.27
4:E:136:GLU:HB2	4:E:235:LEU:CD1	1.66	1.25
1:A:902:MET:O	4:E:93:TYR:HA	1.27	1.24
4:E:136:GLU:CB	4:E:235:LEU:HD11	1.68	1.22
1:A:902:MET:HG3	4:E:93:TYR:CZ	1.73	1.21
1:A:904:SER:N	4:E:95:ASN:OD1	1.76	1.17
1:A:902:MET:HA	4:E:93:TYR:CD1	1.78	1.17
1:A:904:SER:H	4:E:95:ASN:ND2	1.44	1.14
4:E:139:LYS:CE	4:E:382:TYR:HD2	1.60	1.14
4:E:139:LYS:NZ	4:E:382:TYR:CE2	2.16	1.13
4:E:139:LYS:HG2	4:E:382:TYR:CE2	1.83	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:SER:H	4:E:95:ASN:CG	1.53	1.11
4:F:437:PHE:CZ	4:F:460:LYS:CB	2.34	1.10
1:A:903:TYR:C	4:E:95:ASN:OD1	1.88	1.10
3:C:3:MET:HE2	3:C:7:LYS:HE3	1.28	1.10
3:C:3:MET:CE	3:C:7:LYS:CE	2.28	1.09
3:C:3:MET:HE1	3:C:7:LYS:HE3	1.18	1.09
4:F:183:THR:CG2	4:F:228:THR:HG22	1.81	1.09
4:E:132:LEU:O	4:E:235:LEU:HD12	1.51	1.08
4:F:183:THR:HG23	4:F:228:THR:HG21	1.34	1.08
4:F:227:LEU:H	4:F:227:LEU:HD12	1.16	1.07
4:F:149:TYR:CB	4:F:227:LEU:CD2	2.32	1.07
4:F:183:THR:HG23	4:F:228:THR:CG2	1.83	1.07
4:F:226:VAL:HG12	4:F:227:LEU:HD12	1.30	1.06
2:B:57:ARG:NH1	5:P:18:C:OP1	1.89	1.06
4:F:437:PHE:HZ	4:F:460:LYS:HB3	1.23	1.04
1:A:902:MET:SD	2:D:71:TYR:CD1	2.52	1.02
4:E:132:LEU:O	4:E:235:LEU:CD1	2.07	1.01
4:F:439:GLY:O	4:F:461:LEU:HA	1.62	1.00
1:A:903:TYR:CA	4:E:95:ASN:OD1	2.09	1.00
2:B:71:TYR:CZ	4:E:53:PRO:HB3	1.96	1.00
1:A:902:MET:SD	2:D:71:TYR:HD1	1.83	0.99
1:A:904:SER:N	4:E:95:ASN:CG	2.12	0.99
4:F:202:LYS:NZ	4:F:520:ALA:HB1	1.77	0.98
2:D:73:GLN:NE2	4:E:45:VAL:HG21	1.75	0.98
1:A:902:MET:CG	4:E:93:TYR:CE1	2.48	0.96
4:F:183:THR:OG1	4:F:228:THR:HG22	1.63	0.96
4:F:286:THR:HG22	4:F:440:THR:O	1.66	0.96
2:B:71:TYR:OH	4:E:53:PRO:HB2	1.66	0.94
4:F:183:THR:CG2	4:F:228:THR:CG2	2.39	0.94
4:F:202:LYS:HZ3	4:F:520:ALA:HB1	1.31	0.93
4:E:139:LYS:HG2	4:E:382:TYR:HE2	1.32	0.93
4:E:151:ILE:CG2	4:E:226:VAL:HG22	1.99	0.92
2:B:74:ALA:C	2:B:75:ARG:N	2.22	0.92
1:A:902:MET:HE1	4:E:92:LEU:HD13	1.50	0.92
3:C:3:MET:HE1	3:C:7:LYS:CE	1.96	0.91
2:B:71:TYR:CZ	4:E:53:PRO:CB	2.54	0.90
4:F:437:PHE:HZ	4:F:460:LYS:HB2	1.35	0.90
1:A:902:MET:HA	4:E:93:TYR:HD1	1.33	0.90
1:A:902:MET:HE2	4:E:92:LEU:HB3	1.53	0.89
4:E:139:LYS:HE3	4:E:382:TYR:HD2	1.35	0.87
4:E:139:LYS:CE	4:E:382:TYR:CD2	2.44	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:404:GLN:HB3	4:E:537:GLN:NE2	1.90	0.87
1:A:902:MET:HA	4:E:93:TYR:CE1	2.07	0.86
4:F:202:LYS:NZ	4:F:520:ALA:CB	2.38	0.86
4:E:21:ARG:NH1	4:E:232:VAL:HG13	1.90	0.85
1:A:902:MET:CA	4:E:93:TYR:CD1	2.59	0.85
4:E:404:GLN:CB	4:E:537:GLN:NE2	2.39	0.85
4:E:136:GLU:CB	4:E:235:LEU:HD21	2.05	0.85
1:A:902:MET:CE	4:E:92:LEU:HD13	2.06	0.85
4:F:226:VAL:HG12	4:F:227:LEU:CD1	2.06	0.85
4:E:233:MET:HB2	4:E:234:PRO:HD2	1.58	0.85
2:B:74:ALA:O	2:B:77:GLU:N	2.09	0.84
4:F:437:PHE:CZ	4:F:460:LYS:CG	2.60	0.84
4:E:136:GLU:CG	4:E:235:LEU:CD2	2.32	0.83
4:E:136:GLU:HB2	4:E:235:LEU:HD11	0.86	0.82
4:F:453:SER:HB3	4:F:461:LEU:HB2	1.62	0.82
4:F:546:PHE:O	4:F:574:CYS:HA	1.79	0.82
1:A:902:MET:O	4:E:93:TYR:CA	2.21	0.82
1:A:903:TYR:HA	4:E:95:ASN:OD1	1.79	0.82
4:F:437:PHE:CZ	4:F:460:LYS:HB3	2.05	0.82
4:F:183:THR:CB	4:F:228:THR:HG22	2.09	0.81
4:F:189:LYS:HB3	4:F:190:ASN:HB2	1.64	0.80
1:A:902:MET:HG3	4:E:93:TYR:CD1	2.17	0.79
4:E:101:ASP:O	4:E:103:VAL:CG2	2.31	0.79
1:A:904:SER:H	4:E:95:ASN:HD21	1.28	0.78
4:E:101:ASP:O	4:E:103:VAL:HG22	1.82	0.78
4:E:117:ALA:HB2	4:E:414:LYS:O	1.84	0.78
4:F:143:GLU:OE2	4:F:230:HIS:CE1	2.38	0.77
4:E:178:ARG:HD3	4:E:340:VAL:HG22	1.68	0.77
2:D:73:GLN:HE22	4:E:45:VAL:HG22	0.95	0.75
4:F:437:PHE:HZ	4:F:460:LYS:CG	1.99	0.75
4:F:183:THR:OG1	4:F:228:THR:CG2	2.34	0.75
4:F:202:LYS:HZ2	4:F:520:ALA:CB	2.01	0.73
4:F:320:LYS:NZ	9:F:1003:ADP:O1A	2.19	0.73
2:B:74:ALA:O	2:B:77:GLU:HB2	1.87	0.73
4:E:139:LYS:NZ	4:E:382:TYR:HD2	1.40	0.73
4:E:549:THR:HG22	4:E:550:THR:HG23	1.70	0.73
2:D:70:MET:HG3	4:E:45:VAL:HG11	1.69	0.73
4:F:437:PHE:CZ	4:F:460:LYS:HB2	2.14	0.73
4:E:235:LEU:HD23	4:E:235:LEU:N	2.03	0.72
4:F:437:PHE:CZ	4:F:460:LYS:HG2	2.24	0.72
1:A:902:MET:CG	4:E:93:TYR:CD1	2.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:136:GLU:CA	4:E:235:LEU:HD11	2.20	0.71
2:B:71:TYR:CE2	4:F:92:LEU:HD22	2.26	0.71
4:F:500:LEU:O	4:F:507:ARG:NH2	2.23	0.71
4:F:286:THR:CG2	4:F:440:THR:O	2.38	0.70
4:E:189:LYS:H	4:E:190:ASN:HB2	1.56	0.70
2:B:74:ALA:C	2:B:77:GLU:H	1.94	0.70
2:B:71:TYR:OH	4:E:53:PRO:CB	2.38	0.70
4:E:136:GLU:HB2	4:E:235:LEU:CG	2.21	0.70
3:C:56:LEU:HD23	2:D:106:ILE:HD11	1.72	0.69
4:E:552:THR:HG23	4:E:555:SER:H	1.57	0.69
4:F:142:GLU:HG2	4:F:411:LEU:HD23	1.74	0.69
2:D:73:GLN:CD	4:E:45:VAL:HG21	2.13	0.69
4:F:185:TYR:O	4:F:223:ASP:HA	1.92	0.69
4:F:446:ALA:H	4:F:467:LYS:HB3	1.56	0.69
3:C:50:GLU:HB3	2:D:122:LEU:HD22	1.75	0.68
4:E:494:GLY:HA2	4:E:497:ARG:HD3	1.76	0.68
3:C:58:VAL:HG22	2:D:119:ILE:HG12	1.74	0.68
4:F:183:THR:HG21	4:F:228:THR:HG22	1.73	0.68
4:F:405:LEU:HD11	4:F:537:GLN:OE1	1.93	0.67
4:F:510:VAL:HA	4:F:529:PRO:O	1.93	0.67
1:A:904:SER:N	4:E:95:ASN:ND2	2.29	0.67
4:F:489:ASN:HD22	4:F:549:THR:HA	1.59	0.67
2:D:73:GLN:CD	4:E:45:VAL:CG2	2.58	0.67
4:E:136:GLU:HG3	4:E:235:LEU:HD21	0.72	0.66
4:E:404:GLN:HB3	4:E:537:GLN:HE21	1.59	0.65
2:D:70:MET:HE1	4:E:70:TYR:OH	1.96	0.65
4:E:280:LEU:HB3	4:E:399:ILE:HG22	1.77	0.65
4:F:227:LEU:H	4:F:227:LEU:CD1	1.94	0.65
2:D:62:MET:SD	4:E:79:ILE:HG21	2.35	0.65
1:A:83:GLU:HG3	1:A:219:PHE:HB2	1.79	0.65
4:F:201:GLU:H	4:F:209:VAL:HG23	1.62	0.65
5:P:25:C:O2	6:T:112:G:N2	2.19	0.65
4:F:202:LYS:HZ3	4:F:520:ALA:CB	2.02	0.65
4:F:440:THR:HG22	4:F:441:CYS:N	2.11	0.65
4:E:139:LYS:HE3	4:E:382:TYR:CD2	2.26	0.64
4:E:233:MET:HB2	4:E:234:PRO:CD	2.26	0.64
4:F:518:GLN:NE2	4:F:549:THR:OG1	2.30	0.64
1:A:902:MET:CA	4:E:93:TYR:CE1	2.80	0.64
4:E:265:ASN:OD1	4:E:265:ASN:N	2.29	0.64
2:D:25:ALA:O	2:D:29:GLY:N	2.29	0.64
4:E:136:GLU:N	4:E:235:LEU:HD11	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:404:GLN:HB2	4:E:537:GLN:NE2	2.13	0.64
4:F:525:ILE:HG12	4:F:526:LEU:HG	1.78	0.64
1:A:902:MET:HG3	4:E:93:TYR:CE2	2.30	0.64
1:A:902:MET:CE	4:E:92:LEU:HB3	2.28	0.64
4:E:552:THR:OG1	4:E:553:ALA:N	2.31	0.64
1:A:50:LYS:NZ	1:A:53:CYS:SG	2.72	0.63
4:F:470:GLN:O	4:F:571:GLY:HA2	1.99	0.62
4:E:187:VAL:HG12	4:E:192:LYS:HG3	1.80	0.62
4:F:270:GLN:NE2	4:F:298:TYR:OH	2.30	0.62
4:F:520:ALA:O	4:F:524:LYS:NZ	2.24	0.62
4:E:404:GLN:HB2	4:E:537:GLN:HE22	1.63	0.62
2:D:70:MET:CE	4:E:70:TYR:OH	2.48	0.62
4:E:151:ILE:HG22	4:E:226:VAL:HG22	1.78	0.61
2:D:175:ASP:OD1	2:D:175:ASP:N	2.34	0.61
1:A:698:GLN:NE2	1:A:790:ASN:OD1	2.34	0.61
1:A:358:ASP:OD1	1:A:533:ARG:NH1	2.33	0.61
1:A:691:ASN:HB3	1:A:759:SER:O	2.01	0.61
4:E:440:THR:HG22	4:E:441:CYS:N	2.16	0.61
6:T:128:U:H2'	6:T:129:G:H8	1.66	0.61
4:E:60:VAL:HA	4:E:63:LEU:HD12	1.82	0.61
4:F:187:VAL:HG13	4:F:192:LYS:HB2	1.81	0.61
4:F:255:THR:OG1	4:F:256:LEU:N	2.34	0.61
4:E:151:ILE:HG21	4:E:226:VAL:HG22	1.82	0.60
4:E:404:GLN:CB	4:E:537:GLN:HE21	2.12	0.60
3:C:75:MET:HB3	2:D:96:ARG:HD3	1.82	0.60
1:A:116:ARG:HG2	1:A:217:TYR:HB2	1.83	0.60
4:F:440:THR:HG22	4:F:441:CYS:H	1.66	0.60
2:B:51:ARG:O	2:B:55:MET:CE	2.50	0.60
4:F:176:LEU:HB3	4:F:201:GLU:HA	1.84	0.60
4:E:201:GLU:HG3	4:E:210:VAL:HG23	1.84	0.59
3:C:3:MET:CE	3:C:7:LYS:CD	2.80	0.59
2:D:59:LEU:HD11	4:E:81:PHE:HB3	1.82	0.59
1:A:902:MET:CB	4:E:93:TYR:CE1	2.85	0.59
4:E:119:ASP:HA	4:E:122:LEU:HD23	1.85	0.59
4:F:247:VAL:HB	4:F:248:ARG:HD2	1.84	0.59
4:F:287:GLY:O	4:F:291:PHE:N	2.35	0.59
1:A:538:THR:HB	1:A:661:GLN:HG2	1.85	0.59
4:E:155:ARG:HH22	4:F:248:ARG:NH1	2.00	0.59
4:E:233:MET:CB	4:E:234:PRO:HD2	2.30	0.59
4:E:286:THR:HG22	4:E:440:THR:H	1.67	0.59
4:E:331:SER:OG	4:E:332:ARG:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:515:TYR:OH	4:F:550:THR:OG1	2.20	0.59
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.84	0.58
4:E:286:THR:HG22	4:E:440:THR:O	2.03	0.58
1:A:501:SER:OG	6:T:100:A:OP1	2.17	0.58
4:E:163:LEU:HB2	4:E:211:TYR:CD1	2.39	0.58
4:E:377:SER:OG	4:E:401:ASP:O	2.21	0.58
4:F:537:GLN:H	4:F:567:ARG:HD2	1.69	0.58
1:A:698:GLN:OE1	1:A:789:GLN:NE2	2.36	0.58
4:F:513:SER:OG	4:F:515:TYR:O	2.19	0.58
4:F:183:THR:O	4:F:225:PHE:HA	2.03	0.58
4:F:288:LYS:NZ	10:F:1005:AF3:F2	2.27	0.58
5:P:26:U:H2'	5:P:27:A:H8	1.68	0.58
4:E:534:ASP:OD1	4:E:560:ARG:NH1	2.35	0.58
4:F:262:PHE:HB3	4:F:290:HIS:HE1	1.69	0.57
4:F:80:SER:HB3	4:F:81:PHE:HA	1.87	0.57
4:F:496:VAL:HG12	4:F:500:LEU:HD12	1.86	0.57
1:A:589:ILE:HG12	1:A:758:LEU:HD13	1.86	0.57
4:F:2:VAL:HG12	4:F:13:SER:HB2	1.85	0.57
4:F:227:LEU:O	4:F:228:THR:HG23	2.04	0.57
2:D:62:MET:HE1	4:E:67:GLY:HA2	1.87	0.57
4:F:481:THR:O	4:F:482:HIS:ND1	2.38	0.57
1:A:416:ASN:HA	1:A:850:THR:HG23	1.86	0.57
2:D:78:ASP:O	2:D:81:ALA:HB3	2.04	0.57
4:E:283:PRO:HG2	4:E:286:THR:HG21	1.86	0.57
6:T:131:U:H2'	6:T:132:A:H8	1.68	0.56
4:F:197:GLU:O	4:F:214:THR:CB	2.52	0.56
4:F:332:ARG:NH1	4:F:333:ILE:O	2.38	0.56
4:E:155:ARG:HG2	4:E:166:SER:HB2	1.87	0.56
4:F:292:ALA:HB1	4:F:306:TYR:HE2	1.70	0.56
4:E:303:ARG:NH2	4:E:351:THR:O	2.39	0.56
4:F:255:THR:HB	4:F:300:PRO:HD3	1.87	0.56
4:F:519:ASN:OD1	4:F:530:THR:OG1	2.19	0.56
4:F:227:LEU:C	4:F:228:THR:HG23	2.26	0.56
6:T:123:U:H2'	6:T:124:A:H8	1.70	0.56
4:E:201:GLU:H	4:E:209:VAL:HG23	1.71	0.55
1:A:30:VAL:HG13	1:A:51:THR:HG22	1.87	0.55
4:E:136:GLU:CB	4:E:235:LEU:CD2	2.80	0.55
4:F:496:VAL:HG13	4:F:573:LEU:HD23	1.88	0.55
2:D:70:MET:HG3	4:E:45:VAL:CG1	2.37	0.55
2:B:74:ALA:HB2	4:F:45:VAL:HG11	1.88	0.55
4:F:286:THR:N	9:F:1003:ADP:O1B	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:197:GLU:O	4:F:214:THR:HB	2.06	0.55
4:F:280:LEU:HB3	4:F:399:ILE:HG22	1.87	0.55
3:C:3:MET:HE3	3:C:7:LYS:CD	2.37	0.55
2:B:71:TYR:CE1	4:E:53:PRO:HB3	2.42	0.54
2:D:62:MET:CE	4:E:67:GLY:HA2	2.37	0.54
4:E:6:VAL:HG23	4:E:7:LEU:HD23	1.89	0.54
1:A:666:MET:HB3	1:A:673:LEU:HD22	1.89	0.54
3:C:3:MET:HE2	3:C:7:LYS:CE	2.16	0.54
4:F:33:HIS:O	4:F:37:THR:OG1	2.26	0.54
6:T:128:U:H2'	6:T:129:G:C8	2.43	0.54
4:E:151:ILE:CB	4:E:226:VAL:HG22	2.37	0.54
4:F:548:GLN:HE21	4:F:555:SER:HB2	1.72	0.54
4:E:139:LYS:CG	4:E:382:TYR:CE2	2.75	0.53
4:E:139:LYS:HG2	4:E:382:TYR:CD2	2.39	0.53
4:E:155:ARG:HB2	4:E:164:HIS:HB3	1.90	0.53
4:E:21:ARG:HH11	4:E:232:VAL:HG13	1.68	0.53
4:E:465:LYS:NZ	4:E:569:LYS:O	2.38	0.53
4:E:59:ASP:HB3	4:E:62:GLN:HG3	1.90	0.53
4:E:136:GLU:H	4:E:235:LEU:HD11	1.73	0.53
4:F:510:VAL:HB	4:F:544:VAL:HG22	1.90	0.53
1:A:858:ARG:HG2	5:P:32:G:H5'	1.91	0.53
4:F:73:LYS:HZ3	4:F:76:LYS:HD3	1.73	0.53
5:P:25:C:H2'	5:P:26:U:H6	1.74	0.53
1:A:468:GLN:HA	1:A:731:LEU:HD22	1.90	0.53
4:E:379:ALA:O	4:E:423:ASN:ND2	2.42	0.53
4:E:260:ASP:OD1	4:E:260:ASP:N	2.33	0.53
5:P:24:C:H2'	5:P:25:C:H6	1.74	0.53
2:D:73:GLN:NE2	4:E:45:VAL:HG23	2.06	0.52
2:B:74:ALA:O	2:B:77:GLU:CB	2.56	0.52
4:E:184:GLY:HA2	4:E:224:TYR:O	2.10	0.52
4:E:198:TYR:OH	4:E:217:TYR:O	2.27	0.52
4:F:514:PRO:HD3	4:F:546:PHE:HE1	1.74	0.52
1:A:684:ASP:N	1:A:684:ASP:OD1	2.40	0.52
4:E:136:GLU:OE1	4:E:235:LEU:HG	2.09	0.52
4:F:303:ARG:NH2	4:F:351:THR:O	2.38	0.52
5:P:25:C:H2'	5:P:26:U:C6	2.45	0.52
2:B:51:ARG:O	2:B:55:MET:HE1	2.10	0.52
4:F:197:GLU:O	4:F:214:THR:OG1	2.25	0.52
1:A:615:MET:HB2	1:A:766:PHE:HE1	1.73	0.52
4:F:199:THR:HG22	4:F:212:ARG:HB3	1.91	0.52
1:A:824:ASP:OD1	1:A:824:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:286:THR:CG2	4:E:440:THR:H	2.22	0.52
4:E:443:ARG:NH2	4:E:540:GLU:OE1	2.39	0.52
5:P:26:U:H2'	5:P:27:A:C8	2.44	0.52
1:A:837:ILE:O	1:A:884:TYR:OH	2.28	0.52
4:E:405:LEU:HD21	4:E:534:ASP:HA	1.92	0.52
2:B:71:TYR:CE2	4:E:53:PRO:HB3	2.42	0.52
6:T:115:G:H2'	6:T:116:A:H8	1.75	0.52
1:A:653:TYR:O	1:A:657:ASN:ND2	2.37	0.51
1:A:206:THR:OG1	1:A:209:ASN:ND2	2.44	0.51
4:E:151:ILE:HB	4:E:226:VAL:HG22	1.92	0.51
4:F:13:SER:O	4:F:13:SER:OG	2.26	0.51
4:F:127:THR:OG1	4:F:128:GLU:N	2.43	0.51
4:F:451:THR:O	4:F:455:LEU:N	2.42	0.51
2:B:54:ALA:HA	2:B:57:ARG:HD3	1.93	0.51
4:E:446:ALA:O	4:E:450:ASP:HB2	2.11	0.51
4:F:304:ILE:HG12	4:F:370:ILE:HG23	1.92	0.51
1:A:601:MET:O	1:A:605:VAL:HG23	2.11	0.51
4:F:277:TYR:HA	4:F:396:TYR:O	2.10	0.51
4:E:370:ILE:HA	4:E:395:HIS:O	2.10	0.51
4:E:472:PHE:HB3	4:E:590:LEU:HD21	1.93	0.51
4:E:489:ASN:HB2	4:E:549:THR:HG23	1.93	0.51
1:A:636:LEU:HD21	1:A:655:LEU:HD22	1.92	0.50
4:E:189:LYS:N	4:E:190:ASN:HB2	2.24	0.50
1:A:305:ARG:NH1	1:A:470:LEU:O	2.43	0.50
1:A:885:LEU:HG	1:A:916:TRP:HA	1.94	0.50
4:E:153:THR:HG23	4:E:166:SER:HB3	1.94	0.50
6:T:133:C:H2'	6:T:134:G:H8	1.75	0.50
2:D:173:SER:O	2:D:177:SER:OG	2.21	0.50
1:A:149:TYR:HE2	1:A:212:LEU:HD13	1.76	0.50
4:E:49:VAL:HG12	4:E:58:THR:HG22	1.93	0.50
4:E:185:TYR:HB3	4:E:187:VAL:HG13	1.94	0.50
4:E:158:LEU:H	4:E:158:LEU:HD22	1.77	0.50
4:E:21:ARG:HD3	4:E:140:ALA:HB2	1.93	0.49
1:A:109:ASP:N	1:A:109:ASP:OD1	2.45	0.49
1:A:128:VAL:O	1:A:132:ARG:HB2	2.12	0.49
2:D:59:LEU:HD21	4:E:81:PHE:HB3	1.94	0.49
4:F:284:PRO:HD3	4:F:457:TYR:OH	2.12	0.49
6:T:123:U:H2'	6:T:124:A:C8	2.46	0.49
2:B:160:VAL:HG12	2:B:166:ILE:HD13	1.92	0.49
4:F:417:LEU:HD21	4:F:421:TYR:HB2	1.94	0.49
4:E:50:CYS:SG	4:E:72:CYS:N	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:419:PRO:HA	4:F:422:PHE:CZ	2.47	0.49
4:E:132:LEU:O	4:E:235:LEU:HD11	2.08	0.49
4:E:448:ILE:HD11	4:E:566:THR:HA	1.94	0.49
4:E:233:MET:CB	4:E:234:PRO:CD	2.89	0.49
1:A:569:ARG:O	1:A:573:GLN:HB2	2.12	0.49
2:D:70:MET:HG2	4:E:92:LEU:HD21	1.93	0.49
1:A:902:MET:CE	2:D:71:TYR:HD1	2.25	0.48
4:E:101:ASP:HA	4:E:103:VAL:HG22	1.95	0.48
5:P:13:U:H2'	5:P:14:A:H8	1.77	0.48
4:E:503:ASN:HB3	4:E:506:TRP:CD1	2.48	0.48
4:F:363:LEU:HD13	4:F:391:LEU:HD23	1.95	0.48
4:F:458:ASP:H	4:F:460:LYS:NZ	2.10	0.48
1:A:382:ALA:HB3	2:B:117:LEU:HD11	1.95	0.48
6:T:116:A:H2'	6:T:117:A:H8	1.77	0.48
4:E:136:GLU:CG	4:E:235:LEU:CG	2.91	0.48
5:P:18:C:H2'	5:P:19:A:H8	1.79	0.48
2:D:66:ALA:CB	4:E:65:LEU:HD21	2.44	0.48
1:A:501:SER:HB3	6:T:101:A:H5'	1.94	0.48
4:E:80:SER:CB	4:E:81:PHE:HA	2.44	0.48
1:A:72:VAL:HG13	1:A:115:SER:HB2	1.95	0.48
4:E:443:ARG:NH1	4:E:567:ARG:HH21	2.12	0.48
4:F:42:VAL:HB	4:F:60:VAL:HG21	1.96	0.48
1:A:75:HIS:CG	1:A:76:THR:H	2.31	0.48
1:A:202:VAL:HG13	1:A:231:VAL:HG13	1.94	0.48
4:E:479:VAL:HG23	4:E:491:PRO:HG3	1.95	0.48
2:D:83:VAL:HG13	2:D:84:THR:N	2.28	0.48
4:E:2:VAL:HG23	4:E:2:VAL:O	2.12	0.48
4:F:282:GLY:N	4:F:288:LYS:HD3	2.29	0.48
2:B:74:ALA:O	2:B:77:GLU:CA	2.62	0.47
4:F:289:SER:HB2	4:F:320:LYS:HZ2	1.79	0.47
2:D:143:ASP:O	2:D:146:THR:OG1	2.30	0.47
1:A:3:ASP:OD1	1:A:4:ALA:N	2.47	0.47
6:T:133:C:H2'	6:T:134:G:C8	2.48	0.47
4:F:503:ASN:HD22	4:F:506:TRP:HZ2	1.62	0.47
1:A:54:CYS:SG	1:A:74:ARG:NH2	2.86	0.47
1:A:303:ASP:N	1:A:303:ASP:OD1	2.47	0.47
1:A:605:VAL:HG12	1:A:765:CYS:HB2	1.97	0.47
2:B:73:GLN:O	2:B:77:GLU:HG3	2.14	0.47
4:E:405:LEU:CD2	4:E:534:ASP:HA	2.45	0.47
4:F:287:GLY:N	9:F:1003:ADP:O1B	2.26	0.47
1:A:35:PHE:HD2	1:A:48:PHE:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:LEU:HA	1:A:764:VAL:O	2.15	0.47
4:E:243:GLN:HB2	4:E:277:TYR:CE2	2.50	0.47
4:F:437:PHE:CE2	4:F:460:LYS:HG2	2.49	0.47
4:F:202:LYS:NZ	4:F:520:ALA:HB3	2.29	0.47
4:F:203:GLY:HA3	4:F:208:ALA:HB3	1.96	0.47
4:E:519:ASN:OD1	4:E:530:THR:OG1	2.23	0.46
6:T:120:A:H2'	6:T:121:C:C6	2.50	0.46
1:A:867:TYR:O	1:A:870:THR:OG1	2.32	0.46
5:P:3:C:H2'	5:P:4:G:H8	1.80	0.46
4:E:74:SER:O	4:E:74:SER:OG	2.33	0.46
2:D:133:PRO:HA	2:D:183:PRO:HB3	1.97	0.46
4:E:136:GLU:CB	4:E:235:LEU:CG	2.89	0.46
4:F:548:GLN:HB2	4:F:575:ILE:O	2.16	0.46
1:A:605:VAL:HG22	1:A:756:MET:HB2	1.98	0.46
3:C:16:VAL:HG21	2:D:91:LEU:HD22	1.98	0.46
4:F:152:ALA:HB2	4:F:167:TRP:CE3	2.50	0.46
6:T:131:U:H2'	6:T:132:A:C8	2.50	0.46
1:A:756:MET:O	1:A:762:ALA:HA	2.16	0.46
5:P:24:C:H2'	5:P:25:C:C6	2.51	0.46
1:A:8:LEU:HD11	1:A:21:PRO:HD3	1.98	0.46
4:E:132:LEU:C	4:E:235:LEU:HD12	2.32	0.46
4:F:376:ILE:HG21	4:F:398:TYR:HB3	1.98	0.46
4:F:548:GLN:NE2	4:F:555:SER:HB2	2.30	0.46
5:P:8:C:H2'	5:P:9:A:H8	1.81	0.46
4:F:441:CYS:N	4:F:462:LYS:O	2.45	0.46
4:E:255:THR:OG1	4:E:298:TYR:O	2.33	0.45
4:F:5:CYS:HB2	4:F:26:CYS:HB3	1.97	0.45
4:F:65:LEU:HD21	4:F:81:PHE:CE2	2.51	0.45
4:F:459:ASN:N	4:F:459:ASN:OD1	2.48	0.45
1:A:332:LYS:HB2	2:B:107:ILE:HD13	1.98	0.45
1:A:699:ALA:O	1:A:703:ASN:ND2	2.44	0.45
4:E:409:ARG:NH2	4:E:422:PHE:O	2.48	0.45
6:T:116:A:H2'	6:T:117:A:C8	2.52	0.45
1:A:614:LEU:HB2	1:A:802:GLU:HB3	1.98	0.45
4:F:440:THR:CG2	4:F:441:CYS:N	2.79	0.45
1:A:120:THR:OG1	1:A:122:TYR:O	2.34	0.45
5:P:15:C:H2'	5:P:16:G:H8	1.82	0.45
1:A:501:SER:CB	6:T:100:A:H5"	2.47	0.45
4:E:322:LEU:HB2	4:E:346:PHE:HE1	1.82	0.45
4:F:71:TYR:HB3	4:F:75:HIS:HB2	1.99	0.45
4:F:218:LYS:HD2	4:F:218:LYS:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:258:ILE:HG23	4:F:259:SER:H	1.80	0.45
4:E:152:ALA:O	4:E:224:TYR:HB2	2.16	0.45
4:E:546:PHE:O	4:E:574:CYS:HA	2.16	0.45
4:F:202:LYS:HZ2	4:F:520:ALA:HB1	1.62	0.45
4:E:12:THR:OG1	4:E:25:LEU:O	2.35	0.45
4:F:183:THR:HG1	4:F:228:THR:HG22	1.74	0.45
4:F:227:LEU:HD12	4:F:227:LEU:N	2.02	0.45
4:E:443:ARG:HH12	4:E:567:ARG:HH21	1.65	0.45
4:F:183:THR:HG22	4:F:197:GLU:HG2	1.99	0.45
4:E:136:GLU:N	4:E:235:LEU:CD1	2.79	0.45
5:P:22:C:H2'	5:P:23:U:H6	1.81	0.45
1:A:544:LEU:HD12	1:A:544:LEU:HA	1.87	0.44
6:T:112:G:H2'	6:T:113:G:C8	2.53	0.44
6:T:120:A:H2'	6:T:121:C:H6	1.81	0.44
2:B:53:ALA:O	2:B:54:ALA:CA	2.57	0.44
3:C:71:LEU:HD23	2:D:92:PHE:CE2	2.53	0.44
4:E:376:ILE:H	4:E:376:ILE:HG13	1.51	0.44
4:F:420:GLU:H	4:F:420:GLU:HG3	1.52	0.44
6:T:121:C:H2'	6:T:122:G:H8	1.83	0.44
4:E:563:VAL:O	4:E:567:ARG:NH1	2.46	0.44
4:F:167:TRP:CD2	4:F:173:ARG:HD2	2.53	0.44
4:F:297:LEU:HD23	4:F:297:LEU:HA	1.84	0.44
4:F:518:GLN:NE2	4:F:549:THR:HG1	2.14	0.44
1:A:378:PRO:HD2	1:A:537:PRO:HB2	1.99	0.44
4:E:26:CYS:HB2	4:E:97:CYS:SG	2.58	0.44
4:E:120:TYR:CE1	4:E:138:LEU:HD11	2.53	0.44
4:E:332:ARG:NH1	4:E:333:ILE:O	2.51	0.44
4:F:345:LYS:HE2	4:F:345:LYS:HB3	1.86	0.44
4:F:441:CYS:O	4:F:463:ALA:HA	2.17	0.44
2:B:92:PHE:HA	2:B:95:LEU:HD12	1.99	0.44
4:E:478:GLY:HA3	4:E:489:ASN:HD21	1.81	0.44
6:T:124:A:H2'	6:T:125:G:H8	1.82	0.44
2:B:137:THR:O	2:B:141:THR:HG22	2.17	0.44
4:F:380:THR:HG22	4:F:409:ARG:HH22	1.82	0.44
4:F:496:VAL:O	4:F:500:LEU:HB2	2.18	0.44
1:A:82:HIS:NE2	1:A:222:PHE:O	2.45	0.44
1:A:414:ASN:HB2	1:A:844:VAL:HG23	2.00	0.44
4:F:431:THR:HG22	4:F:432:ILE:HG23	2.00	0.44
4:F:580:ASP:O	4:F:584:LYS:HG2	2.17	0.44
1:A:736:ASP:OD1	1:A:736:ASP:N	2.49	0.43
1:A:790:ASN:HB3	1:A:792:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:80:SER:HB3	4:E:81:PHE:HA	2.00	0.43
4:E:163:LEU:N	4:E:209:VAL:O	2.51	0.43
4:E:525:ILE:H	4:E:525:ILE:HG12	1.44	0.43
4:F:65:LEU:HD21	4:F:81:PHE:CZ	2.53	0.43
4:F:129:ARG:HD2	4:F:129:ARG:HA	1.84	0.43
1:A:238:TYR:O	1:A:242:MET:HG3	2.19	0.43
4:F:488:ILE:HA	4:F:518:GLN:HB2	1.99	0.43
1:A:575:LEU:HD13	1:A:641:LYS:HG3	2.00	0.43
4:E:480:ILE:HG12	4:E:550:THR:HG22	1.99	0.43
2:D:134:ASP:OD1	2:D:135:TYR:N	2.51	0.43
4:E:363:LEU:HD13	4:E:391:LEU:HD23	2.00	0.43
4:E:477:LYS:HA	4:E:477:LYS:HD2	1.57	0.43
1:A:903:TYR:CE1	2:D:67:MET:HE3	2.53	0.43
2:B:51:ARG:O	2:B:55:MET:HE2	2.15	0.43
2:D:160:VAL:HG12	2:D:166:ILE:HD13	2.00	0.43
5:P:22:C:H2'	5:P:23:U:C6	2.53	0.43
4:F:449:VAL:HG11	4:F:463:ALA:HB2	2.00	0.43
1:A:371:LEU:HB3	2:B:87:MET:HE3	2.00	0.43
1:A:615:MET:HB2	1:A:766:PHE:CE1	2.52	0.43
1:A:837:ILE:HG21	1:A:866:ALA:HB2	2.01	0.43
4:F:227:LEU:O	4:F:228:THR:OG1	2.28	0.43
4:F:296:ALA:HB2	4:F:306:TYR:OH	2.19	0.43
3:C:22:VAL:HG22	3:C:62:MET:HE1	2.01	0.43
4:F:574:CYS:SG	4:F:575:ILE:N	2.91	0.43
4:F:74:SER:HB3	4:F:75:HIS:CE1	2.54	0.43
4:F:158:LEU:HA	4:F:158:LEU:HD22	1.77	0.43
4:F:180:TYR:OH	4:F:410:THR:HG21	2.19	0.43
4:E:8:CYS:CB	4:E:99:GLY:HA2	2.49	0.42
4:E:497:ARG:HG2	4:E:498:GLU:N	2.32	0.42
5:P:13:U:H2'	5:P:14:A:C8	2.53	0.42
6:T:115:G:H2'	6:T:116:A:C8	2.52	0.42
1:A:501:SER:HB3	6:T:101:A:C5'	2.50	0.42
4:F:287:GLY:HA2	9:F:1003:ADP:H5'1	2.00	0.42
1:A:609:VAL:HG23	1:A:612:PRO:HB3	2.01	0.42
2:D:11:SER:HB3	2:D:49:PHE:HA	2.01	0.42
1:A:462:THR:OG1	1:A:791:ASN:OD1	2.37	0.42
3:C:3:MET:CE	3:C:7:LYS:HG3	2.49	0.42
4:F:281:GLN:HG3	4:F:402:PRO:HD2	2.01	0.42
6:T:118:U:C2	6:T:119:G:C8	3.08	0.42
1:A:225:THR:OG1	1:A:226:THR:N	2.52	0.42
4:F:13:SER:HB3	4:F:92:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:204:ASP:HA	4:F:524:LYS:HE3	1.16	0.42
6:T:112:G:H2'	6:T:113:G:H8	1.84	0.42
4:F:443:ARG:NH1	4:F:567:ARG:HH21	2.17	0.42
5:P:15:C:H2'	5:P:16:G:C8	2.54	0.42
4:E:109:ILE:HD13	4:E:134:ALA:HB2	2.00	0.42
4:E:307:THR:HA	4:E:358:CYS:O	2.20	0.42
4:F:480:ILE:HG22	4:F:482:HIS:HB3	2.02	0.42
4:E:220:ASN:O	4:E:222:GLY:N	2.53	0.42
4:F:163:LEU:HD11	4:F:218:LYS:NZ	2.35	0.42
4:F:552:THR:OG1	4:F:553:ALA:N	2.53	0.42
4:F:139:LYS:HA	4:F:139:LYS:HD3	1.94	0.41
4:F:235:LEU:HD12	4:F:385:SER:HB3	2.02	0.41
4:F:347:LYS:NZ	4:F:347:LYS:HB2	2.34	0.41
4:E:440:THR:CG2	4:E:441:CYS:N	2.82	0.41
4:F:488:ILE:HG23	4:F:518:GLN:HA	2.02	0.41
1:A:568:ASN:OD1	1:A:654:ARG:NH2	2.53	0.41
2:D:69:GLN:OE1	4:E:68:MET:SD	2.78	0.41
4:E:101:ASP:C	4:E:103:VAL:HG22	2.39	0.41
4:E:182:PHE:HB3	4:E:225:PHE:HB3	2.03	0.41
4:F:120:TYR:CE1	4:F:138:LEU:HD11	2.55	0.41
4:F:290:HIS:HB2	4:F:320:LYS:HZ3	1.84	0.41
4:F:440:THR:CG2	4:F:441:CYS:H	2.32	0.41
5:P:3:C:H2'	5:P:4:G:C8	2.55	0.41
5:P:8:C:H2'	5:P:9:A:C8	2.54	0.41
4:E:155:ARG:NH2	4:F:248:ARG:NH1	2.67	0.41
4:E:184:GLY:HA3	4:E:195:ILE:HG12	2.02	0.41
4:E:404:GLN:OE1	10:E:1005:AF3:F2	2.28	0.41
4:F:73:LYS:HD3	4:F:73:LYS:HA	1.88	0.41
4:F:472:PHE:CD1	4:F:590:LEU:HD21	2.55	0.41
4:E:459:ASN:OD1	4:E:459:ASN:N	2.53	0.41
4:F:262:PHE:HB3	4:F:290:HIS:CE1	2.51	0.41
1:A:558:ALA:O	1:A:683:GLY:HA3	2.20	0.41
1:A:840:ALA:O	1:A:858:ARG:NH2	2.49	0.41
2:D:90:MET:O	2:D:94:MET:HG3	2.20	0.41
4:E:474:MET:HB3	4:E:575:ILE:HA	2.02	0.41
4:E:486:SER:HB2	4:E:517:SER:HB3	2.03	0.41
1:A:746:TYR:CZ	1:A:750:ARG:HD2	2.56	0.41
3:C:49:PHE:CD1	2:D:100:ASN:ND2	2.88	0.41
4:E:136:GLU:CD	4:E:235:LEU:HG	2.40	0.41
5:P:18:C:H2'	5:P:19:A:C8	2.56	0.41
5:P:34:U:H2'	5:P:35:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:322:LEU:HD13	4:E:327:ILE:HG13	2.02	0.41
4:F:183:THR:CB	4:F:228:THR:CG2	2.84	0.41
2:D:41:SER:HA	2:D:44:VAL:HG12	2.02	0.41
4:E:136:GLU:CB	4:E:235:LEU:CD1	2.54	0.41
4:E:184:GLY:HA2	4:E:225:PHE:HA	2.02	0.41
4:E:304:ILE:HG12	4:E:370:ILE:HG23	2.03	0.41
4:E:439:GLY:O	4:E:440:THR:OG1	2.36	0.41
4:E:500:LEU:HD21	4:E:528:LEU:HD21	2.03	0.41
4:F:411:LEU:HD13	4:F:411:LEU:HA	1.88	0.41
2:D:68:THR:O	2:D:72:LYS:HG2	2.21	0.41
4:F:21:ARG:NH1	4:F:232:VAL:HG13	2.35	0.41
4:F:262:PHE:HZ	4:F:297:LEU:HD12	1.86	0.41
4:F:489:ASN:H	4:F:518:GLN:HG3	1.85	0.41
4:F:465:LYS:HG2	4:F:466:ASP:H	1.86	0.40
4:F:189:LYS:CB	4:F:190:ASN:HB2	2.40	0.40
5:P:23:U:H2'	5:P:24:C:C6	2.56	0.40
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.90	0.40
1:A:638:LEU:HD12	1:A:638:LEU:HA	1.94	0.40
1:A:864:ILE:HG23	1:A:924:MET:HG2	2.03	0.40
4:E:308:ALA:O	4:E:360:VAL:HG23	2.22	0.40
1:A:902:MET:SD	2:D:71:TYR:CE1	3.10	0.40
2:D:73:GLN:NE2	4:E:46:ASN:OD1	2.49	0.40
4:E:449:VAL:HG11	4:E:463:ALA:HB3	2.02	0.40
1:A:708:LEU:HD11	1:A:731:LEU:HD12	2.04	0.40
2:D:70:MET:HE3	2:D:70:MET:HB2	2.02	0.40
4:E:277:TYR:HA	4:E:396:TYR:O	2.21	0.40
4:E:487:ALA:O	4:E:517:SER:OG	2.39	0.40
4:F:21:ARG:HD3	4:F:140:ALA:HB2	2.03	0.40
4:F:227:LEU:O	4:F:228:THR:CB	2.69	0.40
4:F:405:LEU:HD22	4:F:534:ASP:OD1	2.22	0.40
4:F:458:ASP:H	4:F:460:LYS:HZ1	1.68	0.40
4:F:475:PHE:HA	4:F:576:MET:O	2.21	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%)	887 (96%)	38 (4%)	0	100 100
2	B	182/199 (92%)	177 (97%)	3 (2%)	2 (1%)	14 52
2	D	183/199 (92%)	177 (97%)	6 (3%)	0	100 100
3	C	73/88 (83%)	72 (99%)	1 (1%)	0	100 100
4	E	588/605 (97%)	534 (91%)	53 (9%)	1 (0%)	47 81
4	F	588/605 (97%)	518 (88%)	68 (12%)	2 (0%)	41 75
All	All	2539/2628 (97%)	2365 (93%)	169 (7%)	5 (0%)	50 81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	53	ALA
2	B	54	ALA
4	E	102	ASN
4	F	102	ASN
4	F	228	THR

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%)	785 (96%)	34 (4%)	30 63
2	B	149/168 (89%)	141 (95%)	8 (5%)	22 55
2	D	152/168 (90%)	142 (93%)	10 (7%)	16 49
3	C	70/81 (86%)	69 (99%)	1 (1%)	67 85
4	E	503/526 (96%)	438 (87%)	65 (13%)	4 22
4	F	503/526 (96%)	426 (85%)	77 (15%)	2 17
All	All	2196/2292 (96%)	2001 (91%)	195 (9%)	13 37

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	24	THR
1	A	49	LEU
1	A	114	ILE
1	A	116	ARG
1	A	152	CYS
1	A	153	ASP
1	A	166	VAL
1	A	208	ASP
1	A	231	VAL
1	A	241	LEU
1	A	259	THR
1	A	268	TRP
1	A	302	LEU
1	A	335	VAL
1	A	341	VAL
1	A	343	SER
1	A	459	ASN
1	A	494	ILE
1	A	538	THR
1	A	544	LEU
1	A	613	HIS
1	A	638	LEU
1	A	686	THR
1	A	687	THR
1	A	734	ASN
1	A	758	LEU
1	A	759	SER
1	A	761	ASP
1	A	818	MET
1	A	870	THR
1	A	871	LYS
1	A	891	LEU
1	A	917	GLU
2	B	35	LEU
2	B	51	ARG
2	B	52	ASP
2	B	55	MET
2	B	65	GLN
2	B	107	ILE
2	B	114	CYS
2	B	186	VAL

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Mol	Chain	Res	Type
3	C	71	LEU
2	D	32	GLU
2	D	42	LEU
2	D	78	ASP
2	D	95	LEU
2	D	131	VAL
2	D	137	THR
2	D	146	THR
2	D	163	ASP
2	D	167	VAL
2	D	175	ASP
4	E	7	LEU
4	E	22	ARG
4	E	45	VAL
4	E	72	CYS
4	E	73	LYS
4	E	103	VAL
4	E	122	LEU
4	E	127	THR
4	E	138	LEU
4	E	156	GLU
4	E	158	LEU
4	E	164	HIS
4	E	165	LEU
4	E	178	ARG
4	E	194	GLN
4	E	204	ASP
4	E	209	VAL
4	E	210	VAL
4	E	219	LEU
4	E	221	VAL
4	E	227	LEU
4	E	232	VAL
4	E	235	LEU
4	E	236	SER
4	E	248	ARG
4	E	255	THR
4	E	265	ASN
4	E	290	HIS
4	E	297	LEU
4	E	307	THR
4	E	327	ILE

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Mol	Chain	Res	Type
4	E	334	ILE
4	E	347	LYS
4	E	348	VAL
4	E	359	THR
4	E	366	THR
4	E	382	TYR
4	E	405	LEU
4	E	410	THR
4	E	417	LEU
4	E	438	LEU
4	E	441	CYS
4	E	447	GLU
4	E	448	ILE
4	E	452	VAL
4	E	456	VAL
4	E	479	VAL
4	E	492	GLN
4	E	493	ILE
4	E	497	ARG
4	E	498	GLU
4	E	499	PHE
4	E	501	THR
4	E	503	ASN
4	E	519	ASN
4	E	525	ILE
4	E	526	LEU
4	E	532	THR
4	E	542	ASP
4	E	548	GLN
4	E	552	THR
4	E	562	ASN
4	E	563	VAL
4	E	573	LEU
4	E	581	LEU
4	F	7	LEU
4	F	9	ASN
4	F	10	SER
4	F	15	ARG
4	F	22	ARG
4	F	26	CYS
4	F	37	THR
4	F	63	LEU

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Mol	Chain	Res	Type
4	F	70	TYR
4	F	104	THR
4	F	111	THR
4	F	116	ASN
4	F	121	ILE
4	F	122	LEU
4	F	129	ARG
4	F	130	LEU
4	F	158	LEU
4	F	163	LEU
4	F	164	HIS
4	F	166	SER
4	F	177	ASN
4	F	178	ARG
4	F	181	VAL
4	F	183	THR
4	F	188	THR
4	F	193	VAL
4	F	195	ILE
4	F	199	THR
4	F	207	ASP
4	F	210	VAL
4	F	212	ARG
4	F	219	LEU
4	F	226	VAL
4	F	227	LEU
4	F	232	VAL
4	F	235	LEU
4	F	247	VAL
4	F	248	ARG
4	F	250	THR
4	F	255	THR
4	F	256	LEU
4	F	258	ILE
4	F	262	PHE
4	F	307	THR
4	F	327	ILE
4	F	337	ARG
4	F	344	ASP
4	F	347	LYS
4	F	359	THR
4	F	366	THR

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Mol	Chain	Res	Type
4	F	371	VAL
4	F	382	TYR
4	F	405	LEU
4	F	411	LEU
4	F	416	THR
4	F	417	LEU
4	F	423	ASN
4	F	436	MET
4	F	437	PHE
4	F	438	LEU
4	F	448	ILE
4	F	459	ASN
4	F	460	LYS
4	F	464	HIS
4	F	492	GLN
4	F	499	PHE
4	F	500	LEU
4	F	506	TRP
4	F	525	ILE
4	F	526	LEU
4	F	530	THR
4	F	531	GLN
4	F	574	CYS
4	F	580	ASP
4	F	585	LEU
4	F	588	THR
4	F	590	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	698	GLN
1	A	789	GLN
3	C	19	GLN
4	E	537	GLN
4	F	230	HIS
4	F	518	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	P	33/35 (94%)	1 (3%)	1 (3%)
6	T	36/55 (65%)	0	0
All	All	69/90 (76%)	1 (1%)	1 (1%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	P	25	C

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 16 ligands modelled in this entry, 11 are monoatomic - leaving 5 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	A	2003	8	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
10	AF3	E	1005	-	0,3,3	-	-	-		
9	ADP	E	1003	8	24,29,29	0.95	1 (4%)	29,45,45	1.57	4 (13%)
9	ADP	F	1003	8	24,29,29	0.92	1 (4%)	29,45,45	1.39	4 (13%)
10	AF3	F	1005	-	0,3,3	-	-	-		

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	A	2003	8	-	5/12/32/32	0/3/3/3
9	ADP	F	1003	8	-	2/12/32/32	0/3/3/3
9	ADP	E	1003	8	-	1/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2003	ADP	C5-C4	2.40	1.47	1.40
9	E	1003	ADP	C5-C4	2.37	1.47	1.40
9	F	1003	ADP	C5-C4	2.28	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	1003	ADP	PA-O3A-PB	-4.20	118.42	132.83
9	E	1003	ADP	C3'-C2'-C1'	3.53	106.29	100.98
9	F	1003	ADP	N3-C2-N1	-3.47	123.26	128.68
9	A	2003	ADP	C3'-C2'-C1'	3.41	106.12	100.98
9	A	2003	ADP	N3-C2-N1	-3.28	123.55	128.68
9	E	1003	ADP	N3-C2-N1	-3.24	123.61	128.68
9	F	1003	ADP	PA-O3A-PB	-2.77	123.30	132.83
9	A	2003	ADP	PA-O3A-PB	-2.75	123.38	132.83
9	F	1003	ADP	C4-C5-N7	-2.71	106.57	109.40
9	E	1003	ADP	C4-C5-N7	-2.65	106.64	109.40
9	F	1003	ADP	C3'-C2'-C1'	2.59	104.87	100.98
9	A	2003	ADP	C4-C5-N7	-2.57	106.72	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2003	ADP	C5'-O5'-PA-O1A
9	F	1003	ADP	PB-O3A-PA-O5'
9	A	2003	ADP	C5'-O5'-PA-O3A
9	A	2003	ADP	C5'-O5'-PA-O2A
9	E	1003	ADP	O4'-C4'-C5'-O5'
9	F	1003	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	A	2003	ADP	C3'-C4'-C5'-O5'
9	A	2003	ADP	O4'-C4'-C5'-O5'

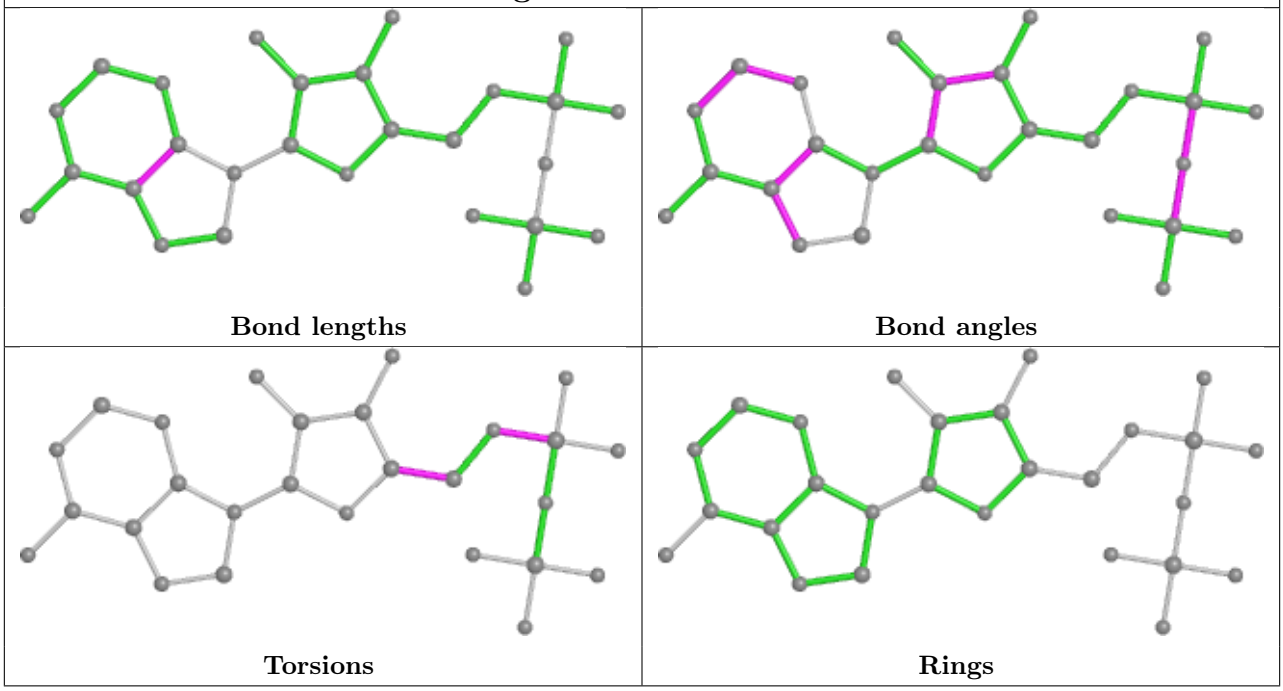
There are no ring outliers.

3 monomers are involved in 6 short contacts:

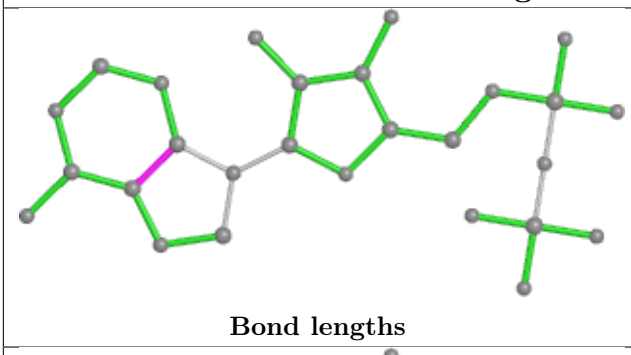
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	1005	AF3	1	0
9	F	1003	ADP	4	0
10	F	1005	AF3	1	0

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.

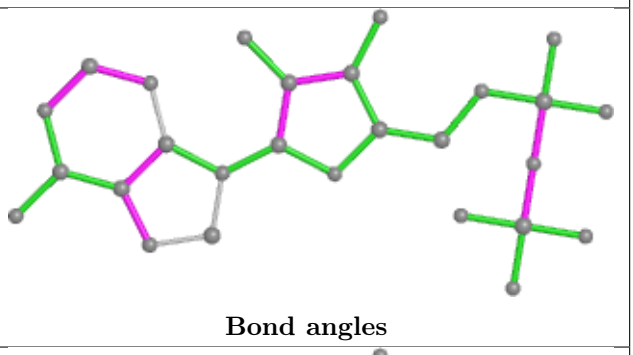
Ligand ADP A 2003



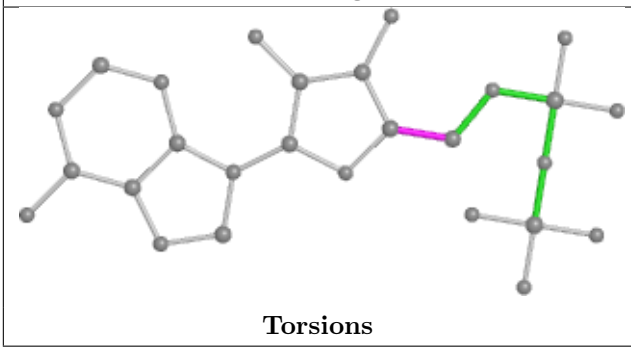
Ligand ADP E 1003



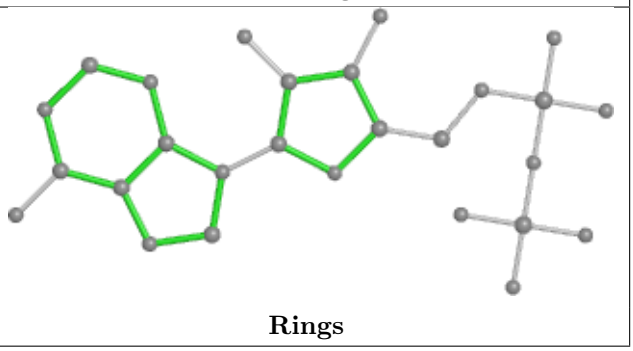
Bond lengths



Bond angles

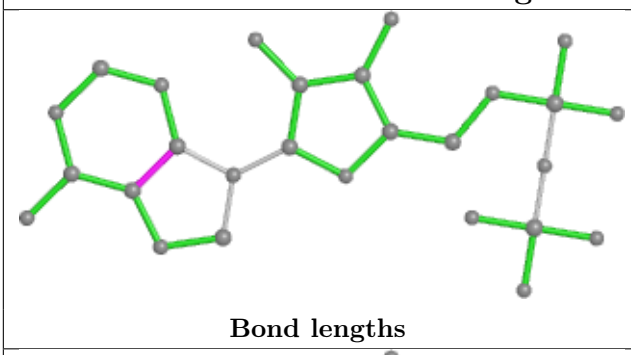


Torsions

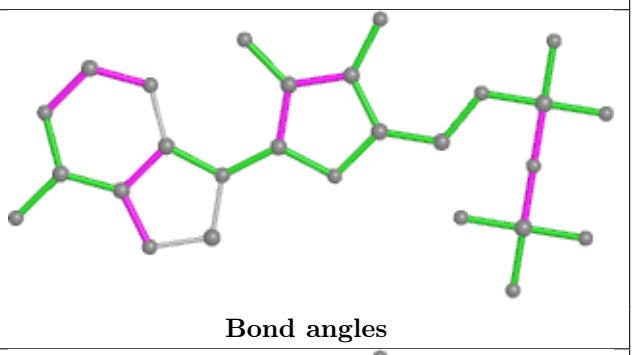


Rings

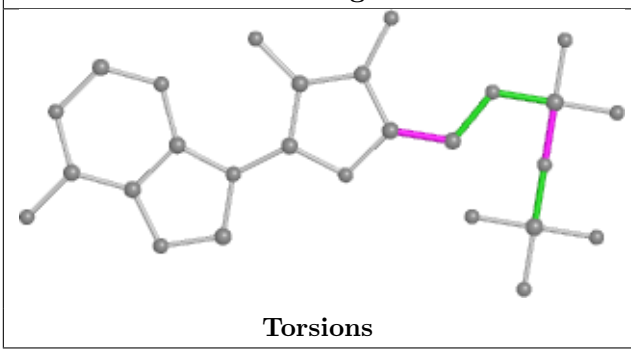
Ligand ADP F 1003



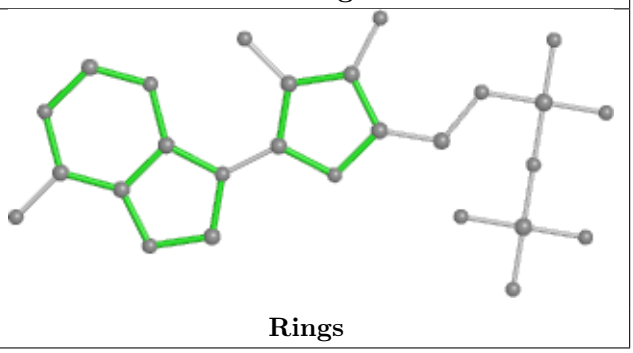
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
4	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	74:ALA	C	75:ARG	N	2.22
1	B	53:ALA	C	54:ALA	N	1.79
1	F	234:PRO	C	235:LEU	N	1.62

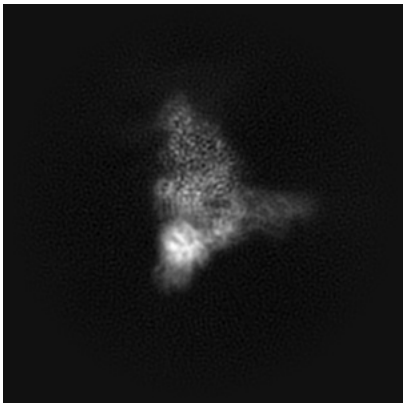
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24429. These allow visual inspection of the internal detail of the map and identification of artifacts.

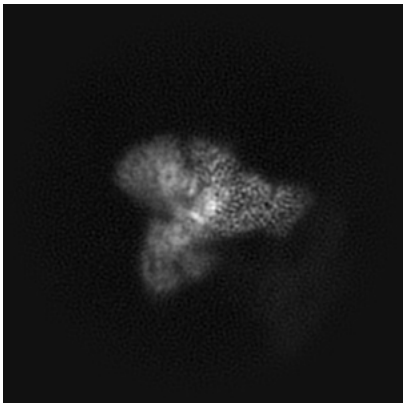
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

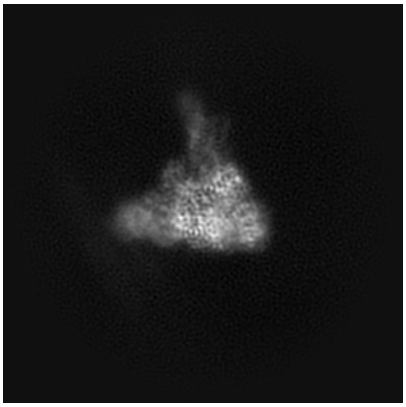
6.1.1 Primary map



X



Y

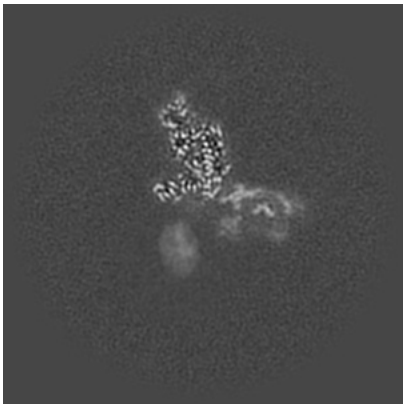


Z

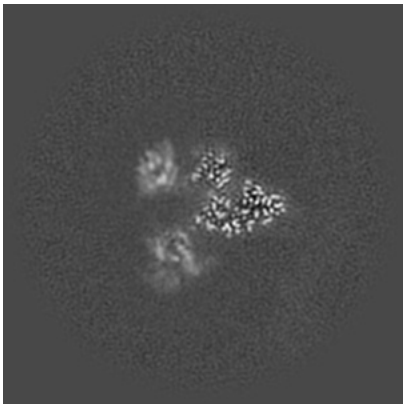
The images above show the map projected in three orthogonal directions.

6.2 Central slices

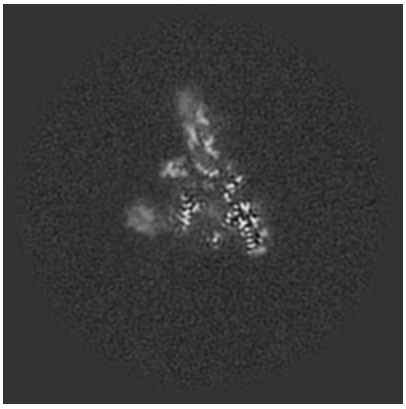
6.2.1 Primary map



X Index: 160



Y Index: 160

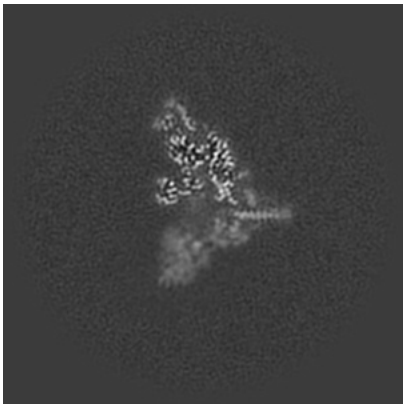


Z Index: 160

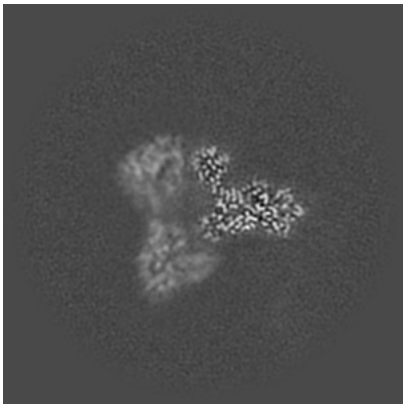
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

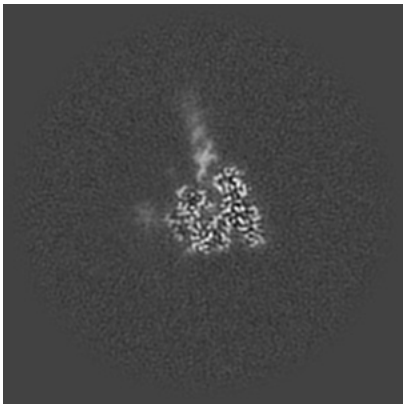
6.3.1 Primary map



X Index: 170



Y Index: 148

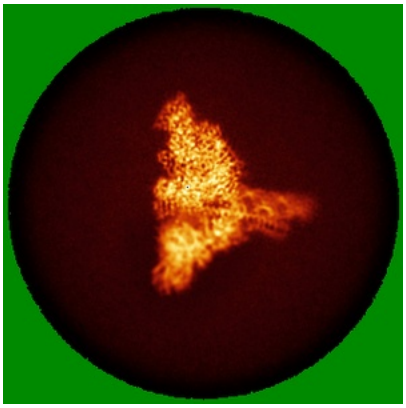


Z Index: 168

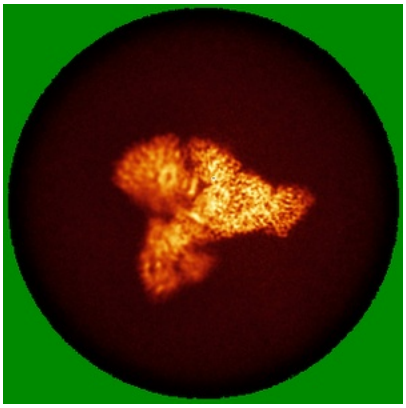
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

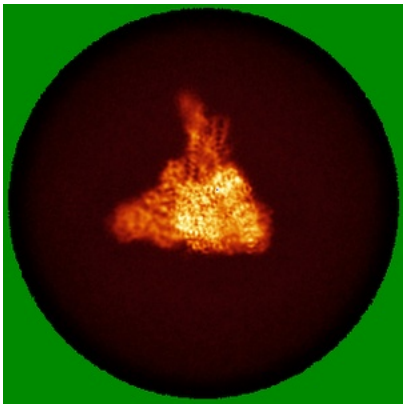
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

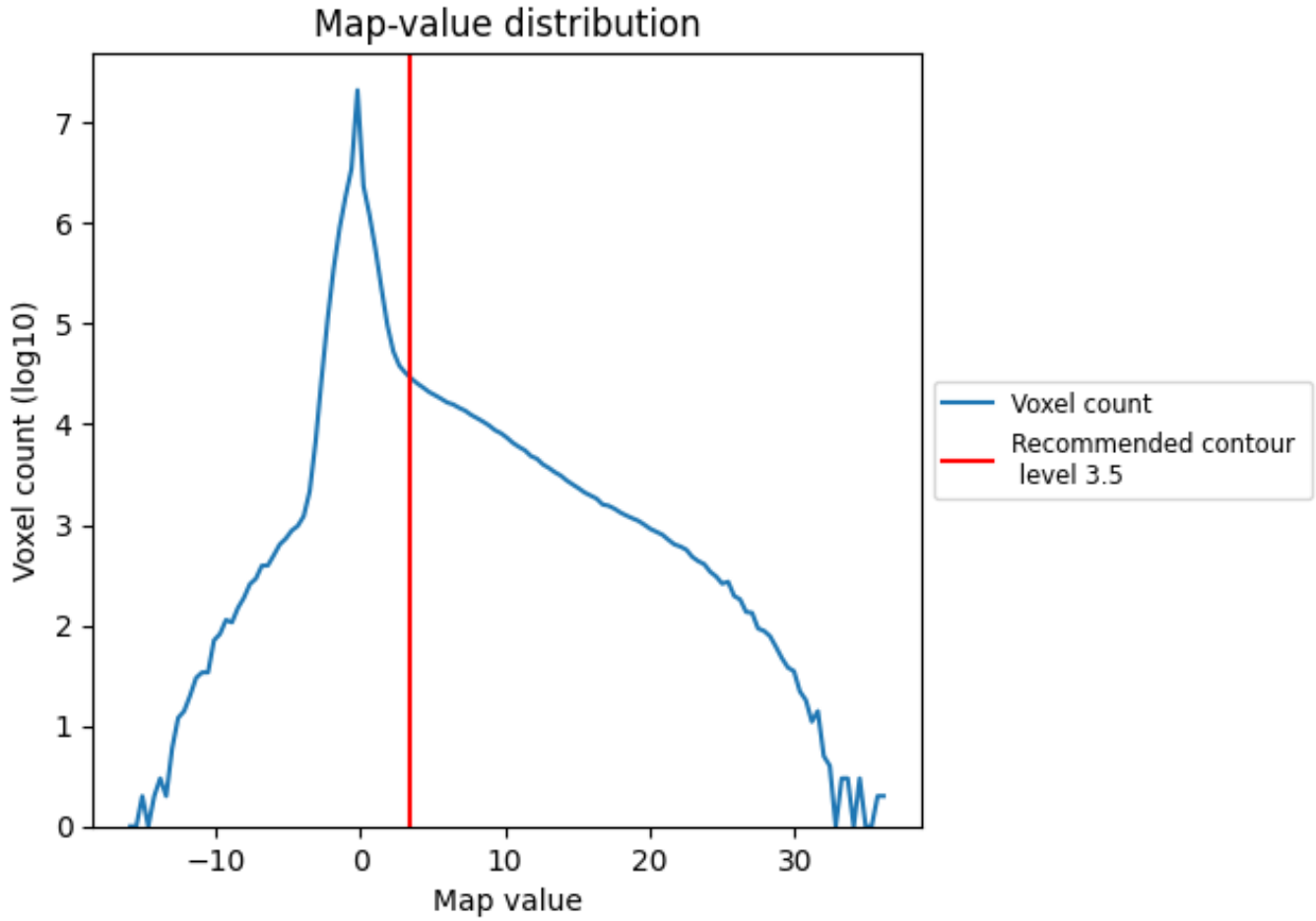
6.6 Mask visualisation (i)

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

7 Map analysis

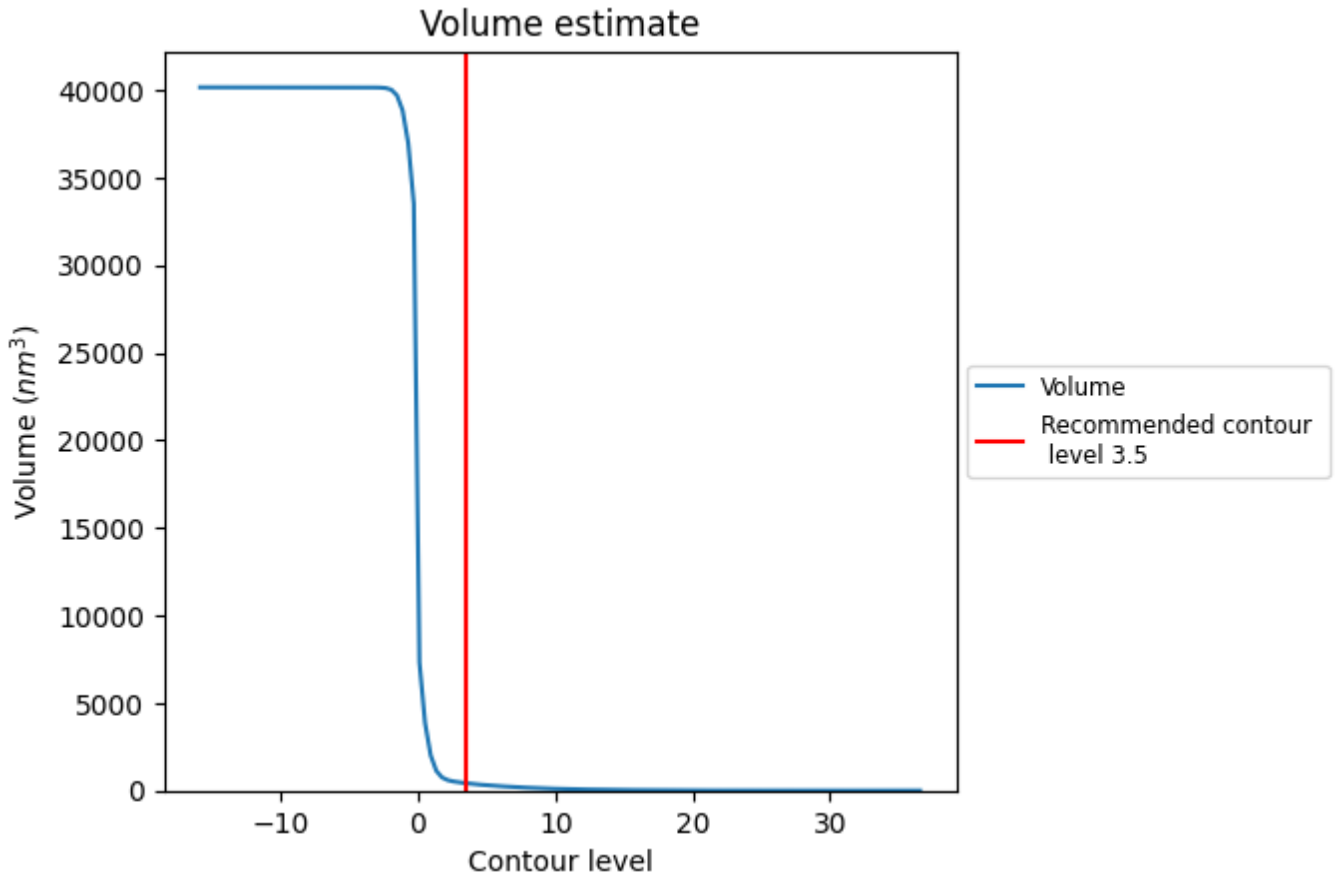
This section contains the results of statistical analysis of the map.

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.

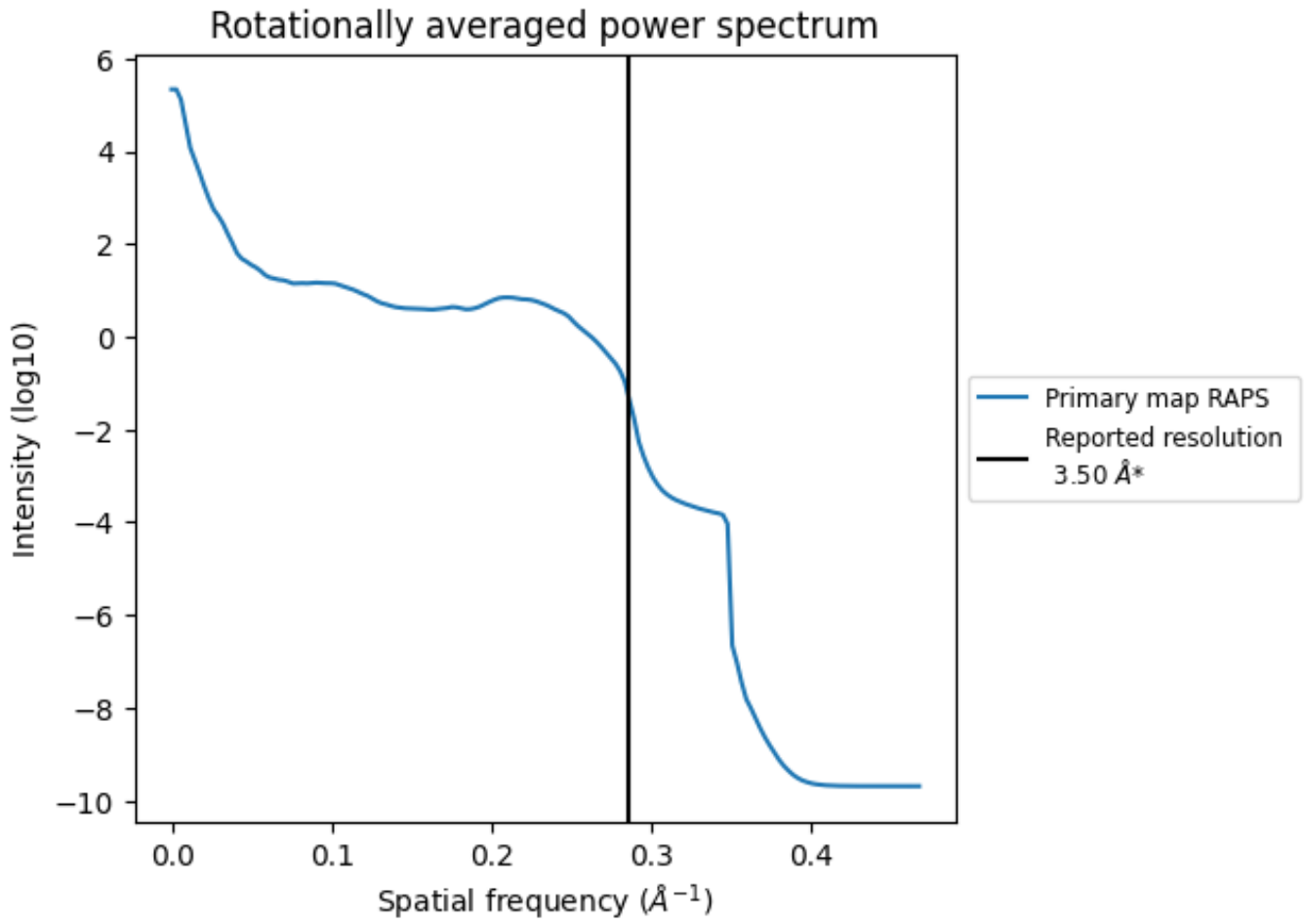
7.2 Volume estimate



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 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)

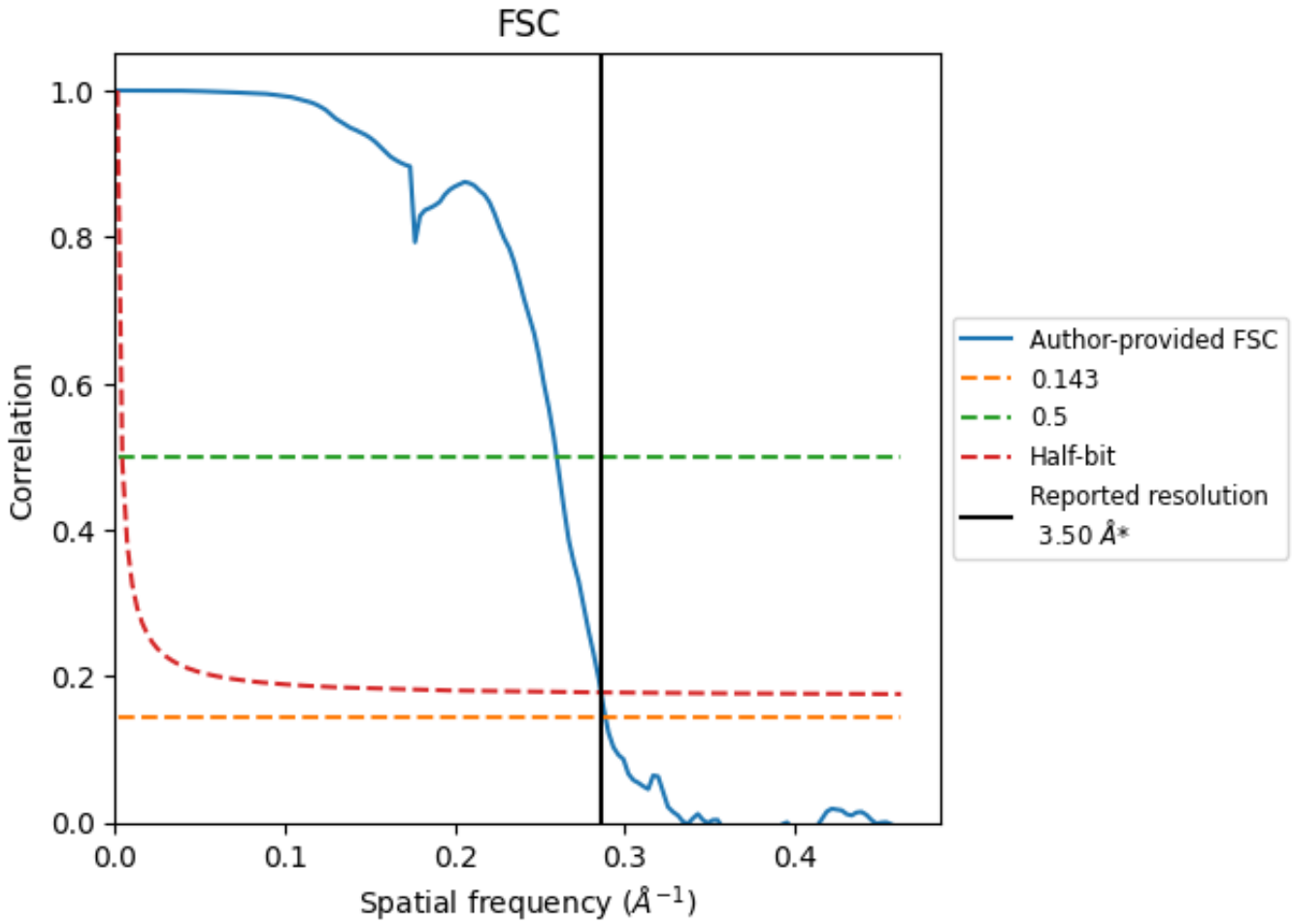


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

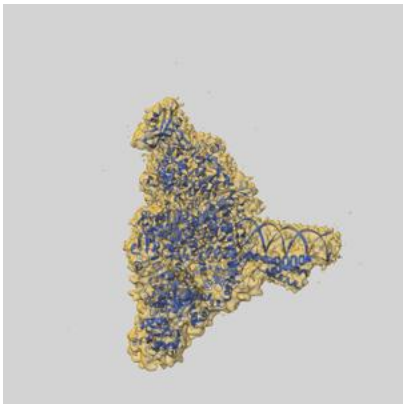
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.85	3.50
Unmasked-calculated*	-	-	-

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

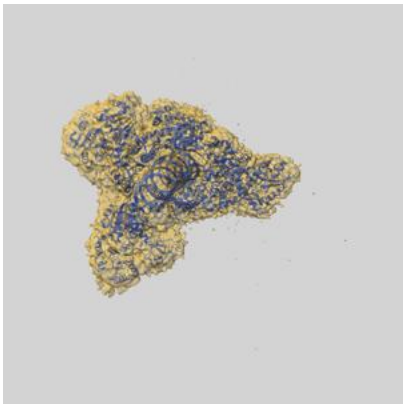
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24429 and PDB model 7RE0. Per-residue inclusion information can be found in section 3 on page 8.

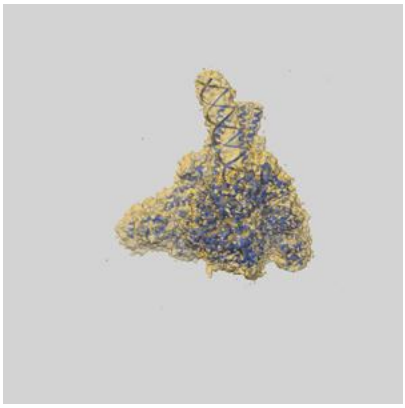
9.1 Map-model overlay



X



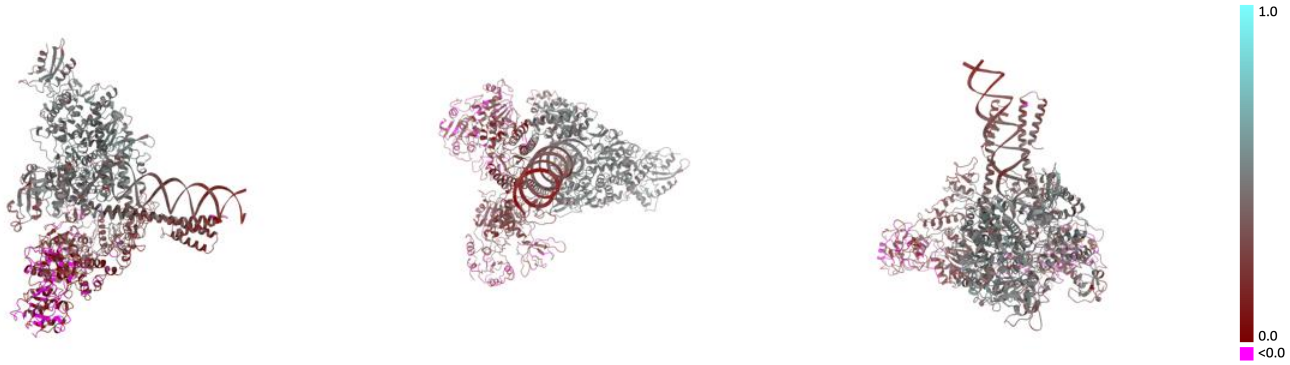
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 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.

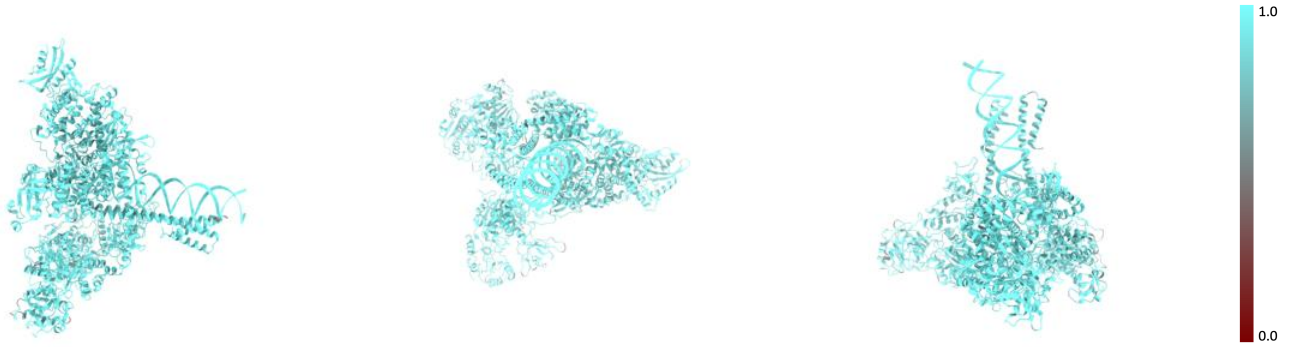
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

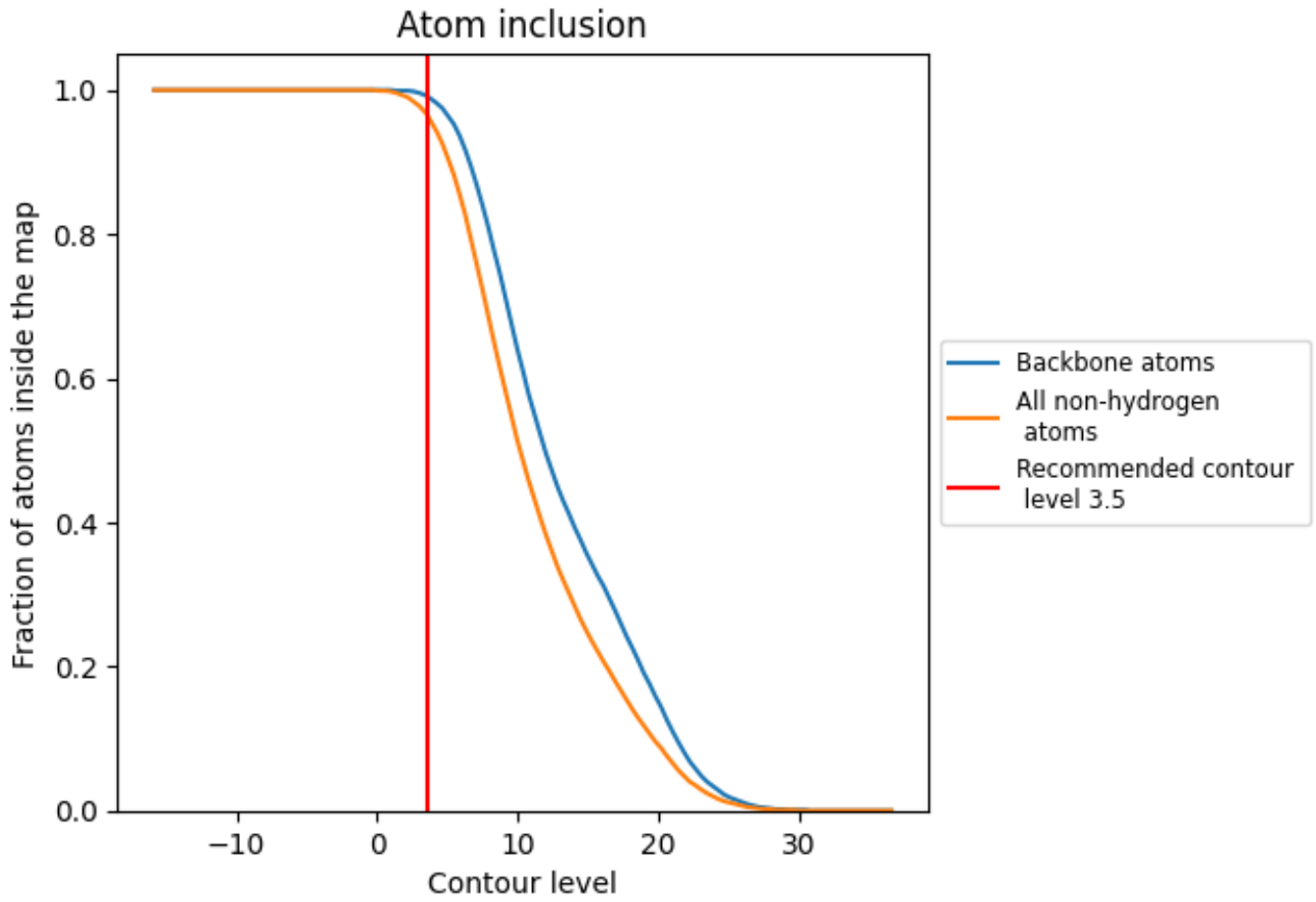
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.3230
A	0.9800	0.4760
B	0.9640	0.3860
C	0.9620	0.4450
D	0.9480	0.3670
E	0.9530	0.1500
F	0.9600	0.1990
P	0.9970	0.3160
T	0.9840	0.3120