



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 08:55 am BST

PDB ID : 6HTS / pdb_00006hts
EMDB ID : EMD-3954
Title : Cryo-EM structure of the human INO80 complex bound to nucleosome
Authors : Ayala, R.; Willhoft, O.; Aramayo, R.J.; Wilkinson, M.; McCormack, E.A.;
Ocloo, L.; Wigley, D.B.; Zhang, X.
Deposited on : 2018-10-04
Resolution : 4.80 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

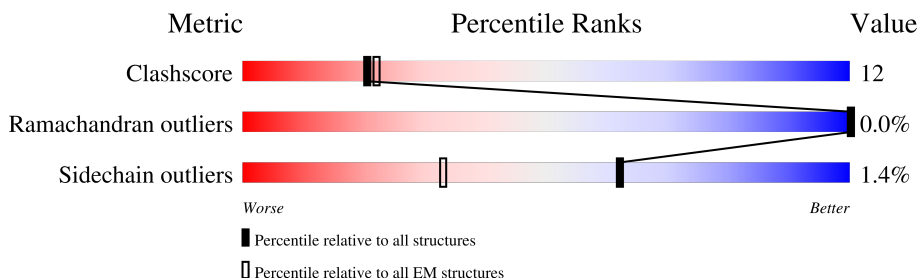
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







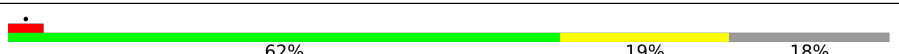
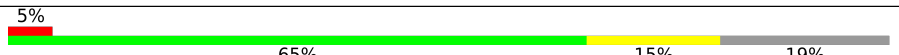
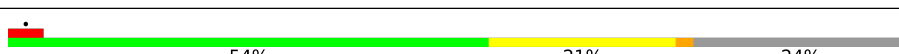


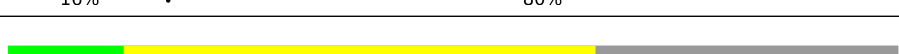
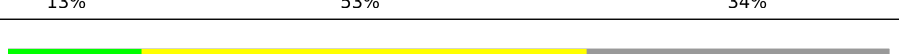
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	456	75% 20% 5%
1	C	456	78% 18% .
1	E	456	77% 20% .
2	B	463	68% 23% . 7%
2	D	463	74% 19% 6%
2	F	463	72% 22% 6%
3	G	1290	46% 6% 47%
4	H	607	52% . 46%

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Mol	Chain	Length	Quality of chain
5	I	136	
5	M	136	
6	J	103	
6	N	103	
7	K	130	
7	O	130	
8	L	126	
8	P	126	
9	R	356	
10	X	228	
11	Y	228	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 38744 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total	C	N	O	S	0	0
			3344	2107	575	646	16		
1	C	437	Total	C	N	O	S	0	0
			3358	2115	577	650	16		
1	E	443	Total	C	N	O	S	0	0
			3403	2144	584	658	17		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3299	2065	575	644	15		
2	D	434	Total	C	N	O	S	0	0
			3347	2095	584	653	15		
2	F	434	Total	C	N	O	S	0	0
			3365	2104	588	657	16		

- Molecule 3 is a protein called Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	680	Total	C	N	O	S	0	0
			4100	2548	778	764	10		

- Molecule 4 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	326	Total	C	N	O	0	0
			1612	960	326	326		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	96	Total	C	N	O	S	0	0
			789	497	152	136	4		
5	M	99	Total	C	N	O	S	0	0
			815	514	158	139	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	82	Total	C	N	O	S	0	0
			652	412	127	112	1		
6	N	86	Total	C	N	O	S	0	0
			694	436	140	117	1		

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	106	Total	C	N	O		0	0
			819	517	160	142			
7	O	105	Total	C	N	O		0	0
			810	511	158	141			

- Molecule 8 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	96	Total	C	N	O	S	0	0
			755	474	138	141	2		
8	P	94	Total	C	N	O	S	0	0
			736	462	134	138	2		

- Molecule 9 is a protein called INO80 complex subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	72	Total	C	N	O	S	0	0
			533	328	104	93	8		

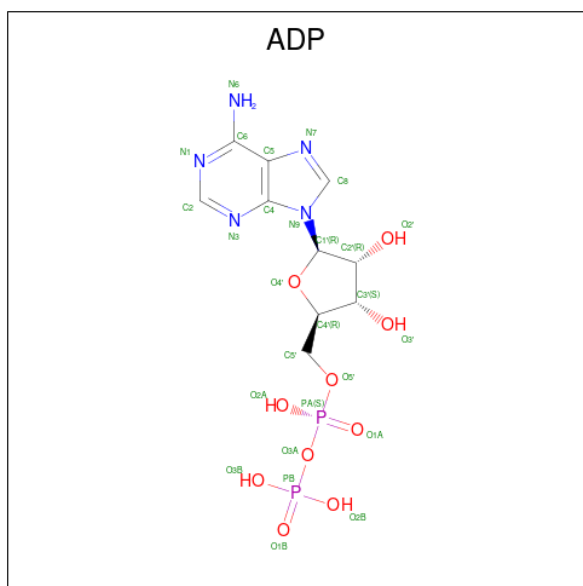
- Molecule 10 is a DNA chain called DNA (150-MER).

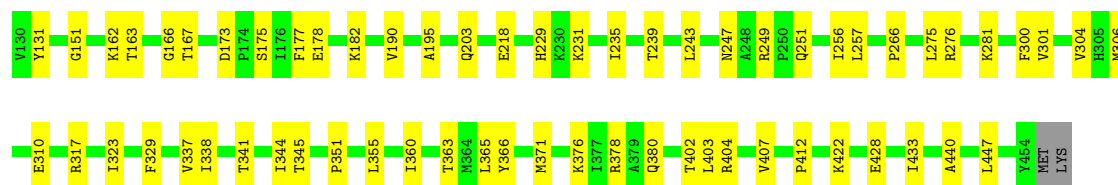
Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	150	Total	C	N	O	P	0	0
			3095	1463	586	896	150		

- Molecule 11 is a DNA chain called DNA (150-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	150	Total	C	N	O	P	0	0
			3055	1451	550	904	150		

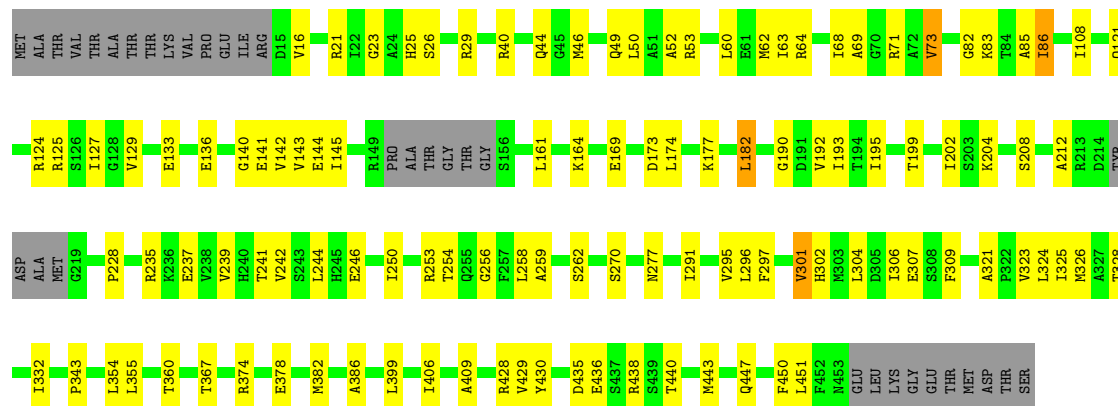
- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).





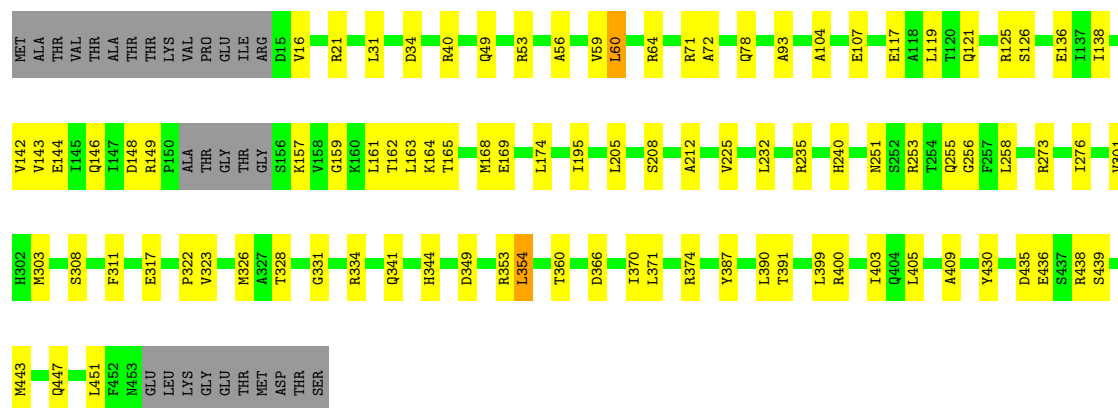
• Molecule 2: RuvB-like 2

Chain B: 68% 23% 7%



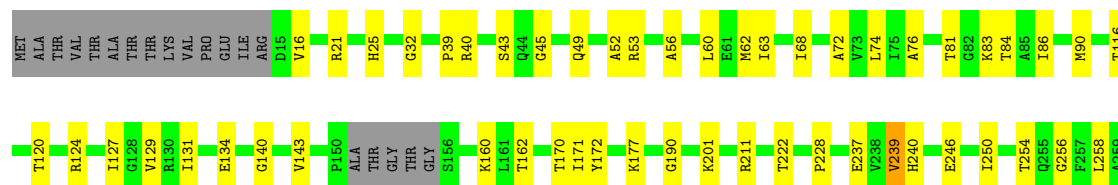
• Molecule 2: RuvB-like 2

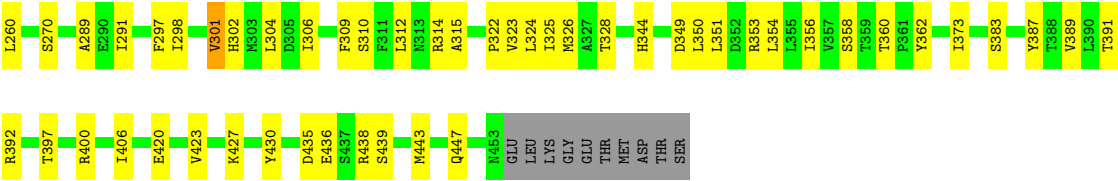
Chain D: 74% 19% 6%



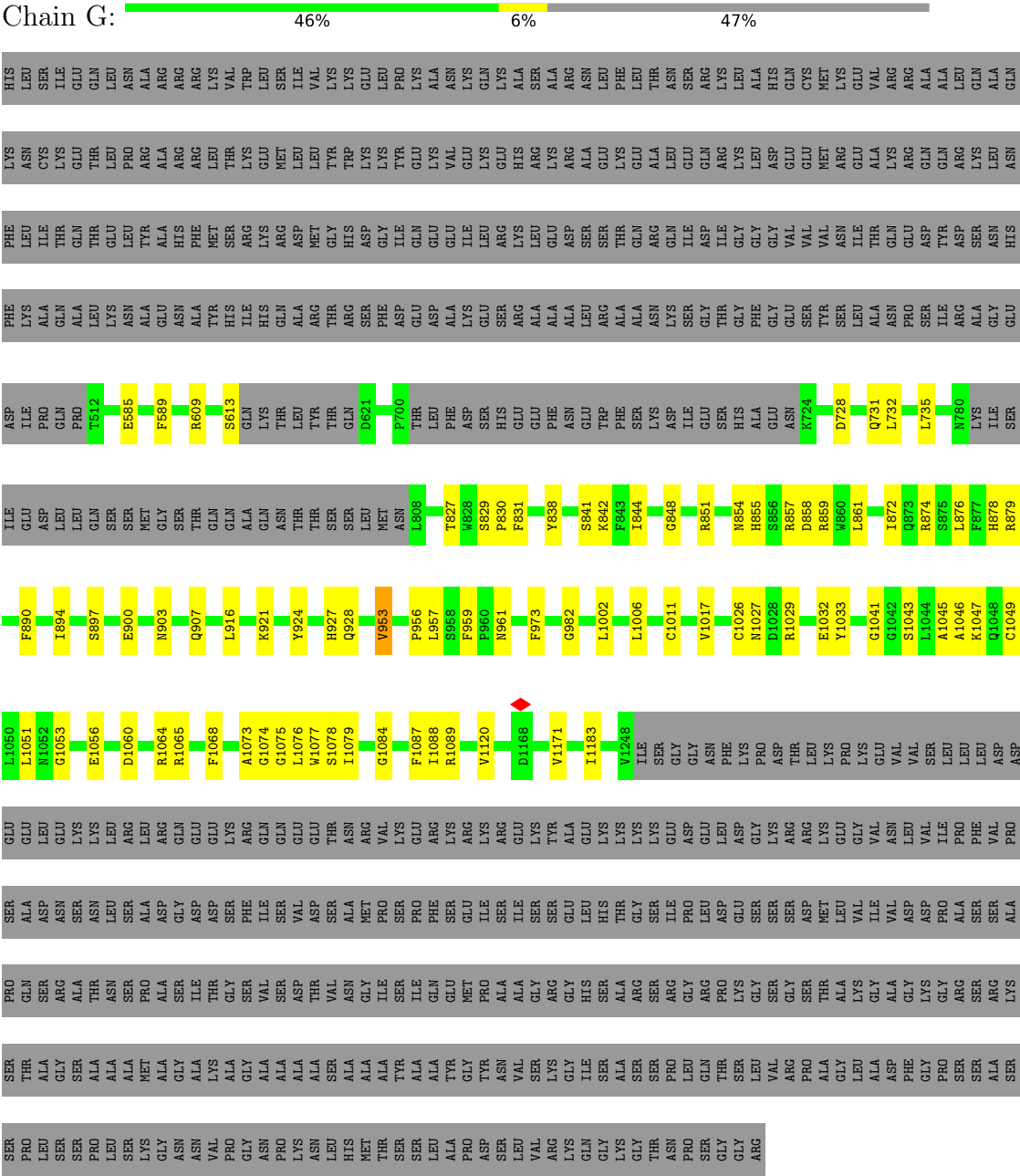
• Molecule 2: RuvB-like 2

Chain F: 72% 22% 6%



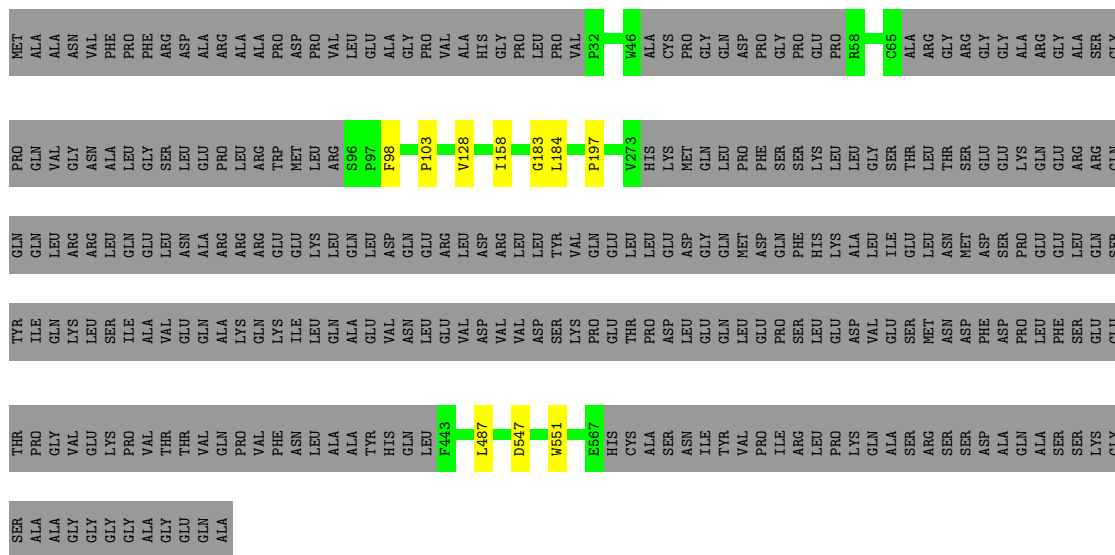


• Molecule 3: Chromatin-remodeling ATPase INO80

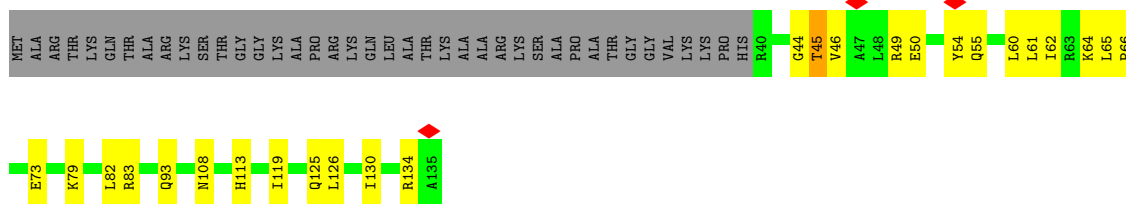


• Molecule 4: Actin-related protein 5

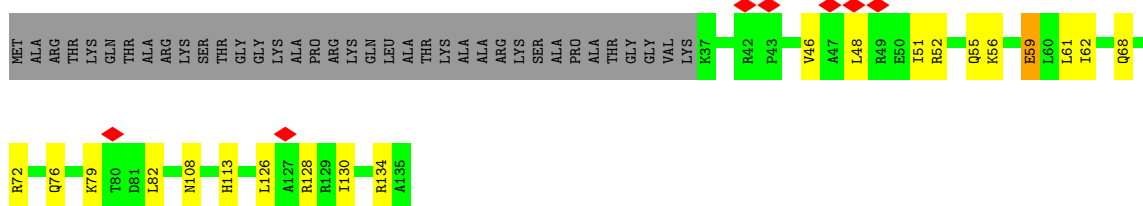




- Molecule 5: Histone H3.1



- Molecule 5: Histone H3.1



- Molecule 6: Histone H4

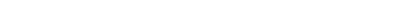


- Molecule 6: Histone H4



[illegible]

- Molecule 10: DNA (150-MER)

Chain X:  13% 53% 34%

[illegible]

- Molecule 11: DNA (150-MER)

Chain Y: 15% 50% 34%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58145	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0155	Depositor
Map size (\AA)	294.30002, 294.30002, 294.30002	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.08	0/3387	0.24	0/4564
1	C	0.09	0/3401	0.24	0/4585
1	E	0.08	0/3449	0.24	0/4650
2	B	0.09	0/3335	0.27	0/4492
2	D	0.09	0/3386	0.27	0/4562
2	F	0.09	0/3404	0.27	0/4584
3	G	0.11	0/4159	0.29	0/5725
4	H	0.11	0/1610	0.35	0/2236
5	I	0.11	0/799	0.37	0/1071
5	M	0.11	0/827	0.31	0/1109
6	J	0.10	0/659	0.33	0/883
6	N	0.10	0/702	0.32	0/937
7	K	0.10	0/829	0.29	0/1118
7	O	0.10	0/820	0.29	0/1107
8	L	0.59	1/766 (0.1%)	0.35	0/1026
8	P	0.59	1/746 (0.1%)	0.34	0/1001
9	R	0.16	0/550	0.45	0/750
10	X	0.30	0/3477	0.49	0/5369
11	Y	0.30	0/3421	0.50	0/5273
All	All	0.19	2/39727 (0.0%)	0.33	0/55042

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
5	I	0	1
9	R	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	36	SER	C-N	15.86	1.58	1.33
8	L	36	SER	C-N	15.85	1.58	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	44	GLY	Peptide
9	R	314	CYS	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	3344	0	3451	60	0
1	C	3358	0	3444	56	0
1	E	3403	0	3495	64	0
2	B	3299	0	3337	79	0
2	D	3347	0	3390	62	0
2	F	3365	0	3421	69	0
3	G	4100	0	2839	67	0
4	H	1612	0	721	5	0
5	I	789	0	829	19	0
5	M	815	0	856	18	0
6	J	652	0	696	11	0
6	N	694	0	742	17	0
7	K	819	0	879	20	0
7	O	810	0	866	17	0
8	L	755	0	784	28	0
8	P	736	0	757	30	0
9	R	533	0	528	11	0
10	X	3095	0	1681	211	0
11	Y	3055	0	1685	216	0
12	A	27	0	12	2	0
12	B	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	27	0	12	3	0
12	D	27	0	12	1	0
12	E	27	0	12	4	0
12	F	27	0	12	2	0
13	R	1	0	0	0	0
All	All	38744	0	34473	870	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 12.

All (870) 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)
10:X:-45:DG:N2	11:Y:46:DA:H2	0.91	1.38
11:Y:37:DC:N1	11:Y:38:DT:H72	1.40	1.35
11:Y:37:DC:C2'	11:Y:38:DT:H73	1.55	1.32
10:X:2:DG:C2	11:Y:-1:DG:N2	1.98	1.29
10:X:-51:DG:C2	11:Y:52:DG:N2	2.01	1.29
11:Y:37:DC:C2'	11:Y:38:DT:C7	2.09	1.28
11:Y:37:DC:C6	11:Y:38:DT:H72	1.68	1.28
10:X:-33:DG:C2'	10:X:-32:DT:H71	1.70	1.22
10:X:38:DG:C2	11:Y:-37:DG:N2	2.08	1.20
10:X:-45:DG:N2	11:Y:46:DA:C2	1.82	1.20
10:X:2:DG:C2	11:Y:-1:DG:C2	2.34	1.15
10:X:-81:DG:H2''	10:X:-80:DT:H71	1.19	1.12
10:X:2:DG:N2	11:Y:-1:DG:C2	2.17	1.11
11:Y:37:DC:H2''	11:Y:38:DT:H73	1.15	1.10
10:X:-33:DG:H2''	10:X:-32:DT:C7	1.83	1.08
10:X:-81:DG:H2''	10:X:-80:DT:C7	1.84	1.04
10:X:-51:DG:C2	11:Y:52:DG:C2	2.46	1.03
11:Y:63:DA:H2''	11:Y:64:DT:H71	1.36	1.02
11:Y:37:DC:H2'	11:Y:38:DT:H73	1.39	1.01
11:Y:37:DC:H2'	11:Y:38:DT:C7	1.86	1.01
11:Y:37:DC:C1'	11:Y:38:DT:H72	1.90	1.01
2:D:443:MET:O	2:D:447:GLN:HB2	1.61	1.00
10:X:4:DG:N2	11:Y:-3:DG:C2	2.28	1.00
2:F:443:MET:O	2:F:447:GLN:HB2	1.63	0.98
2:B:443:MET:O	2:B:447:GLN:HB2	1.64	0.97
11:Y:67:DA:H2''	11:Y:68:DT:H71	1.43	0.96
10:X:2:DG:N3	11:Y:-1:DG:N2	2.13	0.96
11:Y:63:DA:H2''	11:Y:64:DT:C7	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:37:DC:H2''	11:Y:38:DT:C7	1.85	0.94
10:X:-81:DG:C2'	10:X:-80:DT:H71	1.97	0.94
11:Y:-43:DT:H2'	11:Y:-42:DT:H72	1.51	0.93
11:Y:37:DC:C6	11:Y:38:DT:C7	2.52	0.92
10:X:38:DG:N2	11:Y:-37:DG:N2	2.18	0.92
11:Y:-43:DT:C2'	11:Y:-42:DT:H72	2.01	0.90
3:G:874:ARG:O	3:G:878:HIS:HB2	1.73	0.89
10:X:-33:DG:H2''	10:X:-32:DT:H71	0.91	0.89
11:Y:37:DC:N1	11:Y:38:DT:C7	2.33	0.88
10:X:26:DA:C2	11:Y:-25:DA:H2	1.93	0.87
10:X:4:DG:C2	11:Y:-3:DG:C2	2.63	0.85
2:B:443:MET:HE1	1:C:347:PRO:HB3	1.58	0.85
10:X:53:DC:H2''	10:X:54:DT:H71	1.59	0.85
11:Y:63:DA:C2'	11:Y:64:DT:H71	2.08	0.83
3:G:844:ILE:O	3:G:848:GLY:HA3	1.80	0.82
10:X:23:DG:C6	10:X:24:DC:N4	2.47	0.82
11:Y:67:DA:C2'	11:Y:68:DT:H71	2.10	0.82
11:Y:24:DA:C2	11:Y:25:DG:C2	2.68	0.82
10:X:-73:DA:C2	11:Y:74:DG:N2	2.49	0.81
10:X:-56:DG:N2	11:Y:57:DA:H2	1.78	0.81
10:X:26:DA:C2	11:Y:-25:DA:C2	2.69	0.80
10:X:26:DA:N1	11:Y:-25:DA:C2	2.50	0.80
10:X:-51:DG:N3	11:Y:52:DG:N2	2.29	0.79
10:X:-51:DG:N1	11:Y:52:DG:C2	2.49	0.79
11:Y:37:DC:C2'	11:Y:38:DT:H72	1.92	0.79
10:X:-56:DG:N2	11:Y:57:DA:C2	2.50	0.78
10:X:-38:DA:C6	10:X:-37:DG:C6	2.72	0.78
10:X:-24:DT:C6	10:X:-23:DT:H72	2.19	0.78
10:X:-51:DG:N2	11:Y:52:DG:C2	2.52	0.77
10:X:53:DC:H2''	10:X:54:DT:C7	2.14	0.77
8:P:56:SER:H	10:X:-54:DC:H5'	1.49	0.77
10:X:6:DA:H2''	10:X:7:DC:C5	2.20	0.77
10:X:25:DT:O2	11:Y:-24:DG:N2	2.17	0.77
10:X:-45:DG:H2''	10:X:-44:DG:H5''	1.67	0.76
2:B:253:ARG:HG2	2:B:259:ALA:HB2	1.68	0.76
10:X:-28:DC:H2''	10:X:-27:DC:C5	2.21	0.75
10:X:-73:DA:C2	11:Y:74:DG:C2	2.75	0.75
10:X:2:DG:N2	11:Y:-1:DG:N2	2.28	0.75
10:X:36:DA:H2''	10:X:37:DC:C5	2.21	0.75
11:Y:63:DA:H2''	11:Y:64:DT:C5	2.22	0.74
10:X:-51:DG:N1	11:Y:52:DG:N1	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:-58:DC:H2''	10:X:-57:DT:H71	1.68	0.74
2:F:39:PRO:HB3	2:F:53:ARG:HE	1.54	0.73
10:X:-81:DG:H2''	10:X:-80:DT:C5	2.23	0.73
10:X:-81:DG:C2'	10:X:-80:DT:C7	2.62	0.72
11:Y:-43:DT:C6	11:Y:-42:DT:H72	2.23	0.72
2:B:301:VAL:HG21	2:B:326:MET:HB2	1.72	0.72
3:G:842:LYS:HB2	3:G:1027:ASN:HB2	1.71	0.71
11:Y:37:DC:C1'	11:Y:38:DT:C7	2.59	0.71
10:X:-64:DA:H2''	10:X:-63:DT:C7	2.20	0.71
10:X:53:DC:H2''	10:X:54:DT:C5	2.26	0.71
10:X:-58:DC:C2'	10:X:-57:DT:H71	2.21	0.71
2:D:370:ILE:HG21	2:D:399:LEU:HD21	1.73	0.71
11:Y:67:DA:H2''	11:Y:68:DT:C7	2.19	0.70
11:Y:78:DG:C2'	11:Y:79:DT:H72	2.21	0.70
11:Y:-43:DT:C2'	11:Y:-42:DT:C7	2.70	0.70
10:X:44:DT:H2'	10:X:45:DT:H72	1.74	0.70
11:Y:59:DA:H2'	11:Y:60:DT:H71	1.74	0.70
1:E:96:MET:SD	1:E:115:ASN:ND2	2.65	0.70
10:X:-33:DG:C2'	10:X:-32:DT:C7	2.54	0.69
10:X:61:DC:H2''	10:X:62:DG:N7	2.07	0.69
10:X:46:DG:N2	11:Y:-45:DA:C2	2.60	0.69
1:A:96:MET:SD	1:A:115:ASN:ND2	2.65	0.69
10:X:34:DC:C6	10:X:35:DT:H72	2.27	0.69
1:A:280:ASN:O	1:A:284:ASN:ND2	2.25	0.69
10:X:2:DG:N2	11:Y:-1:DG:N3	2.40	0.69
11:Y:42:DC:H2'	11:Y:43:DT:H72	1.75	0.69
10:X:2:DG:N1	11:Y:-1:DG:N1	2.41	0.69
2:B:136:GLU:HG2	2:B:235:ARG:HG2	1.73	0.68
10:X:4:DG:C2	11:Y:-3:DG:N1	2.61	0.68
10:X:-64:DA:C2'	10:X:-63:DT:H72	2.24	0.68
1:E:404:ARG:NH1	12:E:501:ADP:O2A	2.26	0.68
1:E:15:ILE:HB	2:F:68:ILE:HG22	1.76	0.68
11:Y:78:DG:H2'	11:Y:79:DT:H72	1.74	0.68
11:Y:69:DC:H2''	11:Y:70:DC:C5	2.28	0.67
1:C:96:MET:SD	1:C:115:ASN:ND2	2.67	0.67
10:X:-64:DA:H2''	10:X:-63:DT:H72	1.77	0.67
2:D:349:ASP:O	2:D:353:ARG:HB2	1.95	0.67
1:A:244:ASP:O	1:A:248:ALA:HB2	1.95	0.67
3:G:1120:VAL:O	3:G:1171:VAL:HA	1.95	0.66
2:B:124:ARG:HH12	2:B:277:ASN:HD21	1.43	0.66
2:B:164:LYS:HG3	2:B:169:GLU:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:LYS:O	1:E:231:LYS:HA	1.96	0.66
10:X:-51:DG:N1	11:Y:52:DG:N2	2.44	0.66
10:X:4:DG:C2	11:Y:-3:DG:N2	2.63	0.66
10:X:44:DT:C2'	10:X:45:DT:H72	2.26	0.66
2:F:74:LEU:O	2:F:356:ILE:HA	1.95	0.66
10:X:38:DG:N2	11:Y:-37:DG:C2	2.64	0.66
1:C:447:LEU:O	1:C:451:GLN:HB2	1.96	0.66
5:I:60:LEU:HD12	5:I:64:LYS:HE2	1.78	0.66
1:A:196:ASN:O	3:G:859:ARG:NH2	2.29	0.65
1:A:130:VAL:O	1:A:229:HIS:HA	1.96	0.65
2:B:302:HIS:HB3	2:B:328:THR:HG23	1.78	0.65
1:E:371:MET:HG3	1:E:403:LEU:HD13	1.79	0.65
11:Y:0:DC:C2'	11:Y:1:DT:H71	2.26	0.65
2:F:143:VAL:N	2:F:162:THR:O	2.27	0.65
10:X:-30:DA:H2''	10:X:-29:DT:H5''	1.79	0.65
11:Y:59:DA:C8	11:Y:60:DT:H73	2.32	0.65
2:F:350:LEU:HD12	2:F:353:ARG:HD2	1.79	0.65
10:X:-24:DT:C2'	10:X:-23:DT:H72	2.27	0.65
11:Y:59:DA:C8	11:Y:60:DT:C7	2.80	0.65
10:X:-51:DG:H2'	10:X:-50:DT:H71	1.78	0.65
1:C:157:VAL:HG21	1:C:177:PHE:HB2	1.78	0.64
3:G:831:PHE:O	3:G:1017:VAL:HA	1.96	0.64
11:Y:-49:DG:H2''	11:Y:-48:DC:C5	2.31	0.64
10:X:-57:DT:H2''	10:X:-56:DG:N7	2.12	0.64
10:X:35:DT:H2''	10:X:36:DA:N7	2.12	0.64
10:X:56:DG:N2	11:Y:-55:DG:N2	2.45	0.64
2:F:254:THR:HG21	3:G:916:LEU:HD13	1.78	0.64
3:G:1011:CYS:O	3:G:1089:ARG:NH1	2.31	0.64
8:P:40:TYR:OH	11:Y:47:DG:OP1	2.12	0.64
11:Y:7:DC:H2''	11:Y:8:DC:C6	2.33	0.64
11:Y:-43:DT:H2'	11:Y:-42:DT:C7	2.26	0.64
2:F:256:GLY:O	2:F:260:LEU:HB2	1.98	0.63
11:Y:-60:DG:H2''	11:Y:-59:DT:C6	2.34	0.63
1:C:40:VAL:O	12:C:501:ADP:N6	2.32	0.63
2:D:121:GLN:O	2:D:125:ARG:HB2	1.97	0.63
3:G:903:ASN:O	3:G:907:GLN:CB	2.46	0.63
10:X:40:DC:C4	10:X:41:DC:N4	2.65	0.63
2:F:129:VAL:HG22	2:F:291:ILE:HG22	1.79	0.63
11:Y:63:DA:C2'	11:Y:64:DT:C7	2.70	0.63
1:C:65:ALA:HA	1:C:327:VAL:O	1.97	0.63
11:Y:-24:DG:C8	11:Y:-23:DC:C5	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:903:ASN:O	3:G:907:GLN:HB2	1.99	0.63
2:B:40:ARG:O	2:B:53:ARG:NH2	2.31	0.62
1:A:67:LEU:HD23	1:A:360:ILE:HG12	1.81	0.62
11:Y:80:DA:H2''	11:Y:81:DC:C6	2.34	0.62
2:B:143:VAL:HG12	2:B:144:GLU:HG3	1.81	0.62
2:B:409:ALA:HA	2:B:429:VAL:HG21	1.81	0.62
2:D:117:GLU:OE2	2:D:273:ARG:NH2	2.32	0.62
2:B:142:VAL:O	2:B:190:GLY:N	2.32	0.62
10:X:12:DG:H2'	10:X:13:DT:H72	1.81	0.62
2:D:49:GLN:NE2	2:D:360:THR:O	2.32	0.62
10:X:38:DG:C2	11:Y:-37:DG:C2	2.88	0.61
1:A:14:ARG:NH1	2:B:321:ALA:O	2.34	0.61
8:P:35:GLU:HA	8:P:36:SER:HA	1.81	0.61
10:X:14:DT:H2''	10:X:15:DT:H71	1.81	0.61
1:C:215:LEU:HD21	2:D:195:ILE:HG21	1.81	0.61
1:C:371:MET:HG3	1:C:403:LEU:HD13	1.81	0.61
2:F:49:GLN:HB3	2:F:52:ALA:HB3	1.81	0.61
11:Y:59:DA:C5	11:Y:60:DT:C4	2.88	0.61
2:F:81:THR:OG1	2:F:83:LYS:NZ	2.34	0.61
1:A:177:PHE:HA	1:A:180:LEU:HD12	1.83	0.61
5:I:83:ARG:HH21	11:Y:-24:DG:H1'	1.66	0.61
11:Y:-28:DT:H2''	11:Y:-27:DC:C5	2.36	0.61
11:Y:-7:DG:H2''	11:Y:-6:DT:C5	2.36	0.61
2:F:49:GLN:NE2	2:F:360:THR:O	2.33	0.61
4:H:547:ASP:O	4:H:551:TRP:CB	2.49	0.61
10:X:42:DA:C2	11:Y:-41:DG:N2	2.69	0.61
2:F:170:THR:OG1	9:R:321:ALA:O	2.18	0.61
10:X:4:DG:H2''	10:X:5:DT:C6	2.36	0.61
2:B:129:VAL:HG22	2:B:291:ILE:HG22	1.82	0.60
10:X:8:DG:C2	11:Y:-7:DG:N2	2.69	0.60
11:Y:-60:DG:H2''	11:Y:-59:DT:C5	2.35	0.60
11:Y:0:DC:H2'	11:Y:1:DT:H71	1.82	0.60
1:E:281:LYS:NZ	3:G:982:GLY:O	2.33	0.60
10:X:26:DA:N1	11:Y:-25:DA:H2	1.92	0.60
10:X:-68:DA:H2'	10:X:-67:DT:H72	1.83	0.60
10:X:50:DG:C2	11:Y:-49:DG:N2	2.69	0.60
4:H:183:GLY:HA2	4:H:487:LEU:HA	1.82	0.60
11:Y:38:DT:H5'	11:Y:38:DT:H6	1.67	0.60
2:B:297:PHE:HD1	2:B:325:ILE:HG13	1.67	0.59
1:C:232:LYS:NZ	3:G:827:THR:OG1	2.35	0.59
7:K:112:GLN:HB2	7:K:115:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:OE1	2:D:78:GLN:NE2	2.36	0.59
3:G:609:ARG:O	3:G:613:SER:CB	2.49	0.59
6:N:92:ARG:NH2	8:P:100:LEU:O	2.34	0.59
8:P:80:LEU:O	8:P:86:ARG:NH1	2.26	0.59
10:X:-8:DG:C2	10:X:-7:DG:N2	2.69	0.59
10:X:-28:DC:H2''	10:X:-27:DC:H5	1.63	0.59
11:Y:-24:DG:C8	11:Y:-23:DC:H5	2.19	0.59
3:G:1045:ALA:O	3:G:1049:CYS:HB2	2.02	0.59
10:X:-47:DC:H2''	10:X:-46:DT:C5	2.37	0.59
11:Y:-52:DG:C4	11:Y:-51:DC:C5	2.90	0.59
11:Y:5:DC:H2''	11:Y:6:DC:C5	2.38	0.59
10:X:2:DG:N1	11:Y:-1:DG:C2	2.71	0.59
1:A:214:ASP:HB2	2:B:173:ASP:H	1.67	0.59
3:G:854:ASN:O	3:G:858:ASP:N	2.28	0.59
5:I:108:ASN:ND2	6:J:42:GLY:O	2.35	0.59
6:N:87:VAL:HG11	6:N:102:GLY:HA3	1.84	0.58
4:H:98:PHE:HA	4:H:103:PRO:HA	1.84	0.58
8:L:37:TYR:O	8:L:41:VAL:HB	2.04	0.58
7:O:112:GLN:HB2	7:O:115:LEU:HG	1.84	0.58
10:X:-68:DA:H2''	10:X:-67:DT:C6	2.38	0.58
10:X:53:DC:H2''	10:X:54:DT:C6	2.39	0.58
2:F:301:VAL:HG21	2:F:326:MET:HB3	1.85	0.58
5:I:73:GLU:OE1	6:J:25:ASN:ND2	2.36	0.58
2:B:440:THR:HA	2:B:443:MET:HE2	1.84	0.58
1:C:184:ARG:NH1	3:G:1077:TRP:O	2.36	0.58
8:P:37:TYR:O	8:P:41:VAL:HB	2.04	0.58
11:Y:18:DC:C2	11:Y:19:DC:C5	2.92	0.58
3:G:830:PRO:HG2	3:G:1087:PHE:HB2	1.85	0.58
11:Y:34:DT:H2''	11:Y:35:DC:C5	2.39	0.58
7:K:47:ALA:HB1	8:L:94:ILE:HG13	1.85	0.58
3:G:927:HIS:HB2	3:G:953:VAL:HG11	1.84	0.57
7:K:54:VAL:HG21	8:L:98:VAL:HG21	1.84	0.57
1:A:16:ALA:HB3	1:A:19:SER:HB3	1.85	0.57
1:E:151:GLY:H	9:R:288:PRO:HD3	1.68	0.57
11:Y:81:DC:C2'	11:Y:82:DT:H72	2.35	0.57
2:B:140:GLY:HA2	2:B:228:PRO:HG2	1.86	0.57
1:C:304:VAL:HG21	1:C:329:PHE:HB3	1.86	0.57
2:D:208:SER:O	2:D:212:ALA:HB3	2.04	0.57
11:Y:72:DG:C2'	11:Y:73:DT:H72	2.34	0.57
1:C:16:ALA:HB3	1:C:19:SER:HB3	1.87	0.57
2:D:164:LYS:HG3	2:D:169:GLU:HG2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:956:PRO:O	3:G:961:ASN:ND2	2.37	0.57
8:L:87:SER:N	11:Y:34:DG:OP1	2.32	0.57
9:R:329:LEU:HD11	9:R:338:ASN:HD22	1.68	0.57
1:C:201:LYS:NZ	3:G:1088:ILE:O	2.36	0.57
1:E:100:GLU:HG2	2:F:116:THR:HG21	1.86	0.57
8:P:36:SER:N	11:Y:48:DG:OP1	2.37	0.57
1:A:426:GLU:HB2	1:A:429:HIS:HD2	1.69	0.57
2:B:199:THR:OG1	3:G:1026:CYS:O	2.21	0.57
2:B:258:LEU:O	2:B:262:SER:CB	2.53	0.57
2:B:258:LEU:O	2:B:262:SER:HB2	2.05	0.57
4:H:128:VAL:HA	4:H:158:ILE:HA	1.86	0.57
1:C:249:ARG:NH1	1:C:267:LYS:O	2.38	0.57
2:D:400:ARG:NH1	12:D:501:ADP:O2A	2.38	0.57
4:H:184:LEU:HA	4:H:197:PRO:HA	1.87	0.57
10:X:-76:DT:H2''	10:X:-75:DG:C8	2.40	0.57
10:X:-18:DG:H2'	10:X:-17:DT:H71	1.85	0.57
1:A:378:ARG:NH2	12:A:501:ADP:O3'	2.37	0.57
2:B:49:GLN:NE2	2:B:360:THR:O	2.36	0.57
7:O:88:ARG:NH2	7:O:100:VAL:O	2.37	0.57
10:X:-59:DT:H2''	10:X:-58:DC:C5	2.40	0.57
2:B:83:LYS:NZ	2:B:328:THR:O	2.36	0.56
8:L:61:ILE:HA	6:N:98:TYR:HB3	1.86	0.56
2:B:382:MET:HE2	2:B:386:ALA:HB1	1.87	0.56
1:C:232:LYS:HE3	1:C:234:ILE:HD11	1.87	0.56
2:D:34:ASP:OD1	2:D:40:ARG:NH2	2.34	0.56
3:G:831:PHE:HB3	3:G:1017:VAL:HG12	1.87	0.56
10:X:-77:DA:C8	10:X:-76:DT:H72	2.40	0.56
2:D:253:ARG:HB3	2:D:256:GLY:HA3	1.88	0.56
11:Y:63:DA:H2''	11:Y:64:DT:C6	2.40	0.56
2:B:195:ILE:HG12	2:B:202:ILE:HG13	1.88	0.56
1:E:422:LYS:NZ	1:E:428:GLU:OE2	2.38	0.56
7:K:88:ARG:NH2	7:K:100:VAL:O	2.37	0.56
11:Y:72:DG:H2'	11:Y:73:DT:H72	1.86	0.56
2:B:21:ARG:HE	1:C:62:ALA:HB2	1.71	0.56
2:B:177:LYS:NZ	3:G:1033:TYR:OH	2.30	0.56
1:C:159:ILE:HD12	1:C:172:LEU:HD12	1.87	0.56
1:E:16:ALA:HB3	1:E:19:SER:HB3	1.87	0.56
7:K:57:TYR:HE2	8:L:106:LEU:HA	1.71	0.56
10:X:-73:DA:N3	11:Y:74:DG:N2	2.52	0.56
2:D:165:THR:OG1	2:D:168:MET:O	2.20	0.56
3:G:1060:ASP:O	3:G:1064:ARG:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:69:ALA:O	7:K:73:ASN:ND2	2.34	0.56
11:Y:37:DC:C2	11:Y:38:DT:H72	2.33	0.56
7:K:51:LEU:HB2	8:L:94:ILE:HG21	1.88	0.56
1:C:125:LYS:HG2	1:C:235:ILE:HG12	1.87	0.56
3:G:872:ILE:O	3:G:876:LEU:HB3	2.06	0.56
8:P:107:ALA:O	8:P:111:VAL:HB	2.07	0.55
2:B:50:LEU:HD23	2:B:53:ARG:HH21	1.71	0.55
2:D:387:TYR:O	2:D:391:THR:OG1	2.21	0.55
6:N:38:ALA:HB1	6:N:43:VAL:HB	1.88	0.55
10:X:56:DG:C2	11:Y:-55:DG:N2	2.74	0.55
1:C:263:LEU:HB3	1:E:257:LEU:HD12	1.88	0.55
5:M:72:ARG:O	5:M:76:GLN:HB2	2.06	0.55
10:X:42:DA:C2	11:Y:-41:DG:C2	2.94	0.55
10:X:53:DC:C2'	10:X:54:DT:H71	2.33	0.55
2:B:142:VAL:O	2:B:190:GLY:CA	2.55	0.55
1:C:33:LYS:O	1:C:46:ARG:NH1	2.38	0.55
1:A:40:VAL:O	12:A:501:ADP:N6	2.40	0.55
2:B:108:ILE:HD11	2:B:304:LEU:HD11	1.89	0.55
2:D:144:GLU:HG2	9:R:278:GLY:HA2	1.88	0.55
11:Y:60:DT:H2'	11:Y:61:DA:C8	2.41	0.55
11:Y:78:DG:H2''	11:Y:79:DT:C7	2.36	0.55
1:E:306:MET:HE1	2:F:306:ILE:HG23	1.88	0.55
2:F:250:ILE:HD13	3:G:894:ILE:HD11	1.87	0.55
5:M:61:LEU:HD12	6:N:37:LEU:HD23	1.89	0.55
11:Y:-28:DT:H2''	11:Y:-27:DC:C6	2.42	0.55
7:O:69:ALA:O	7:O:73:ASN:ND2	2.34	0.55
10:X:-18:DG:C2'	10:X:-17:DT:H71	2.37	0.55
10:X:15:DT:H2''	10:X:16:DA:C8	2.42	0.55
1:A:371:MET:HG3	1:A:403:LEU:HD13	1.89	0.54
2:D:303:MET:HE1	1:E:310:GLU:HA	1.88	0.54
1:E:100:GLU:OE2	2:F:314:ARG:NH1	2.40	0.54
2:F:240:HIS:HA	3:G:879:ARG:HH22	1.72	0.54
3:G:1073:ALA:HB3	3:G:1078:SER:HB3	1.89	0.54
1:E:53:VAL:HG12	1:E:83:ILE:HG23	1.90	0.54
2:F:302:HIS:HB3	2:F:328:THR:HG23	1.89	0.54
11:Y:-52:DG:C5	11:Y:-51:DC:N4	2.76	0.54
11:Y:49:DC:H2''	11:Y:50:DA:C8	2.42	0.54
5:M:59:GLU:OE2	6:N:40:ARG:NH2	2.40	0.54
7:O:54:VAL:HG21	8:P:98:VAL:HG21	1.90	0.54
1:A:118:ARG:NH1	2:B:270:SER:OG	2.40	0.54
6:N:47:SER:HB3	6:N:50:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:75:HIS:HD2	8:P:80:LEU:HD22	1.71	0.54
2:D:148:ASP:O	2:D:157:LYS:HA	2.08	0.54
8:L:107:ALA:O	8:L:111:VAL:HB	2.06	0.54
6:N:59:LYS:NZ	6:N:63:GLU:OE2	2.35	0.54
2:B:161:LEU:HG	2:B:174:LEU:HD11	1.90	0.54
5:I:61:LEU:HD12	6:J:37:LEU:HD23	1.89	0.54
10:X:-49:DG:C6	10:X:-48:DC:N4	2.75	0.54
2:B:374:ARG:NH2	2:B:378:GLU:OE2	2.40	0.54
2:F:239:VAL:O	3:G:879:ARG:NH1	2.41	0.54
2:F:383:SER:N	2:F:420:GLU:OE2	2.41	0.54
7:K:54:VAL:HG22	8:L:110:ALA:HB1	1.89	0.54
10:X:-38:DA:N1	10:X:-37:DG:C6	2.76	0.54
10:X:23:DG:C6	10:X:24:DC:C4	2.96	0.54
1:E:67:LEU:HD23	1:E:360:ILE:HG12	1.90	0.54
7:K:21:ALA:HB1	8:L:117:ALA:HB1	1.90	0.54
7:K:102:ILE:HG23	8:L:61:ILE:HD13	1.89	0.54
11:Y:42:DC:H2'	11:Y:43:DT:C7	2.38	0.54
2:B:332:ILE:HG12	2:B:343:PRO:HA	1.90	0.54
1:E:20:HIS:NE2	12:E:501:ADP:O2'	2.38	0.54
7:O:59:THR:HG21	8:P:41:VAL:HG22	1.89	0.53
10:X:-60:DA:H2'	10:X:-59:DT:H71	1.89	0.53
1:E:71:PRO:HD2	1:E:74:THR:HG21	1.91	0.53
2:D:205:LEU:HG	2:D:225:VAL:HG21	1.88	0.53
10:X:-38:DA:C2	10:X:-37:DG:C4	2.96	0.53
11:Y:67:DA:C2'	11:Y:68:DT:C7	2.84	0.53
2:D:146:GLN:OE1	9:R:274:ARG:NH2	2.41	0.53
10:X:4:DG:H2''	10:X:5:DT:C5	2.43	0.53
11:Y:46:DA:H2''	11:Y:47:DG:C8	2.44	0.53
9:R:332:LEU:HA	9:R:335:TYR:HB3	1.91	0.53
11:Y:29:DA:H2'	11:Y:30:DT:H71	1.90	0.53
11:Y:37:DC:C2	11:Y:38:DT:C5	2.97	0.53
5:I:62:ILE:O	5:I:93:GLN:NE2	2.41	0.53
7:K:29:ARG:NH2	8:L:40:TYR:OH	2.42	0.53
10:X:12:DG:C2'	10:X:13:DT:H72	2.39	0.53
11:Y:12:DT:C6	11:Y:13:DT:H72	2.44	0.53
11:Y:69:DC:H2''	11:Y:70:DC:H5	1.73	0.53
2:B:133:GLU:O	2:B:237:GLU:HA	2.09	0.52
1:C:205:ARG:NH2	1:C:212:GLU:OE2	2.42	0.52
2:D:371:LEU:HD13	2:D:390:LEU:HG	1.90	0.52
10:X:-25:DC:H2''	10:X:-24:DT:C6	2.44	0.52
2:B:29:ARG:O	2:B:44:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:LEU:HD13	2:D:64:ARG:HH22	1.75	0.52
2:F:400:ARG:NH2	12:F:501:ADP:O2A	2.42	0.52
10:X:-36:DG:N2	11:Y:37:DC:O2	2.42	0.52
11:Y:64:DT:H2"	11:Y:65:DA:C8	2.44	0.52
5:M:79:LYS:HB3	5:M:82:LEU:HD11	1.91	0.52
10:X:4:DG:N3	11:Y:-3:DG:N2	2.58	0.52
11:Y:-43:DT:H2"	11:Y:-42:DT:C7	2.40	0.52
1:A:416:LEU:O	1:A:420:ASN:ND2	2.33	0.52
7:O:59:THR:HG23	8:P:62:MET:HE2	1.92	0.52
10:X:2:DG:H2"	10:X:3:DC:C5	2.44	0.52
8:P:84:ASN:HB2	8:P:86:ARG:NH1	2.25	0.52
2:B:25:HIS:HE1	1:C:320:GLU:HB3	1.74	0.52
2:D:317:GLU:OE2	2:D:353:ARG:NH2	2.43	0.52
11:Y:-22:DA:C4	11:Y:-21:DC:C5	2.98	0.52
2:B:250:ILE:HA	2:B:256:GLY:HA3	1.90	0.52
2:B:367:THR:HG23	2:B:399:LEU:HD13	1.92	0.52
2:F:190:GLY:HA3	2:F:211:ARG:HG2	1.91	0.52
3:G:1056:GLU:O	3:G:1060:ASP:HB2	2.10	0.52
2:F:72:ALA:HA	2:F:324:LEU:HB2	1.91	0.52
3:G:973:PHE:HB3	3:G:1002:LEU:HD23	1.92	0.52
7:O:26:PRO:HD3	8:P:40:TYR:CD2	2.45	0.52
10:X:-6:DG:H2"	10:X:-5:DG:C8	2.45	0.52
11:Y:3:DT:H2"	11:Y:4:DC:C6	2.45	0.52
1:E:440:ALA:HB1	2:F:351:LEU:HG	1.92	0.52
5:M:51:ILE:O	5:M:55:GLN:HB2	2.09	0.52
10:X:-8:DG:C2	10:X:-7:DG:C2	2.98	0.52
11:Y:80:DA:H2"	11:Y:81:DC:C5	2.45	0.52
1:A:356:ASP:OD2	2:F:400:ARG:NH1	2.42	0.51
1:C:71:PRO:HD2	1:C:74:THR:HG21	1.92	0.51
3:G:872:ILE:O	3:G:876:LEU:CB	2.58	0.51
10:X:-1:DA:C2	11:Y:2:DG:C2	2.98	0.51
10:X:4:DG:N2	11:Y:-3:DG:N1	2.58	0.51
11:Y:7:DC:H2"	11:Y:8:DC:C5	2.46	0.51
2:B:296:LEU:HB3	2:B:324:LEU:HB3	1.93	0.51
7:K:17:ARG:HH21	7:K:28:GLY:HA2	1.75	0.51
10:X:-75:DG:H2"	10:X:-74:DC:C5	2.45	0.51
11:Y:5:DC:H2"	11:Y:6:DC:C6	2.45	0.51
2:B:451:LEU:HB2	1:C:333:ARG:HG2	1.93	0.51
1:A:433:ILE:HD13	1:A:436:LEU:HD12	1.91	0.51
10:X:-64:DA:H2"	10:X:-63:DT:C5	2.45	0.51
11:Y:-24:DG:C5	11:Y:-23:DC:C5	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:HA	1:A:327:VAL:O	2.11	0.51
2:D:443:MET:O	2:D:447:GLN:CB	2.48	0.51
7:O:17:ARG:HH21	7:O:28:GLY:HA2	1.75	0.51
10:X:-12:DA:C4	10:X:-11:DC:C5	2.99	0.51
11:Y:-34:DG:H2''	11:Y:-33:DA:C8	2.46	0.51
11:Y:-5:DA:H2''	11:Y:-4:DC:C5	2.46	0.51
1:A:159:ILE:HD12	1:A:172:LEU:HD12	1.92	0.51
1:E:163:THR:OG1	1:E:166:GLY:O	2.27	0.51
8:P:33:ARG:NH2	10:X:-43:DA:OP1	2.44	0.51
5:I:49:ARG:HH22	10:X:-65:DT:H2'	1.76	0.51
7:O:29:ARG:HD2	8:P:35:GLU:OE2	2.11	0.51
10:X:-25:DC:H2''	10:X:-24:DT:C5	2.45	0.51
1:E:17:SER:O	1:E:378:ARG:NH2	2.43	0.50
3:G:841:SER:HB2	3:G:844:ILE:HG12	1.92	0.50
3:G:1045:ALA:O	3:G:1049:CYS:CB	2.59	0.50
10:X:-58:DC:C6	10:X:-57:DT:H73	2.46	0.50
2:D:334:ARG:HA	2:D:341:GLN:HA	1.92	0.50
2:F:387:TYR:O	2:F:391:THR:OG1	2.24	0.50
11:Y:83:DC:H2''	11:Y:84:DG:C8	2.46	0.50
2:D:143:VAL:HG12	2:D:144:GLU:HG3	1.92	0.50
1:E:182:LYS:NZ	3:G:1060:ASP:OD1	2.43	0.50
1:A:71:PRO:HD2	1:A:74:THR:HG21	1.94	0.50
5:I:55:GLN:NE2	6:J:39:ARG:O	2.44	0.50
8:L:54:ILE:HG12	8:L:55:SER:H	1.76	0.50
2:D:301:VAL:HG21	2:D:326:MET:HE3	1.92	0.50
11:Y:45:DC:H1'	11:Y:46:DA:H5'	1.94	0.50
11:Y:59:DA:C2'	11:Y:60:DT:H71	2.41	0.50
2:D:435:ASP:OD1	2:D:436:GLU:N	2.44	0.50
2:F:62:MET:HE3	2:F:68:ILE:HD11	1.94	0.50
8:P:54:ILE:HG12	8:P:55:SER:H	1.76	0.50
10:X:34:DC:H2'	10:X:35:DT:H72	1.92	0.50
2:B:435:ASP:OD1	2:B:436:GLU:N	2.43	0.50
5:M:72:ARG:HD3	6:N:19:ARG:HH12	1.77	0.50
10:X:56:DG:N2	11:Y:-55:DG:H21	2.09	0.50
11:Y:-52:DG:H2''	11:Y:-51:DC:C6	2.46	0.50
2:F:362:TYR:OH	12:F:501:ADP:N7	2.33	0.49
2:B:73:VAL:HG13	2:B:325:ILE:HG22	1.95	0.49
10:X:-24:DT:H2''	10:X:-23:DT:C7	2.42	0.49
10:X:33:DT:H2''	10:X:34:DC:C6	2.47	0.49
3:G:921:LYS:HA	3:G:924:TYR:HD2	1.77	0.49
10:X:-68:DA:C2'	10:X:-67:DT:H72	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:-64:DA:H2''	10:X:-63:DT:C6	2.47	0.49
2:F:430:TYR:OH	2:F:438:ARG:NH2	2.45	0.49
2:B:62:MET:HE1	2:B:71:ARG:HB3	1.93	0.49
5:M:48:LEU:HD23	5:M:51:ILE:HD12	1.94	0.49
7:O:55:LEU:HD13	8:P:66:VAL:HG13	1.93	0.49
11:Y:29:DA:C4	11:Y:30:DT:C5	3.00	0.49
11:Y:61:DA:H2'	11:Y:62:DT:H72	1.94	0.49
2:D:146:GLN:O	2:D:159:GLY:HA3	2.12	0.49
1:E:366:TYR:OH	12:E:501:ADP:N7	2.46	0.49
2:F:389:VAL:HG13	2:F:392:ARG:HH21	1.76	0.49
7:K:67:GLY:HA3	8:L:49:HIS:NE2	2.26	0.49
10:X:-81:DG:H2''	10:X:-80:DT:C6	2.47	0.49
10:X:-75:DG:H2''	10:X:-74:DC:C6	2.48	0.49
2:B:68:ILE:HG12	2:B:69:ALA:H	1.78	0.49
1:C:97:VAL:HG11	2:D:311:PHE:HA	1.94	0.49
2:F:134:GLU:HA	2:F:237:GLU:HA	1.94	0.49
10:X:-63:DT:H2''	10:X:-62:DA:C8	2.48	0.49
11:Y:71:DT:H2''	11:Y:72:DG:C8	2.48	0.49
1:A:110:GLU:HG2	1:A:270:GLU:HA	1.94	0.49
2:F:349:ASP:OD1	2:F:350:LEU:N	2.46	0.49
10:X:-51:DG:C4	11:Y:52:DG:N2	2.80	0.49
10:X:24:DC:C2'	10:X:25:DT:H72	2.42	0.49
11:Y:-37:DG:H2''	11:Y:-36:DT:C5	2.48	0.49
2:D:121:GLN:O	2:D:125:ARG:CB	2.61	0.49
1:E:131:TYR:HE1	1:E:195:ALA:HB2	1.78	0.49
1:E:304:VAL:HG21	1:E:329:PHE:HB3	1.95	0.49
3:G:728:ASP:O	3:G:732:LEU:CB	2.61	0.49
3:G:851:ARG:O	3:G:855:HIS:HB2	2.13	0.49
5:M:52:ARG:O	5:M:56:LYS:HB2	2.13	0.49
1:A:20:HIS:HB3	1:A:381:THR:HG21	1.93	0.49
1:A:306:MET:HE1	2:B:307:GLU:HA	1.95	0.49
1:A:408:GLN:OE1	2:B:71:ARG:NH2	2.45	0.49
2:D:430:TYR:OH	2:D:438:ARG:NH2	2.43	0.49
1:E:162:LYS:HG3	1:E:167:THR:HG22	1.95	0.49
3:G:1051:LEU:HD22	3:G:1077:TRP:HZ3	1.78	0.49
8:L:95:GLN:HG3	8:L:111:VAL:HG22	1.94	0.49
11:Y:-62:DC:H2''	11:Y:-61:DG:C8	2.48	0.49
11:Y:78:DG:C2'	11:Y:79:DT:C7	2.91	0.49
1:C:107:LYS:HG3	1:C:110:GLU:H	1.78	0.48
1:E:243:LEU:HD23	3:G:957:LEU:HD11	1.95	0.48
1:E:301:VAL:HG12	1:E:304:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:246:GLU:HG2	2:F:260:LEU:HD11	1.93	0.48
3:G:1075:GLY:O	3:G:1078:SER:N	2.45	0.48
10:X:-24:DT:C2	10:X:-23:DT:C4	3.01	0.48
10:X:4:DG:N1	11:Y:-3:DG:N1	2.61	0.48
2:F:45:GLY:HA2	2:F:373:ILE:HD13	1.94	0.48
10:X:8:DG:N1	11:Y:-7:DG:N2	2.61	0.48
10:X:51:DG:C5	10:X:52:DC:C4	3.01	0.48
6:N:75:HIS:CE1	8:P:93:GLU:HA	2.49	0.48
8:P:95:GLN:HG3	8:P:111:VAL:HG22	1.94	0.48
1:A:17:SER:O	1:A:378:ARG:NH2	2.45	0.48
1:C:182:LYS:HE2	3:G:1076:LEU:HD13	1.95	0.48
1:C:366:TYR:OH	12:C:501:ADP:N7	2.45	0.48
3:G:1049:CYS:O	3:G:1053:GLY:CA	2.61	0.48
10:X:-12:DA:C4	10:X:-11:DC:C4	3.00	0.48
11:Y:67:DA:H2''	11:Y:68:DT:C5	2.48	0.48
2:D:142:VAL:HA	2:D:163:LEU:HD23	1.95	0.48
2:D:328:THR:HG21	2:D:344:HIS:HB3	1.96	0.48
2:D:405:LEU:O	2:D:409:ALA:HB2	2.13	0.48
5:I:79:LYS:HB3	5:I:82:LEU:HD11	1.95	0.48
6:J:30:THR:HG21	11:Y:-13:DA:H5''	1.95	0.48
6:J:38:ALA:HB1	6:J:43:VAL:HB	1.94	0.48
2:B:306:ILE:HA	2:B:309:PHE:HB2	1.94	0.48
2:D:405:LEU:O	2:D:409:ALA:CB	2.61	0.48
1:E:249:ARG:HH12	1:E:266:PRO:HA	1.79	0.48
2:F:43:SER:OG	2:F:53:ARG:NH1	2.47	0.48
1:C:247:ASN:HB3	1:C:275:LEU:HD11	1.94	0.48
1:C:372:LYS:HG2	1:C:395:GLY:HA3	1.96	0.48
1:C:404:ARG:NH2	12:C:501:ADP:O2A	2.46	0.48
1:E:121:GLY:HA2	1:E:239:THR:HA	1.94	0.48
6:N:75:HIS:CE1	8:P:93:GLU:HG3	2.49	0.48
7:O:50:TYR:HB3	8:P:94:ILE:HG21	1.95	0.48
10:X:-6:DG:H2''	10:X:-5:DG:N7	2.29	0.48
1:A:114:GLU:HG3	1:A:241:HIS:CD2	2.49	0.48
2:F:435:ASP:OD1	2:F:436:GLU:N	2.45	0.48
1:A:15:ILE:HB	2:B:68:ILE:HG13	1.96	0.48
11:Y:8:DC:H2''	11:Y:9:DG:C8	2.48	0.48
2:B:142:VAL:O	2:B:190:GLY:HA2	2.13	0.48
1:E:67:LEU:HB3	1:E:360:ILE:HA	1.95	0.48
1:A:266:PRO:HD3	2:B:253:ARG:NH1	2.29	0.47
3:G:844:ILE:O	3:G:848:GLY:CA	2.58	0.47
10:X:53:DC:C2'	10:X:54:DT:C7	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:-30:DG:H1'	11:Y:-29:DC:H5'	1.96	0.47
11:Y:24:DA:C2	11:Y:25:DG:N2	2.82	0.47
11:Y:67:DA:H2''	11:Y:68:DT:C6	2.49	0.47
2:D:240:HIS:CD2	3:G:1006:LEU:HD11	2.50	0.47
1:E:129:GLU:HB3	1:E:229:HIS:HE1	1.80	0.47
7:O:85:LEU:O	7:O:89:ASN:HB2	2.14	0.47
10:X:3:DC:H2''	10:X:4:DG:C8	2.49	0.47
10:X:49:DC:H2''	10:X:50:DG:C8	2.49	0.47
2:F:443:MET:O	2:F:447:GLN:CB	2.49	0.47
1:A:110:GLU:OE1	1:A:276:ARG:NH2	2.48	0.47
2:B:127:ILE:HG23	2:B:244:LEU:HD13	1.95	0.47
1:C:272:THR:HG23	1:C:275:LEU:H	1.78	0.47
2:D:21:ARG:HE	1:E:62:ALA:HB2	1.79	0.47
2:D:374:ARG:HH11	2:D:403:ILE:HD13	1.79	0.47
3:G:903:ASN:O	3:G:907:GLN:HB3	2.14	0.47
10:X:38:DG:N2	11:Y:-37:DG:H21	2.08	0.47
1:C:409:LEU:HD22	1:C:433:ILE:HG22	1.96	0.47
2:D:31:LEU:O	2:D:53:ARG:NE	2.48	0.47
1:E:190:VAL:O	1:E:203:GLN:HB3	2.15	0.47
11:Y:-27:DC:H2''	11:Y:-26:DT:C7	2.45	0.47
1:C:55:LEU:HD11	1:C:61:MET:HB2	1.97	0.47
2:D:387:TYR:O	2:D:391:THR:CB	2.63	0.47
10:X:-66:DG:C2	11:Y:67:DA:C2	3.03	0.47
10:X:5:DT:H2''	10:X:6:DA:C8	2.49	0.47
1:A:229:HIS:CE1	1:A:231:LYS:HG3	2.49	0.47
2:D:136:GLU:OE2	2:D:235:ARG:NH1	2.48	0.47
10:X:1:DC:H2''	10:X:2:DG:C8	2.50	0.47
10:X:23:DG:C5	10:X:24:DC:C4	3.03	0.47
11:Y:78:DG:H2''	11:Y:79:DT:C6	2.50	0.47
11:Y:81:DC:H2''	11:Y:82:DT:C7	2.45	0.47
2:D:104:ALA:HB3	2:D:107:GLU:HG3	1.97	0.47
2:D:149:ARG:NH2	3:G:1065:ARG:O	2.48	0.47
10:X:23:DG:C5	10:X:24:DC:N4	2.83	0.47
11:Y:59:DA:C4	11:Y:60:DT:C4	3.02	0.47
1:A:279:ILE:HA	1:A:282:VAL:HG22	1.95	0.47
2:D:71:ARG:HB2	2:D:323:VAL:HG12	1.96	0.47
2:D:119:LEU:HD11	2:D:308:SER:HB3	1.97	0.47
10:X:-60:DA:N6	11:Y:59:DA:N6	2.63	0.47
10:X:17:DA:H2''	10:X:18:DG:H8	1.80	0.47
1:A:62:ALA:HB2	2:F:21:ARG:HE	1.80	0.46
2:F:32:GLY:O	2:F:53:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:13:DT:C2'	10:X:14:DT:H71	2.45	0.46
10:X:59:DA:C6	11:Y:-58:DG:N2	2.83	0.46
2:B:141:GLU:HA	2:B:192:VAL:HA	1.96	0.46
11:Y:-8:DC:H2''	11:Y:-7:DG:C8	2.50	0.46
2:B:25:HIS:HD2	2:B:85:ALA:HA	1.79	0.46
2:F:304:LEU:HB3	2:F:309:PHE:CZ	2.51	0.46
10:X:-84:DC:H2''	10:X:-83:DG:C8	2.50	0.46
10:X:-53:DA:N3	11:Y:54:DG:N2	2.63	0.46
11:Y:-43:DT:N1	11:Y:-42:DT:H72	2.30	0.46
1:E:173:ASP:OD2	1:E:175:SER:OG	2.32	0.46
10:X:61:DC:H2''	10:X:62:DG:C8	2.51	0.46
11:Y:84:DG:H2''	11:Y:85:DG:C8	2.49	0.46
1:A:386:ILE:HG22	1:A:425:ILE:HD12	1.96	0.46
2:B:246:GLU:OE2	3:G:838:TYR:OH	2.23	0.46
11:Y:-56:DC:H2''	11:Y:-55:DG:N7	2.30	0.46
11:Y:81:DC:H2'	11:Y:82:DT:H72	1.97	0.46
1:C:337:VAL:HA	1:C:345:THR:HA	1.98	0.46
2:B:296:LEU:O	2:B:324:LEU:HA	2.15	0.46
1:E:151:GLY:HA3	9:R:288:PRO:HG3	1.97	0.46
7:K:85:LEU:O	7:K:89:ASN:HB2	2.15	0.46
10:X:-72:DC:H2''	10:X:-71:DA:C8	2.51	0.46
1:E:301:VAL:HB	1:E:329:PHE:HD1	1.80	0.46
2:F:40:ARG:HB2	2:F:43:SER:HB3	1.97	0.46
10:X:0:DG:C5	10:X:1:DC:C4	3.04	0.46
10:X:24:DC:H2''	10:X:25:DT:C7	2.46	0.46
2:D:251:ASN:HD22	2:D:276:ILE:HD11	1.81	0.46
1:E:338:ILE:HD13	1:E:351:PRO:HG3	1.98	0.46
2:F:74:LEU:HB2	2:F:354:LEU:HD22	1.97	0.46
1:E:378:ARG:HG2	1:E:407:VAL:HG13	1.97	0.46
10:X:0:DG:C6	10:X:1:DC:N4	2.83	0.46
11:Y:-21:DC:C2	11:Y:-20:DC:C5	3.04	0.46
11:Y:56:DC:C2	11:Y:57:DA:C6	3.03	0.46
11:Y:56:DC:O2	11:Y:57:DA:C2	2.68	0.46
1:C:43:GLU:HG3	1:C:46:ARG:HH11	1.81	0.45
1:E:118:ARG:HH22	2:F:270:SER:HB2	1.82	0.45
5:M:128:ARG:HH12	5:M:134:ARG:HB3	1.82	0.45
10:X:-23:DT:H5''	10:X:-23:DT:H6	1.81	0.45
11:Y:-54:DA:H2''	11:Y:-53:DG:C8	2.51	0.45
1:A:172:LEU:HD13	1:A:176:ILE:HD13	1.99	0.45
2:B:63:ILE:HG21	2:B:295:VAL:HG22	1.98	0.45
2:B:258:LEU:O	2:B:262:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:61:ILE:HG23	6:N:98:TYR:HD2	1.81	0.45
10:X:-64:DA:H2'	10:X:-63:DT:H72	1.97	0.45
10:X:-7:DG:H2''	10:X:-6:DG:C8	2.50	0.45
10:X:38:DG:N1	11:Y:-37:DG:N2	2.60	0.45
11:Y:49:DC:H2''	11:Y:50:DA:H8	1.81	0.45
1:E:247:ASN:HB3	1:E:275:LEU:HD11	1.98	0.45
7:O:16:THR:HA	10:X:-42:DG:H5''	1.98	0.45
10:X:-8:DG:H2''	10:X:-7:DG:C8	2.52	0.45
11:Y:-52:DG:N9	11:Y:-51:DC:C5	2.84	0.45
11:Y:56:DC:C2	11:Y:57:DA:N1	2.84	0.45
1:A:249:ARG:NH2	1:A:267:LYS:O	2.50	0.45
1:A:426:GLU:HB2	1:A:429:HIS:CD2	2.50	0.45
2:B:60:LEU:HG	2:B:64:ARG:HH22	1.81	0.45
2:B:82:GLY:HA3	12:B:501:ADP:H8	1.81	0.45
2:F:56:ALA:HB2	2:F:86:ILE:HD11	1.97	0.45
6:N:91:LYS:HA	6:N:96:THR:OG1	2.17	0.45
10:X:44:DT:H2''	10:X:45:DT:C7	2.46	0.45
10:X:54:DT:OP2	10:X:54:DT:H6	1.98	0.45
2:D:143:VAL:N	2:D:162:THR:O	2.43	0.45
2:F:160:LYS:HD3	2:F:171:ILE:HD12	1.99	0.45
5:I:125:GLN:HB3	5:I:134:ARG:HH21	1.81	0.45
8:P:102:LEU:HB2	8:P:107:ALA:HB2	1.99	0.45
10:X:-8:DG:C5	10:X:-7:DG:N1	2.85	0.45
11:Y:-24:DG:C4	11:Y:-23:DC:C5	3.04	0.45
1:C:128:LYS:NZ	3:G:829:SER:OG	2.36	0.45
2:F:201:LYS:HD3	3:G:897:SER:HB2	1.98	0.45
5:M:62:ILE:HD11	6:N:37:LEU:HD11	1.99	0.45
10:X:-21:DG:C5	10:X:-20:DC:N4	2.84	0.45
1:A:49:CYS:HA	1:A:52:ILE:HD12	1.98	0.45
1:C:315:LEU:HA	1:C:318:ALA:HB3	1.98	0.45
5:I:50:GLU:O	5:I:54:TYR:HB2	2.17	0.45
10:X:-26:DC:H2''	10:X:-25:DC:C5	2.51	0.45
2:B:145:ILE:HG21	2:B:182:LEU:HD11	1.98	0.45
1:C:160:GLY:HA2	1:C:169:GLN:HA	1.98	0.45
8:L:102:LEU:HB2	8:L:107:ALA:HB2	1.98	0.45
5:I:113:HIS:CG	5:M:126:LEU:HD22	2.52	0.45
5:I:119:ILE:HG13	6:J:50:ILE:HG13	1.98	0.45
10:X:-51:DG:N2	11:Y:52:DG:N3	2.65	0.45
11:Y:-52:DG:C4	11:Y:-51:DC:C4	3.04	0.45
11:Y:29:DA:C6	11:Y:30:DT:C4	3.05	0.45
5:I:130:ILE:HD12	5:M:130:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:-32:DC:H2''	11:Y:-31:DA:C8	2.51	0.44
1:E:218:GLU:OE2	2:F:177:LYS:NZ	2.39	0.44
10:X:-67:DT:H2''	10:X:-66:DG:C8	2.52	0.44
1:A:427:LYS:HA	1:A:430:VAL:HG12	1.99	0.44
2:B:428:ARG:NH1	1:C:47:GLU:OE2	2.48	0.44
5:I:125:GLN:HB3	5:I:134:ARG:NH2	2.33	0.44
10:X:-58:DC:C2	10:X:-57:DT:C4	3.05	0.44
10:X:-28:DC:C2'	10:X:-27:DC:C5	2.97	0.44
11:Y:37:DC:H2''	11:Y:38:DT:C5	2.50	0.44
1:C:26:LEU:HD21	1:C:46:ARG:HB3	1.99	0.44
1:C:113:MET:SD	1:C:314:TYR:OH	2.75	0.44
2:F:297:PHE:HA	2:F:325:ILE:O	2.17	0.44
10:X:-18:DG:C6	11:Y:17:DA:N6	2.85	0.44
1:A:272:THR:HG23	1:A:275:LEU:H	1.83	0.44
1:A:444:ALA:HA	1:A:447:LEU:HD12	2.00	0.44
1:E:99:SER:OG	2:F:310:SER:OG	2.33	0.44
3:G:924:TYR:O	3:G:928:GLN:HG2	2.18	0.44
3:G:1029:ARG:NH2	3:G:1032:GLU:HG2	2.33	0.44
5:I:45:THR:HB	5:I:46:VAL:H	1.52	0.44
10:X:-79:DA:C2	11:Y:80:DA:C2	3.06	0.44
10:X:-36:DG:H2''	10:X:-35:DG:C8	2.53	0.44
10:X:4:DG:N2	11:Y:-3:DG:N3	2.63	0.44
10:X:24:DC:H2''	10:X:25:DT:C6	2.53	0.44
11:Y:61:DA:C2'	11:Y:62:DT:H72	2.47	0.44
1:C:177:PHE:HA	1:C:180:LEU:HD12	2.00	0.44
10:X:-3:DA:H2''	10:X:-2:DC:C6	2.52	0.44
1:A:70:GLY:HA3	1:A:363:THR:HB	1.99	0.44
2:B:23:GLY:H	2:B:26:SER:HB3	1.82	0.44
1:C:192:TYR:HB3	1:C:201:LYS:HB3	1.98	0.44
5:I:126:LEU:HD22	5:M:113:HIS:CG	2.52	0.44
11:Y:-41:DG:C6	11:Y:-40:DG:O6	2.71	0.44
2:B:129:VAL:O	2:B:241:THR:HA	2.17	0.44
1:E:251:GLN:HB3	3:G:959:PHE:HB2	1.99	0.44
8:L:79:ARG:HB3	8:L:83:TYR:CZ	2.53	0.44
1:A:199:ALA:HB2	3:G:855:HIS:CD2	2.53	0.44
2:B:83:LYS:HZ1	2:B:328:THR:C	2.24	0.44
1:C:162:LYS:HA	1:C:167:THR:HG22	2.00	0.44
10:X:-24:DT:H2''	10:X:-23:DT:H72	2.00	0.44
2:B:208:SER:O	2:B:212:ALA:CB	2.66	0.43
2:F:120:THR:O	2:F:124:ARG:HG2	2.18	0.43
8:P:79:ARG:HB3	8:P:83:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:-21:DG:C6	10:X:-20:DC:N4	2.86	0.43
11:Y:72:DG:H2''	11:Y:73:DT:C6	2.53	0.43
2:D:64:ARG:NH1	2:D:93:ALA:O	2.50	0.43
1:E:178:GLU:OE2	3:G:1068:PHE:N	2.51	0.43
2:F:298:ILE:HG22	2:F:301:VAL:HG22	1.99	0.43
5:I:65:LEU:HB3	5:I:66:PRO:HD3	2.00	0.43
5:M:68:GLN:HE21	5:M:72:ARG:HE	1.66	0.43
10:X:36:DA:C2'	10:X:37:DC:C5	2.99	0.43
11:Y:37:DC:H2''	11:Y:38:DT:C6	2.52	0.43
2:B:443:MET:HG3	2:B:450:PHE:CE2	2.53	0.43
1:E:376:LYS:HE3	1:E:380:GLN:HE21	1.84	0.43
2:F:298:ILE:HB	2:F:326:MET:HG2	2.00	0.43
1:A:122:LEU:HG	1:A:294:LEU:HD23	2.01	0.43
1:C:451:GLN:HA	1:C:454:TYR:HD2	1.82	0.43
3:G:585:GLU:O	3:G:589:PHE:CB	2.67	0.43
7:K:90:ASP:HB3	7:K:93:LEU:HB2	1.99	0.43
10:X:43:DA:C8	10:X:44:DT:H72	2.54	0.43
2:D:161:LEU:HB2	2:D:174:LEU:HD11	2.00	0.43
1:E:75:GLY:N	12:E:501:ADP:O2B	2.51	0.43
11:Y:25:DG:H2''	11:Y:26:DG:C8	2.53	0.43
1:A:415:LEU:HD11	2:B:62:MET:HB2	2.00	0.43
1:E:412:PRO:HB2	1:E:433:ILE:HD12	2.01	0.43
7:K:32:ARG:NH2	8:L:35:GLU:OE2	2.52	0.43
8:L:87:SER:OG	11:Y:-35:DA:O3'	2.36	0.43
11:Y:-13:DA:C4	11:Y:-12:DC:C5	3.07	0.43
1:A:123:ARG:HB3	1:A:293:GLU:HG3	2.01	0.43
7:O:90:ASP:HB3	7:O:93:LEU:HB2	1.99	0.43
1:C:130:VAL:O	1:C:229:HIS:HA	2.18	0.43
2:D:60:LEU:HD23	2:D:60:LEU:HA	1.82	0.43
1:E:49:CYS:HA	1:E:52:ILE:HD12	1.99	0.43
2:F:63:ILE:HG12	2:F:323:VAL:HG21	2.01	0.43
2:F:74:LEU:HD22	2:F:354:LEU:HD13	2.00	0.43
5:M:56:LYS:NZ	11:Y:-64:DC:OP1	2.52	0.43
10:X:44:DT:C2'	10:X:45:DT:C7	2.96	0.43
11:Y:0:DC:H2''	11:Y:1:DT:H71	1.98	0.43
11:Y:59:DA:C4	11:Y:60:DT:C5	3.06	0.43
11:Y:74:DG:H2''	11:Y:75:DC:C6	2.53	0.43
1:A:157:VAL:HG21	1:A:177:PHE:CG	2.54	0.43
1:C:355:LEU:HA	1:C:358:VAL:HG22	2.00	0.43
1:E:117:ARG:HG3	1:E:276:ARG:NH1	2.34	0.43
9:R:309:CYS:HB3	9:R:315:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:-38:DA:N6	10:X:-37:DG:O6	2.51	0.43
6:J:91:LYS:HA	6:J:96:THR:OG1	2.18	0.43
8:L:42:TYR:OH	11:Y:-53:DG:H3'	2.17	0.43
8:L:106:LEU:O	8:L:110:ALA:CB	2.67	0.43
10:X:-18:DG:H2''	10:X:-17:DT:H5'	2.01	0.43
10:X:13:DT:H2'	10:X:14:DT:H71	1.99	0.43
10:X:23:DG:C4	10:X:24:DC:C5	3.07	0.43
10:X:28:DA:C6	10:X:29:DG:C6	3.07	0.43
10:X:40:DC:H2''	10:X:41:DC:C6	2.54	0.43
10:X:40:DC:H2''	10:X:41:DC:H6	1.83	0.43
11:Y:-60:DG:H2''	11:Y:-59:DT:H71	2.01	0.43
11:Y:21:DC:H2''	11:Y:22:DC:C6	2.53	0.43
1:A:139:THR:HB	1:A:158:ILE:HB	2.01	0.42
2:F:60:LEU:HD13	2:F:90:MET:HG2	2.00	0.42
11:Y:38:DT:H5'	11:Y:38:DT:C6	2.50	0.42
2:D:107:GLU:OE2	1:E:317:ARG:NH1	2.52	0.42
1:E:447:LEU:HD11	2:F:344:HIS:NE2	2.33	0.42
3:G:1043:SER:HB3	3:G:1046:ALA:HB3	2.01	0.42
11:Y:-47:DT:H2''	11:Y:-46:DC:C5	2.54	0.42
1:A:131:TYR:HA	1:A:228:VAL:O	2.19	0.42
2:D:71:ARG:O	2:D:323:VAL:HA	2.19	0.42
8:P:106:LEU:O	8:P:110:ALA:CB	2.67	0.42
9:R:312:PRO:HA	9:R:315:PRO:HD3	2.01	0.42
11:Y:-60:DG:H2''	11:Y:-59:DT:C7	2.48	0.42
11:Y:-24:DG:H2''	11:Y:-23:DC:H6	1.82	0.42
1:A:20:HIS:CE1	1:A:378:ARG:HH21	2.37	0.42
1:A:256:ILE:HG23	2:B:254:THR:HG23	2.00	0.42
6:J:31:LYS:HG3	6:J:51:TYR:CE1	2.55	0.42
10:X:-62:DA:H2'	10:X:-61:DT:H71	2.01	0.42
11:Y:-52:DG:H2''	11:Y:-51:DC:H6	1.84	0.42
11:Y:6:DC:H2''	11:Y:7:DC:C6	2.54	0.42
1:A:263:LEU:HD13	1:C:260:MET:HG2	2.02	0.42
1:A:304:VAL:HG21	1:A:329:PHE:HB3	2.02	0.42
7:O:25:PHE:HE2	8:P:66:VAL:HG11	1.84	0.42
10:X:12:DG:C8	10:X:13:DT:H72	2.54	0.42
1:A:122:LEU:O	1:A:237:ASP:HA	2.18	0.42
2:F:25:HIS:CE1	2:F:84:THR:HB	2.54	0.42
5:I:108:ASN:HB2	6:J:43:VAL:HG22	2.01	0.42
8:L:72:ARG:HB3	8:L:101:LEU:HD21	2.01	0.42
10:X:59:DA:C5	11:Y:-58:DG:N2	2.87	0.42
3:G:1049:CYS:O	3:G:1053:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:0:DG:C4	10:X:1:DC:C5	3.08	0.42
10:X:34:DC:C2'	10:X:35:DT:H72	2.49	0.42
10:X:42:DA:C6	10:X:43:DA:C6	3.08	0.42
1:A:117:ARG:HG3	1:A:276:ARG:NH1	2.34	0.42
1:E:96:MET:O	1:E:301:VAL:HA	2.20	0.42
2:F:306:ILE:HA	2:F:309:PHE:HD2	1.85	0.42
10:X:-48:DC:H6	10:X:-48:DC:H2'	1.74	0.42
2:F:140:GLY:HA2	2:F:228:PRO:HG2	2.02	0.42
3:G:731:GLN:O	3:G:735:LEU:CB	2.68	0.42
8:P:37:TYR:HB2	8:P:63:ASN:OD1	2.20	0.42
10:X:-24:DT:N1	10:X:-23:DT:H72	2.34	0.42
10:X:0:DG:C6	10:X:1:DC:C4	3.08	0.42
10:X:16:DA:H1'	10:X:17:DA:C8	2.55	0.42
10:X:36:DA:H2''	10:X:37:DC:C6	2.52	0.42
1:A:447:LEU:O	1:A:451:GLN:HB2	2.20	0.42
2:B:121:GLN:HE21	2:B:125:ARG:HH21	1.68	0.42
1:E:337:VAL:HG12	1:E:345:THR:HG22	2.02	0.42
1:E:71:PRO:HG2	1:E:365:LEU:HG	2.02	0.41
1:E:95:PRO:HA	1:E:300:PHE:HB3	2.01	0.41
3:G:857:ARG:O	3:G:861:LEU:HG	2.20	0.41
7:K:29:ARG:NH1	8:L:35:GLU:HB3	2.35	0.41
5:M:46:VAL:HG21	11:Y:9:DG:H3'	2.01	0.41
7:O:29:ARG:HE	8:P:33:ARG:HH21	1.68	0.41
10:X:-79:DA:H2''	10:X:-78:DC:C6	2.55	0.41
10:X:-12:DA:C5	10:X:-11:DC:N4	2.88	0.41
10:X:57:DG:H2''	10:X:58:DC:C6	2.55	0.41
1:A:96:MET:HE2	1:A:301:VAL:HG22	2.02	0.41
2:B:49:GLN:HB3	2:B:52:ALA:HB3	2.02	0.41
10:X:5:DT:H2''	10:X:6:DA:N7	2.35	0.41
10:X:21:DG:C6	10:X:22:DT:C4	3.08	0.41
1:E:125:LYS:HB3	1:E:235:ILE:HG12	2.02	0.41
7:K:43:VAL:N	10:X:39:DA:OP1	2.50	0.41
5:M:108:ASN:ND2	6:N:42:GLY:O	2.53	0.41
11:Y:-35:DA:C6	11:Y:-34:DG:C6	3.08	0.41
11:Y:42:DC:H2''	11:Y:43:DT:C6	2.55	0.41
1:E:341:THR:HG21	1:E:344:ILE:HD12	2.02	0.41
2:F:76:ALA:O	2:F:358:SER:HA	2.20	0.41
2:F:439:SER:O	2:F:443:MET:HB2	2.19	0.41
10:X:31:DT:H2''	10:X:32:DG:C8	2.55	0.41
11:Y:72:DG:H2''	11:Y:73:DT:C7	2.51	0.41
1:A:205:ARG:NH2	1:A:212:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:CG	2:B:355:LEU:HD23	2.55	0.41
1:C:335:ASN:N	1:C:335:ASN:OD1	2.54	0.41
2:D:126:SER:HB2	2:D:322:PRO:HG3	2.01	0.41
3:G:890:PHE:O	3:G:894:ILE:HG13	2.21	0.41
10:X:24:DC:H2''	10:X:25:DT:H72	2.02	0.41
11:Y:-53:DG:C2	11:Y:-52:DG:C6	3.08	0.41
11:Y:-10:DC:H2''	11:Y:-9:DA:C8	2.56	0.41
1:C:182:LYS:HE2	3:G:1076:LEU:HB3	2.02	0.41
1:E:21:VAL:HG21	1:E:78:ALA:HB1	2.03	0.41
2:F:127:ILE:HG13	2:F:322:PRO:HG3	2.03	0.41
7:O:55:LEU:HD22	8:P:66:VAL:HA	2.01	0.41
11:Y:7:DC:C2'	11:Y:8:DC:C5	3.03	0.41
11:Y:82:DT:H2''	11:Y:83:DC:C6	2.56	0.41
2:B:193:ILE:HG22	2:B:204:LYS:HA	2.02	0.41
1:C:201:LYS:HE3	3:G:1084:GLY:HA3	2.02	0.41
1:E:113:MET:O	1:E:117:ARG:HG2	2.20	0.41
10:X:59:DA:C6	11:Y:-58:DG:C2	3.09	0.41
11:Y:-30:DG:C5	11:Y:-29:DC:N4	2.88	0.41
2:B:82:GLY:HA3	12:B:501:ADP:C8	2.55	0.41
2:B:82:GLY:O	2:B:86:ILE:HG23	2.21	0.41
2:B:295:VAL:HA	2:B:323:VAL:O	2.21	0.41
2:D:255:GLN:HE22	3:G:1079:ILE:HG23	1.85	0.41
1:E:177:PHE:CE2	9:R:294:THR:HG22	2.55	0.41
2:F:423:VAL:HG12	2:F:427:LYS:HE3	2.02	0.41
8:P:72:ARG:HB3	8:P:101:LEU:HD21	2.01	0.41
11:Y:-50:DC:C4	11:Y:-49:DG:C6	3.09	0.41
2:D:72:ALA:HB3	2:D:354:LEU:HB3	2.02	0.41
2:D:138:ILE:HG23	2:D:232:LEU:HG	2.01	0.41
1:E:74:THR:O	1:E:366:TYR:OH	2.38	0.41
1:E:351:PRO:O	1:E:355:LEU:HB2	2.21	0.41
2:F:131:ILE:HG23	2:F:289:ALA:HB2	2.03	0.41
3:G:1041:GLY:HA2	3:G:1047:LYS:HD2	2.03	0.41
5:M:72:ARG:O	5:M:76:GLN:CB	2.69	0.41
6:N:31:LYS:HG3	6:N:51:TYR:CE1	2.56	0.41
10:X:17:DA:H2''	10:X:18:DG:C8	2.55	0.41
2:B:430:TYR:OH	2:B:438:ARG:NH2	2.51	0.41
2:D:331:GLY:HA2	2:D:344:HIS:HA	2.03	0.41
2:F:312:LEU:HA	2:F:315:ALA:HB3	2.02	0.41
8:L:37:TYR:HB2	8:L:63:ASN:OD1	2.20	0.41
2:B:443:MET:O	2:B:447:GLN:CB	2.51	0.40
1:C:128:LYS:HD2	1:C:234:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:HG13	1:C:307:LEU:HD12	2.03	0.40
1:E:256:ILE:HG23	3:G:1074:GLY:O	2.20	0.40
11:Y:50:DA:H1'	11:Y:51:DC:H5'	2.03	0.40
1:A:250:PRO:HG3	2:F:258:LEU:HD22	2.04	0.40
1:C:181:GLN:HG2	3:G:1077:TRP:HZ2	1.86	0.40
8:L:46:LYS:HD3	8:L:46:LYS:HA	1.95	0.40
2:D:366:ASP:O	2:D:370:ILE:HG13	2.22	0.40
2:D:439:SER:O	2:D:443:MET:HB2	2.21	0.40
2:F:172:TYR:CZ	9:R:320:TYR:HB3	2.57	0.40
7:K:58:LEU:HD21	8:L:102:LEU:HD13	2.03	0.40
10:X:-10:DG:C2	11:Y:11:DG:C2	3.10	0.40
11:Y:47:DG:H2''	11:Y:48:DG:C8	2.56	0.40
6:J:46:ILE:O	10:X:7:DC:H3'	2.22	0.40
7:K:76:THR:O	8:L:52:THR:HA	2.21	0.40
10:X:-50:DT:C4	10:X:-49:DG:C6	3.10	0.40
11:Y:48:DG:H2''	11:Y:49:DC:H5''	2.04	0.40
11:Y:72:DG:C2'	11:Y:73:DT:C7	2.99	0.40
2:B:46:MET:HE2	2:B:53:ARG:HD3	2.04	0.40
2:D:56:ALA:HA	2:D:59:VAL:HG22	2.03	0.40
2:D:303:MET:HE3	2:D:303:MET:HB2	1.93	0.40
10:X:-66:DG:H2'	10:X:-65:DT:H71	2.02	0.40
10:X:-14:DA:H2''	10:X:-13:DA:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/456 (94%)	424 (99%)	6 (1%)	0	100	100
1	C	433/456 (95%)	428 (99%)	5 (1%)	0	100	100
1	E	441/456 (97%)	437 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	423/463 (91%)	419 (99%)	4 (1%)	0	100	100
2	D	430/463 (93%)	423 (98%)	7 (2%)	0	100	100
2	F	430/463 (93%)	426 (99%)	4 (1%)	0	100	100
3	G	672/1290 (52%)	649 (97%)	22 (3%)	1 (0%)	48	83
4	H	318/607 (52%)	311 (98%)	7 (2%)	0	100	100
5	I	94/136 (69%)	92 (98%)	2 (2%)	0	100	100
5	M	97/136 (71%)	97 (100%)	0	0	100	100
6	J	80/103 (78%)	80 (100%)	0	0	100	100
6	N	84/103 (82%)	84 (100%)	0	0	100	100
7	K	104/130 (80%)	103 (99%)	1 (1%)	0	100	100
7	O	103/130 (79%)	102 (99%)	1 (1%)	0	100	100
8	L	94/126 (75%)	89 (95%)	5 (5%)	0	100	100
8	P	90/126 (71%)	85 (94%)	5 (6%)	0	100	100
9	R	70/356 (20%)	68 (97%)	2 (3%)	0	100	100
All	All	4393/6000 (73%)	4317 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	1183	ILE

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	367/387 (95%)	363 (99%)	4 (1%)	70	80
1	C	366/387 (95%)	363 (99%)	3 (1%)	79	85
1	E	371/387 (96%)	367 (99%)	4 (1%)	70	80
2	B	353/390 (90%)	344 (98%)	9 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	359/390 (92%)	354 (99%)	5 (1%)	62	76
2	F	364/390 (93%)	358 (98%)	6 (2%)	58	74
3	G	205/1118 (18%)	203 (99%)	2 (1%)	73	82
4	H	2/520 (0%)	2 (100%)	0	100	100
5	I	83/111 (75%)	82 (99%)	1 (1%)	67	79
5	M	86/111 (78%)	85 (99%)	1 (1%)	67	79
6	J	67/79 (85%)	67 (100%)	0	100	100
6	N	71/79 (90%)	71 (100%)	0	100	100
7	K	84/100 (84%)	83 (99%)	1 (1%)	67	79
7	O	83/100 (83%)	83 (100%)	0	100	100
8	L	82/105 (78%)	79 (96%)	3 (4%)	29	50
8	P	80/105 (76%)	76 (95%)	4 (5%)	20	42
9	R	61/288 (21%)	61 (100%)	0	100	100
All	All	3084/5047 (61%)	3041 (99%)	43 (1%)	62	76

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	238	VAL
1	A	295	VAL
1	A	402	THR
2	B	16	VAL
2	B	73	VAL
2	B	86	ILE
2	B	182	LEU
2	B	239	VAL
2	B	242	VAL
2	B	301	VAL
2	B	354	LEU
2	B	406	ILE
1	C	42	GLN
1	C	136	THR
1	C	402	THR
2	D	16	VAL
2	D	60	LEU
2	D	258	LEU

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Mol	Chain	Res	Type
2	D	354	LEU
2	D	451	LEU
1	E	42	GLN
1	E	323	ILE
1	E	363	THR
1	E	402	THR
2	F	16	VAL
2	F	222	THR
2	F	239	VAL
2	F	301	VAL
2	F	397	THR
2	F	406	ILE
3	G	900	GLU
3	G	953	VAL
5	I	45	THR
7	K	118	LYS
8	L	90	THR
8	L	101	LEU
8	L	111	VAL
5	M	59	GLU
8	P	33	ARG
8	P	90	THR
8	P	101	LEU
8	P	111	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	236	GLN
1	A	262	GLN
1	A	429	HIS
2	B	44	GLN
2	B	121	GLN
2	B	233	GLN
2	B	240	HIS
2	B	245	HIS
2	B	255	GLN
1	C	20	HIS
1	C	34	GLN
1	C	115	ASN
1	C	241	HIS

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Mol	Chain	Res	Type
1	C	380	GLN
1	C	420	ASN
2	D	233	GLN
2	D	245	HIS
2	D	255	GLN
1	E	18	HIS
1	E	115	ASN
1	E	229	HIS
1	E	380	GLN
2	F	25	HIS
2	F	78	GLN
2	F	240	HIS
2	F	245	HIS
2	F	341	GLN
2	F	404	GLN
3	G	855	HIS
5	I	85	GLN
5	I	108	ASN
6	J	75	HIS
7	K	82	HIS
7	K	84	GLN
7	K	104	GLN
7	K	112	GLN
8	L	95	GLN
5	M	39	HIS
5	M	68	GLN
5	M	76	GLN
5	M	85	GLN
5	M	108	ASN
6	N	75	HIS
7	O	38	ASN
7	O	82	HIS
7	O	84	GLN
7	O	112	GLN
8	P	95	GLN
9	R	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	ADP	F	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
12	ADP	E	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
12	ADP	B	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
12	ADP	D	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
12	ADP	C	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
12	ADP	A	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)

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
12	ADP	F	501	-	-	2/12/32/32	0/3/3/3
12	ADP	E	501	-	-	2/12/32/32	0/3/3/3
12	ADP	B	501	-	-	0/12/32/32	0/3/3/3
12	ADP	D	501	-	-	2/12/32/32	0/3/3/3
12	ADP	C	501	-	-	2/12/32/32	0/3/3/3
12	ADP	A	501	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	501	ADP	C5-C4	2.53	1.47	1.40
12	B	501	ADP	C5-C4	2.51	1.47	1.40
12	C	501	ADP	C5-C4	2.51	1.47	1.40
12	D	501	ADP	C5-C4	2.50	1.47	1.40
12	F	501	ADP	C5-C4	2.49	1.47	1.40
12	E	501	ADP	C5-C4	2.46	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	501	ADP	PA-O3A-PB	-3.61	120.44	132.83
12	A	501	ADP	PA-O3A-PB	-3.56	120.62	132.83
12	F	501	ADP	PA-O3A-PB	-3.53	120.71	132.83
12	B	501	ADP	PA-O3A-PB	-3.53	120.72	132.83
12	D	501	ADP	PA-O3A-PB	-3.50	120.81	132.83
12	C	501	ADP	PA-O3A-PB	-3.49	120.85	132.83
12	A	501	ADP	C3'-C2'-C1'	3.46	106.19	100.98
12	B	501	ADP	C3'-C2'-C1'	3.35	106.02	100.98
12	E	501	ADP	C3'-C2'-C1'	3.22	105.82	100.98
12	D	501	ADP	C3'-C2'-C1'	3.21	105.81	100.98
12	C	501	ADP	N3-C2-N1	-3.19	123.69	128.68
12	D	501	ADP	N3-C2-N1	-3.19	123.69	128.68
12	F	501	ADP	N3-C2-N1	-3.18	123.72	128.68
12	E	501	ADP	N3-C2-N1	-3.17	123.72	128.68
12	A	501	ADP	N3-C2-N1	-3.14	123.78	128.68
12	B	501	ADP	N3-C2-N1	-3.12	123.79	128.68
12	C	501	ADP	C3'-C2'-C1'	3.07	105.60	100.98
12	F	501	ADP	C3'-C2'-C1'	3.02	105.53	100.98
12	F	501	ADP	C4-C5-N7	-2.72	106.57	109.40
12	E	501	ADP	C4-C5-N7	-2.70	106.58	109.40
12	D	501	ADP	C4-C5-N7	-2.70	106.59	109.40
12	C	501	ADP	C4-C5-N7	-2.69	106.60	109.40
12	A	501	ADP	C4-C5-N7	-2.60	106.69	109.40
12	B	501	ADP	C4-C5-N7	-2.58	106.71	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	501	ADP	C5'-O5'-PA-O3A
12	D	501	ADP	C5'-O5'-PA-O3A

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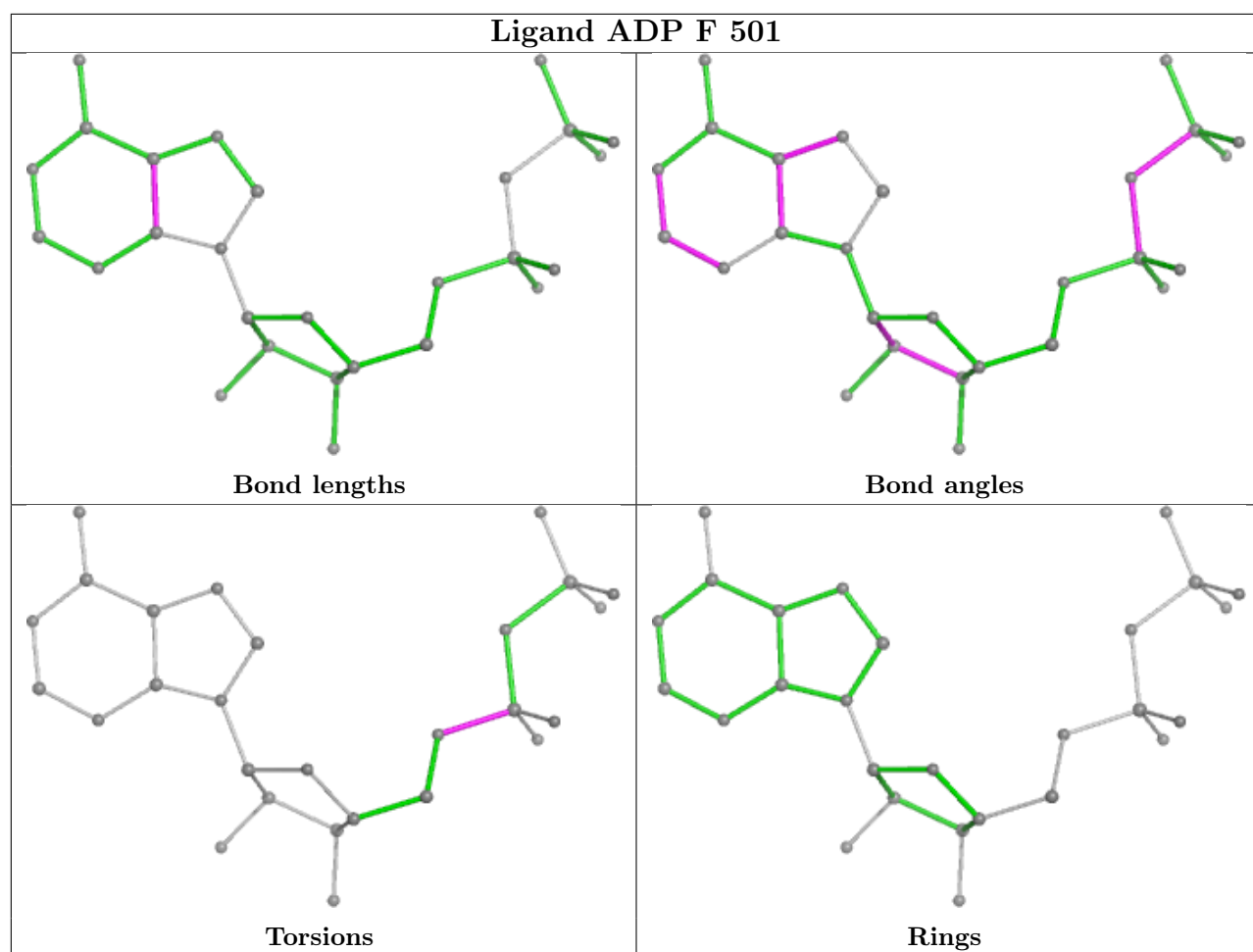
Mol	Chain	Res	Type	Atoms
12	E	501	ADP	C5'-O5'-PA-O1A
12	F	501	ADP	C5'-O5'-PA-O1A
12	F	501	ADP	C5'-O5'-PA-O3A
12	E	501	ADP	C5'-O5'-PA-O3A
12	C	501	ADP	C5'-O5'-PA-O1A
12	D	501	ADP	C5'-O5'-PA-O1A
12	A	501	ADP	C5'-O5'-PA-O1A

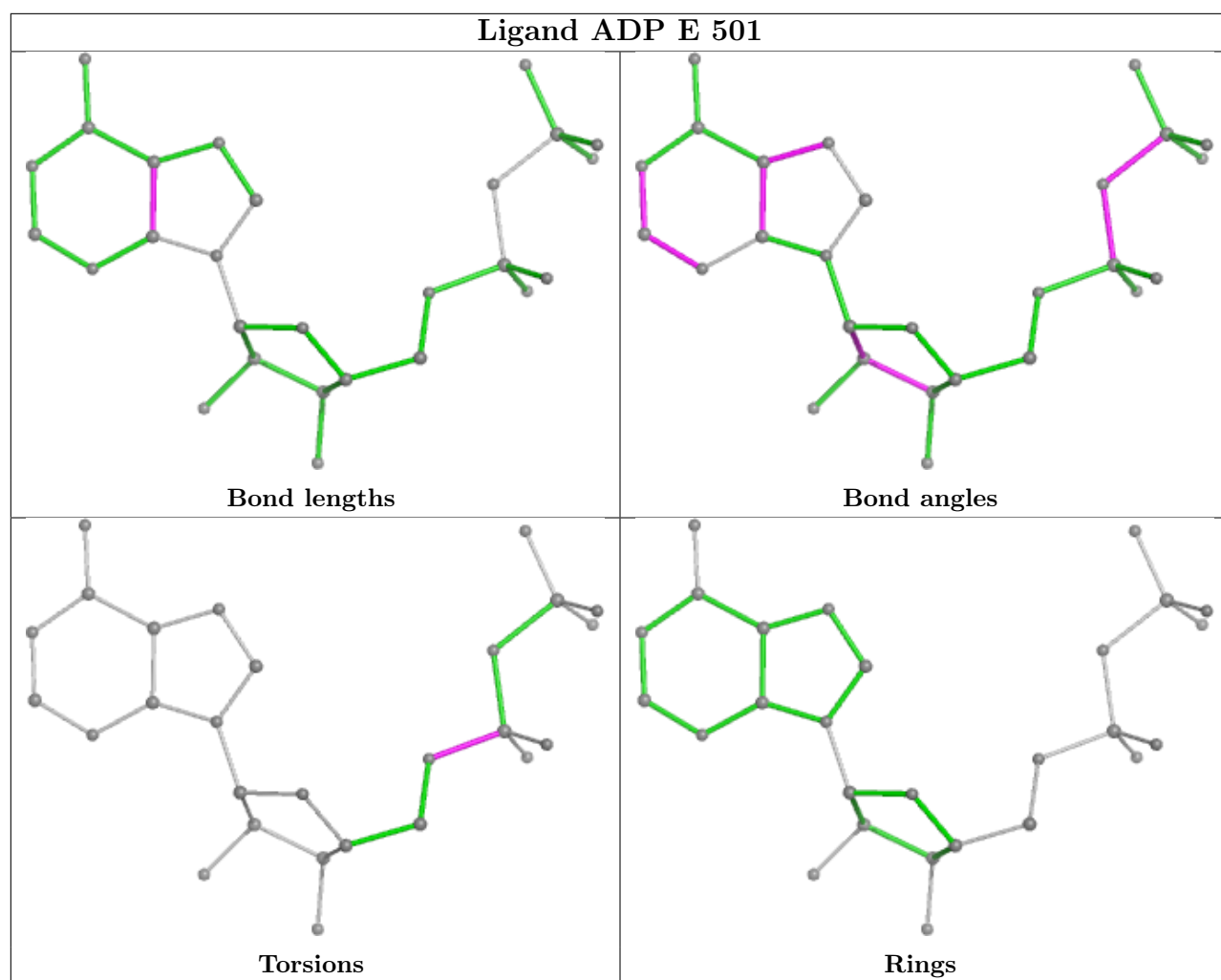
There are no ring outliers.

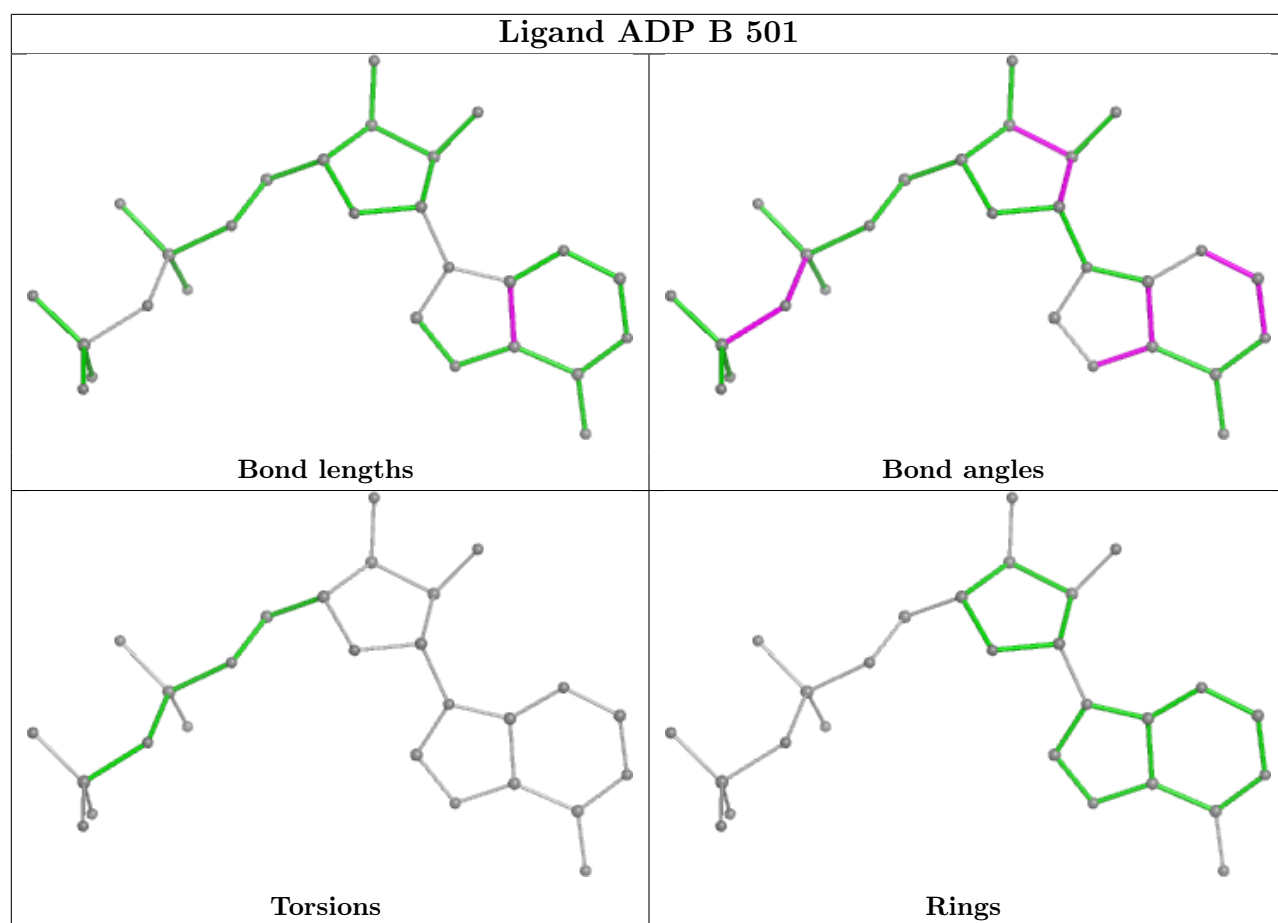
6 monomers are involved in 14 short contacts:

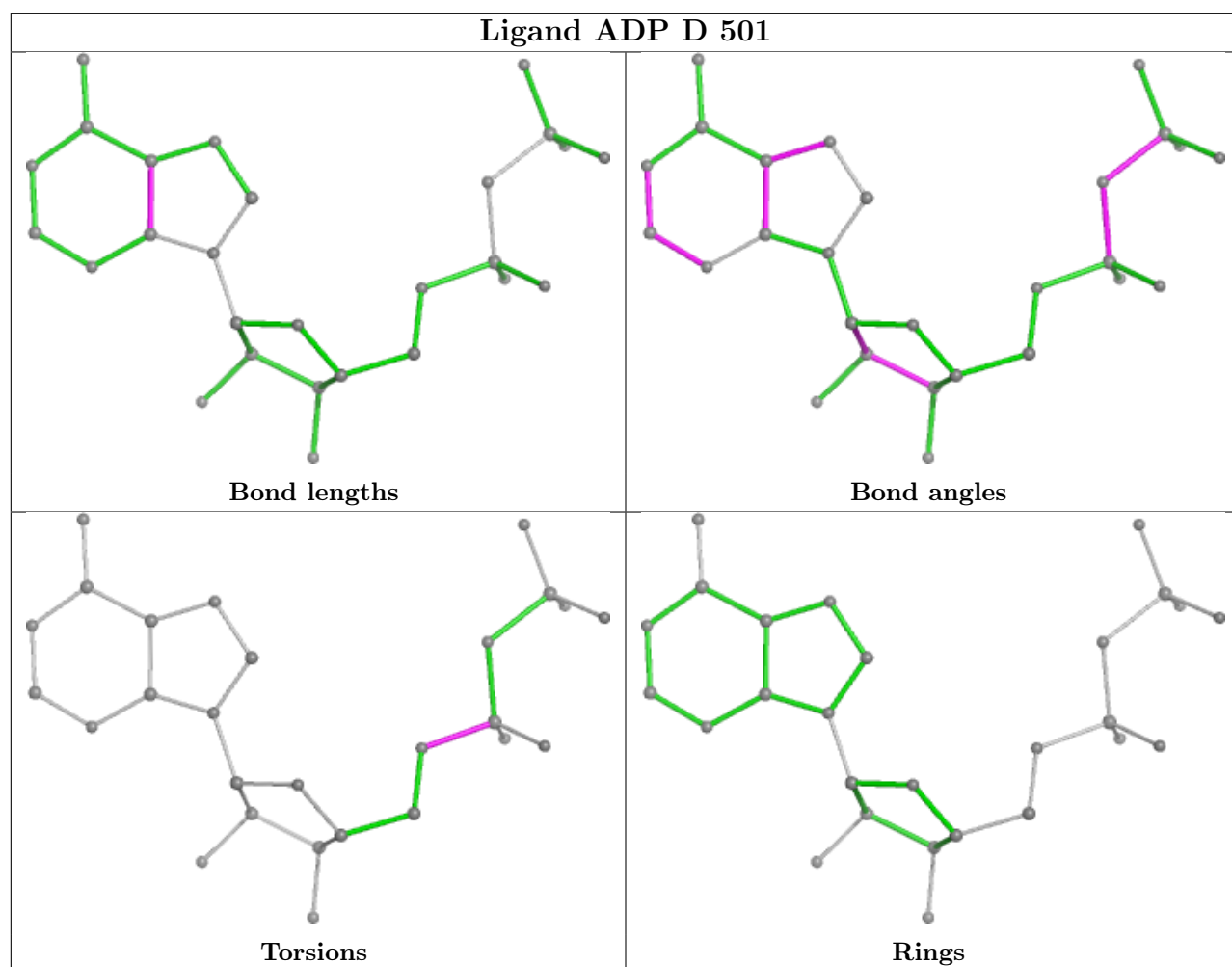
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	501	ADP	2	0
12	E	501	ADP	4	0
12	B	501	ADP	2	0
12	D	501	ADP	1	0
12	C	501	ADP	3	0
12	A	501	ADP	2	0

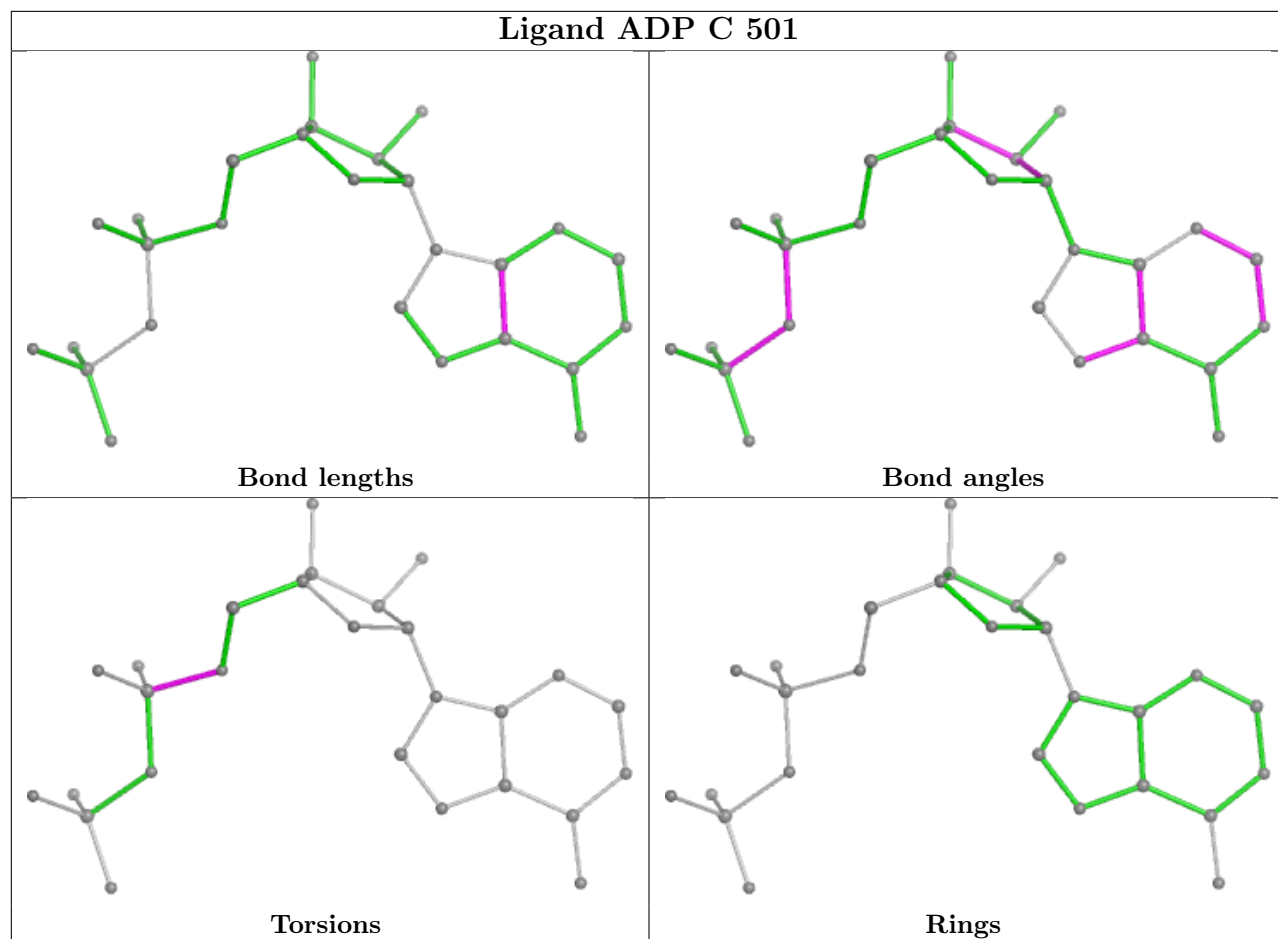
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

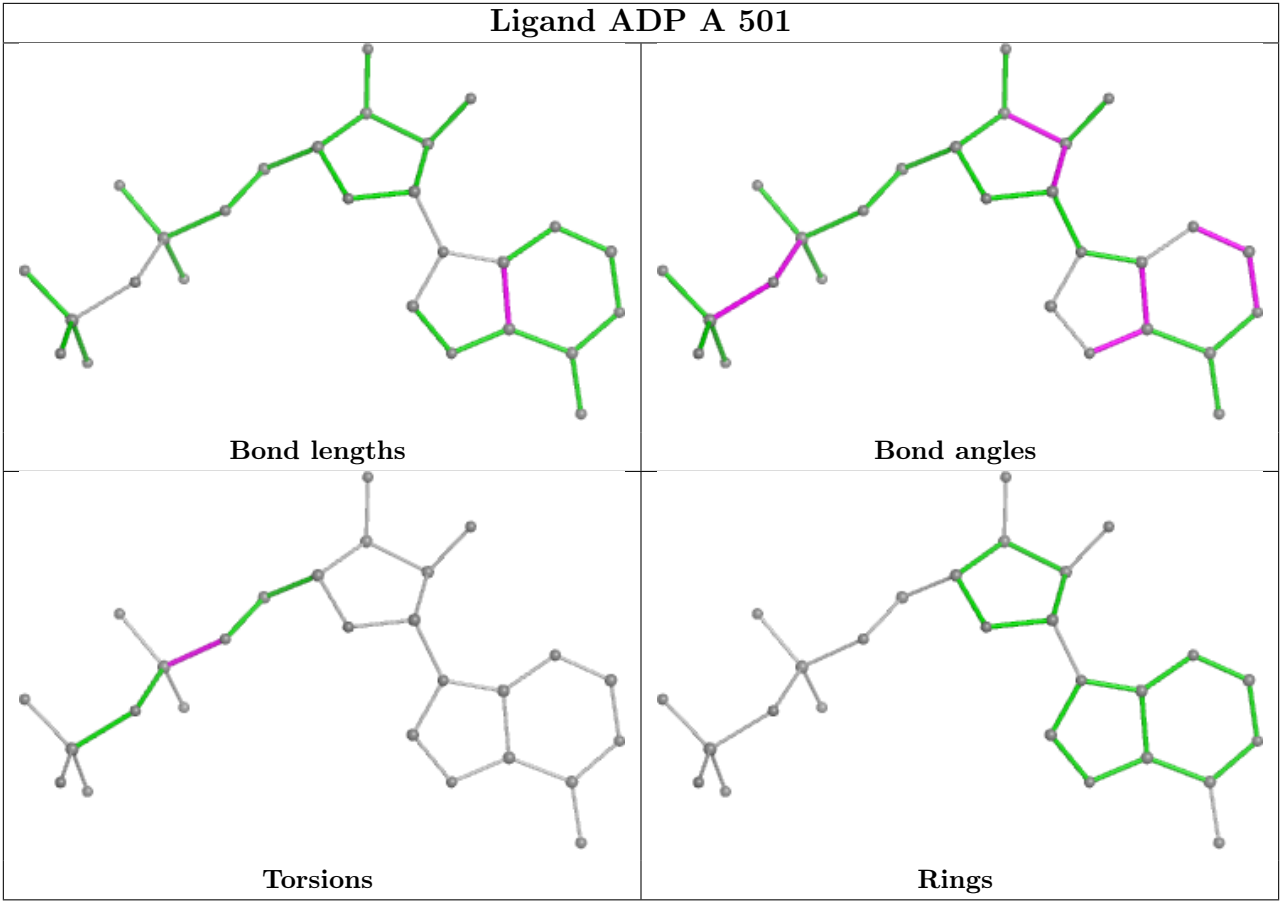












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	35:GLU	C	36:SER	N	4.83

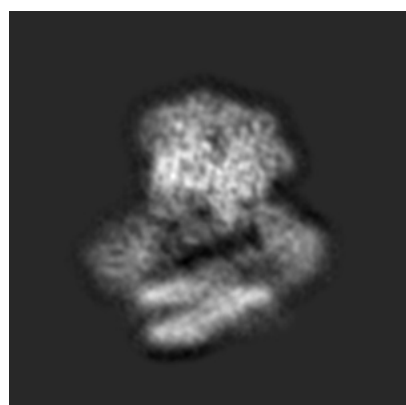
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3954. These allow visual inspection of the internal detail of the map and identification of artifacts.

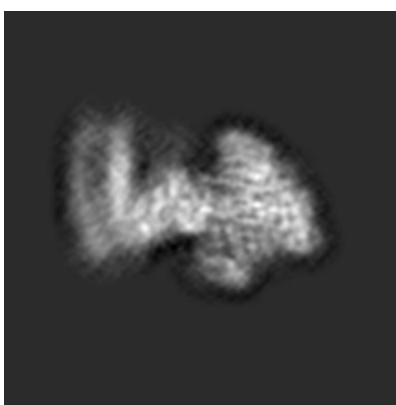
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

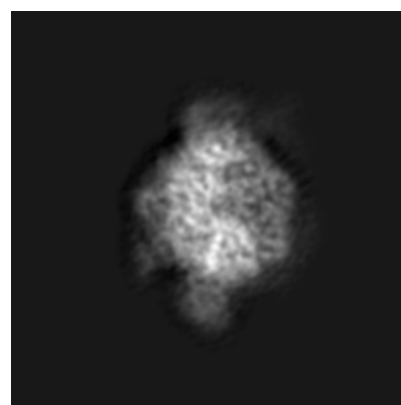
6.1.1 Primary map



X



Y

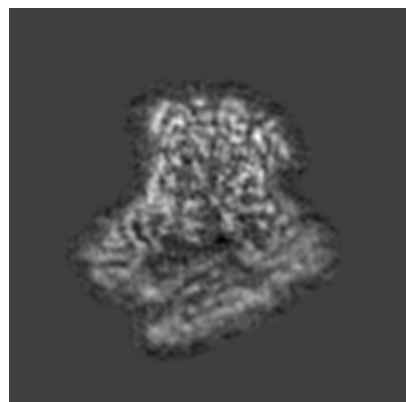


Z

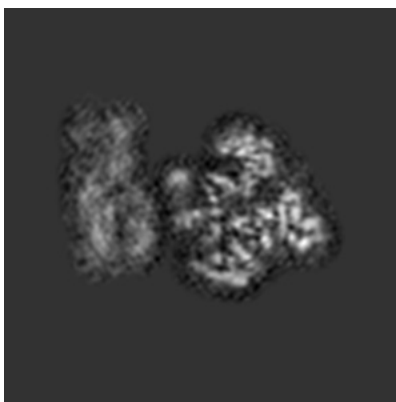
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

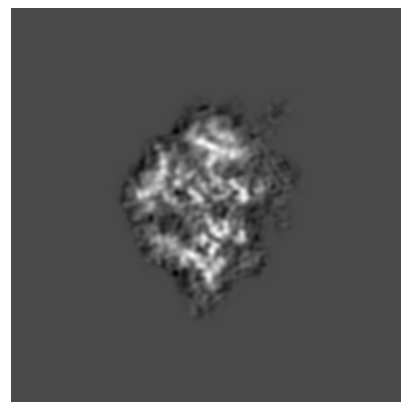
6.2.1 Primary map



X Index: 135



Y Index: 135

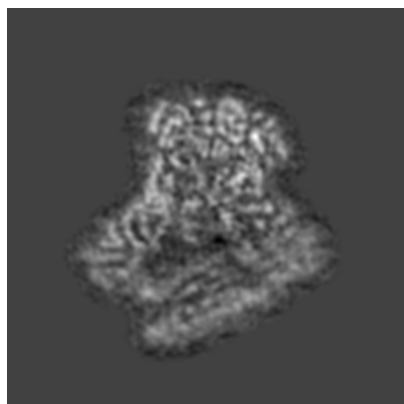


Z Index: 135

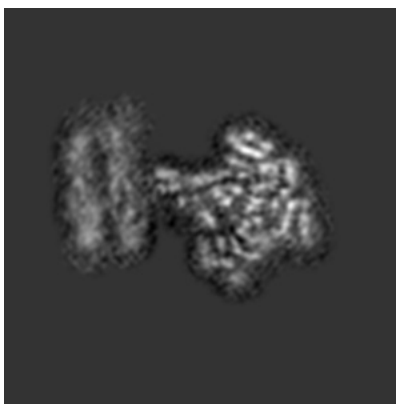
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

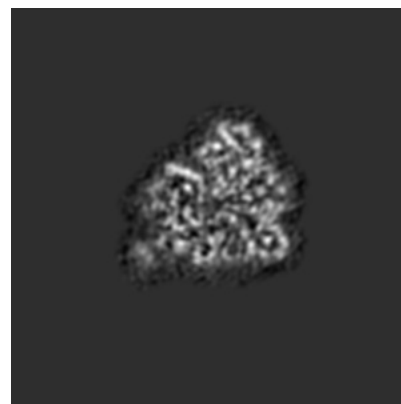
6.3.1 Primary map



X Index: 134



Y Index: 113



Z Index: 166

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

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

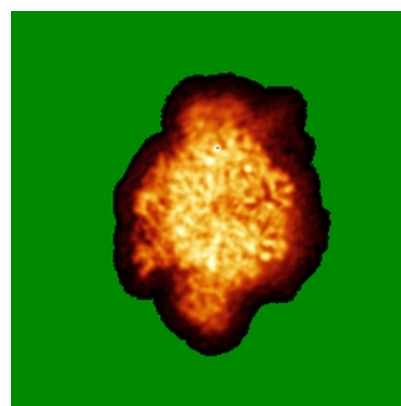
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

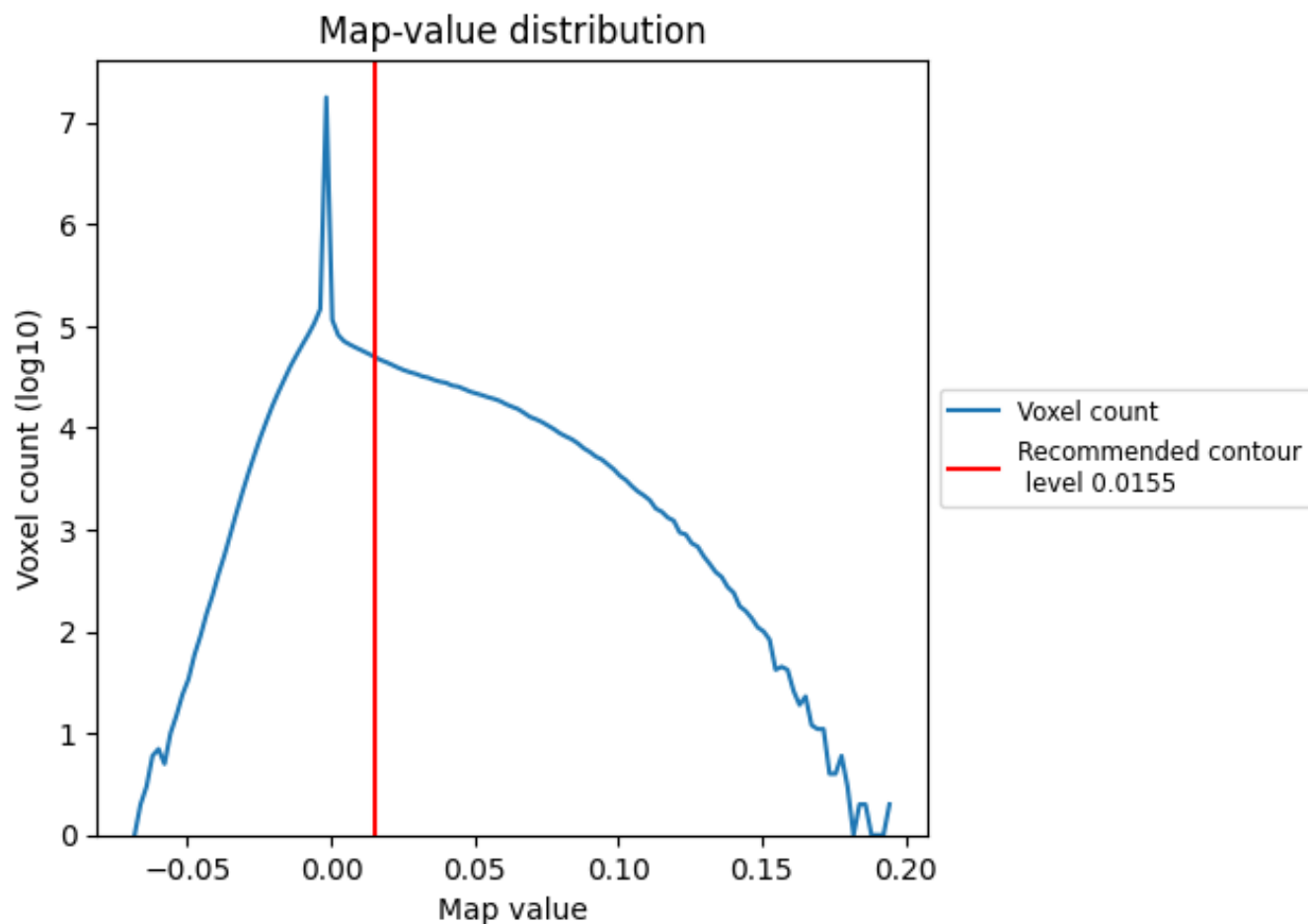
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

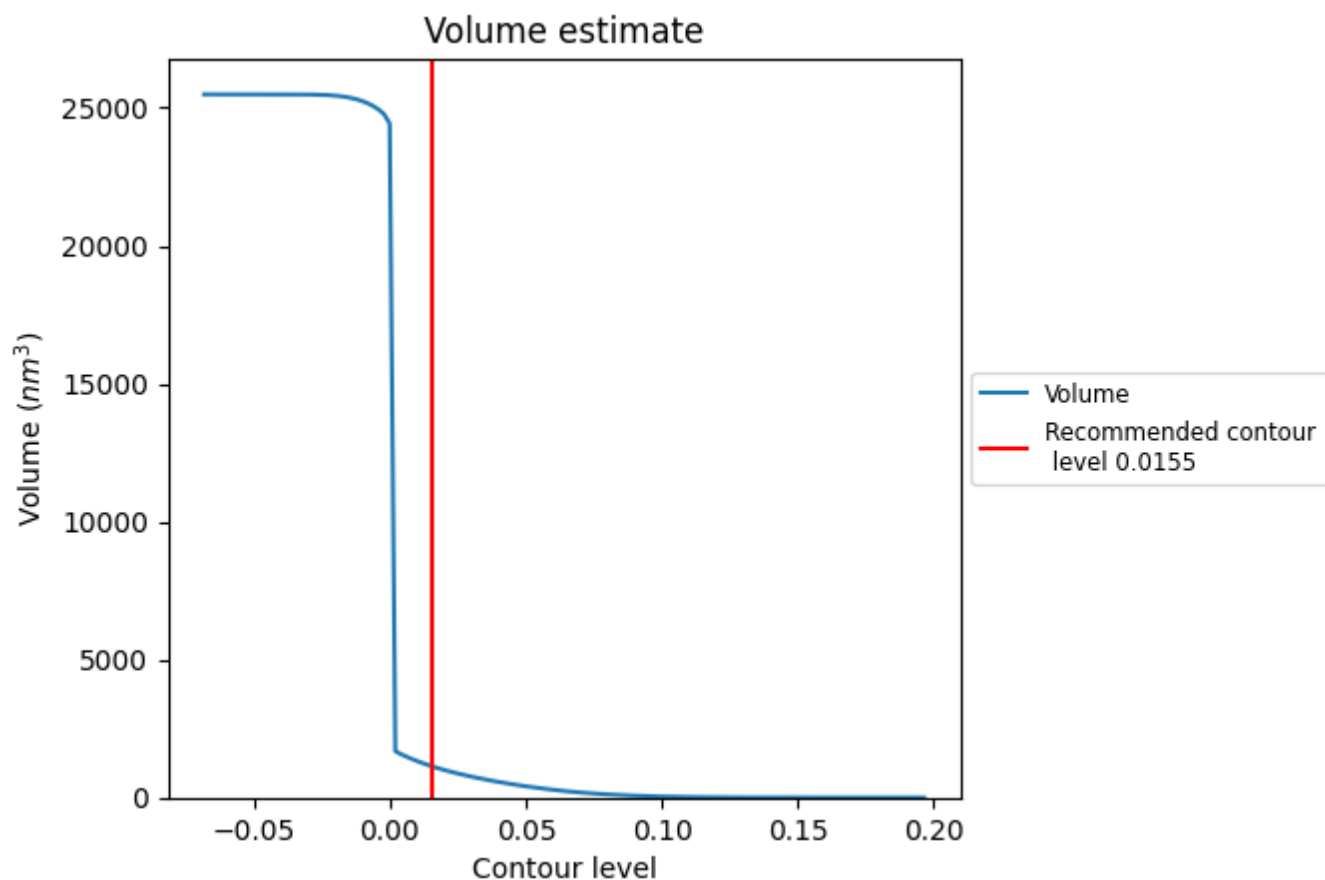
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

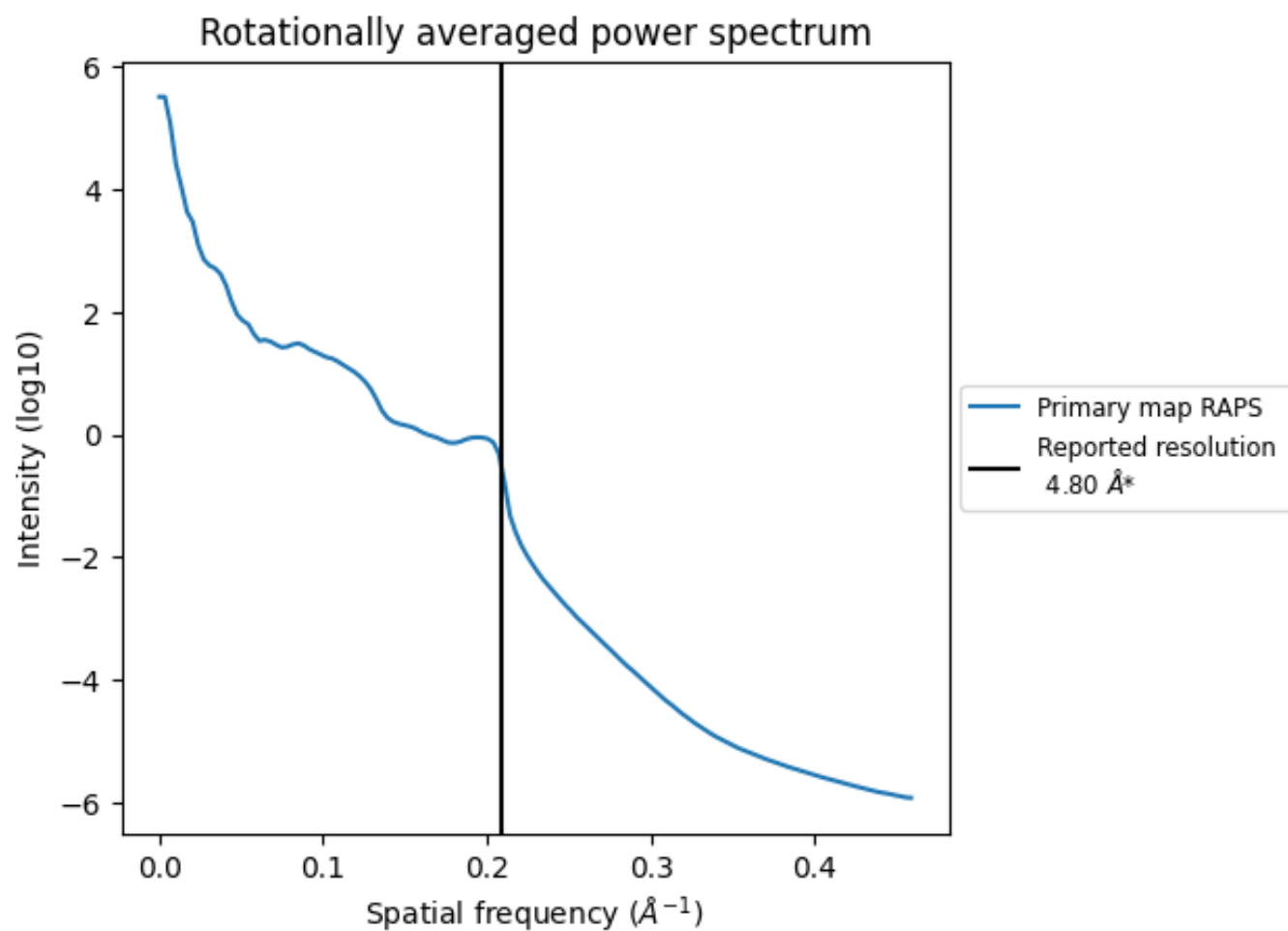
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1132 nm^3 ; this corresponds to an approximate mass of 1023 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 ⓘ

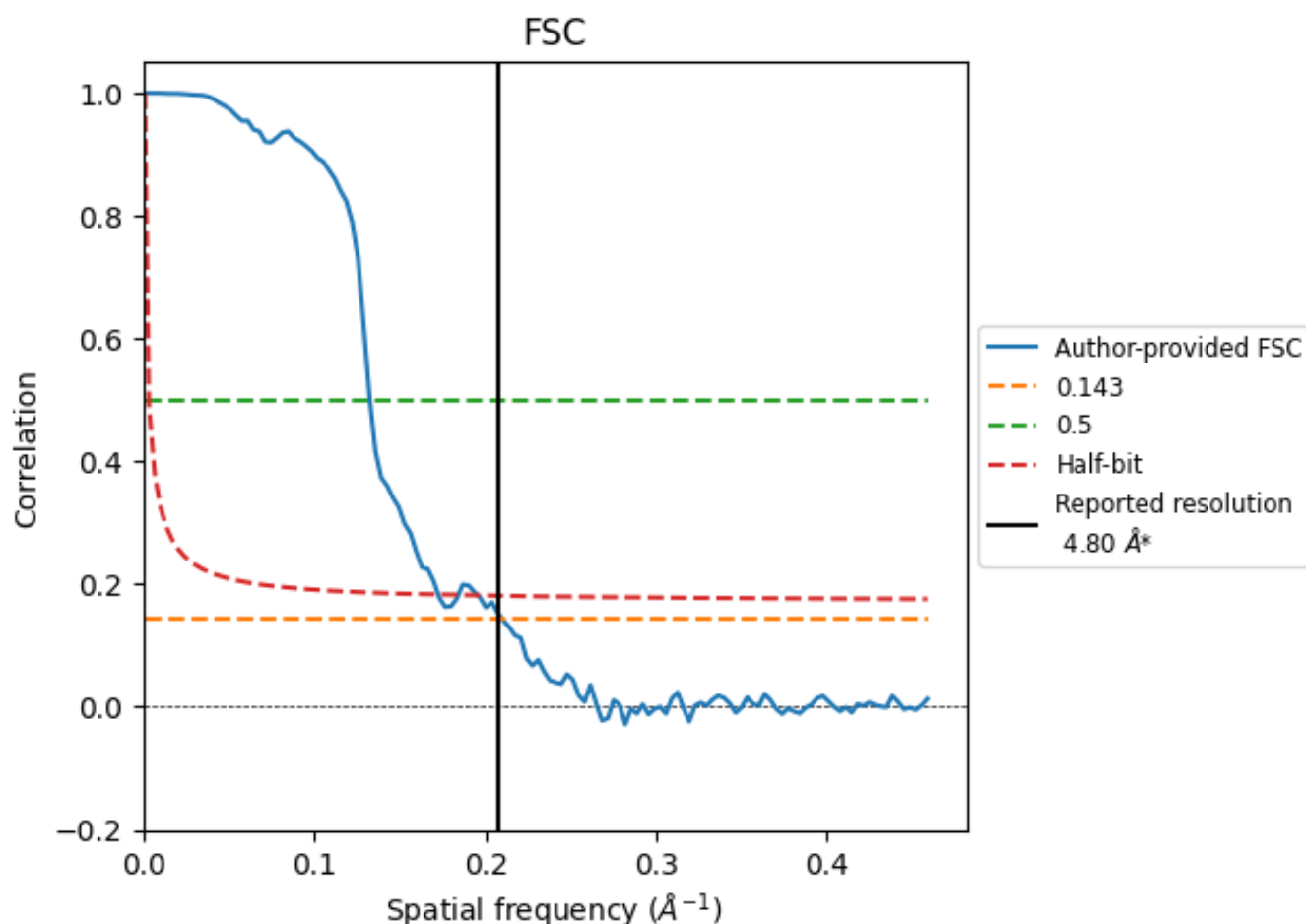


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

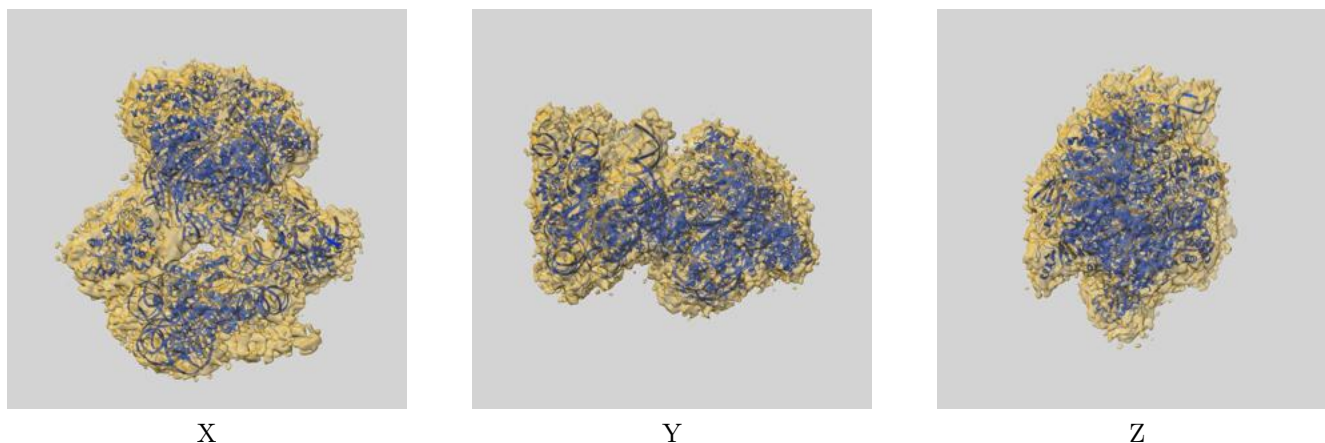
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.76	7.54	5.79
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3954 and PDB model 6HTS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



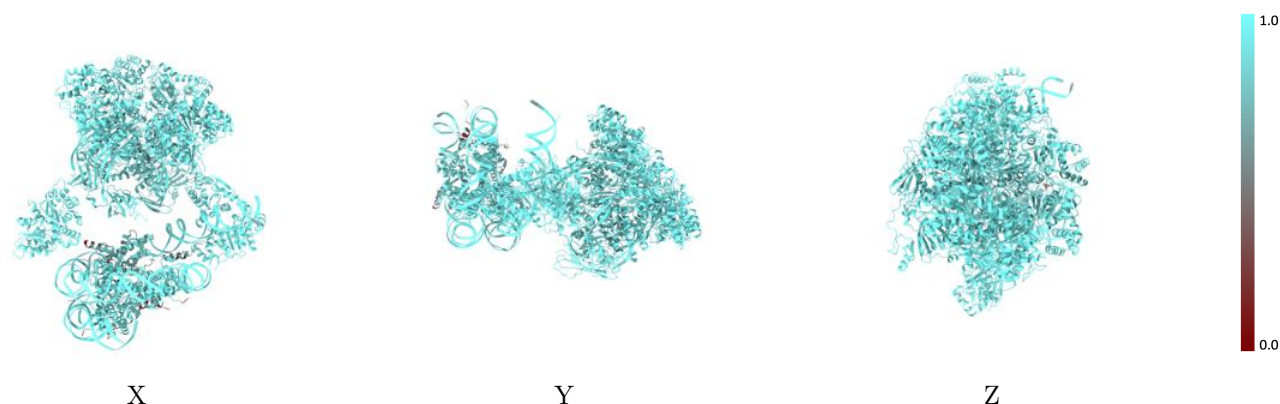
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



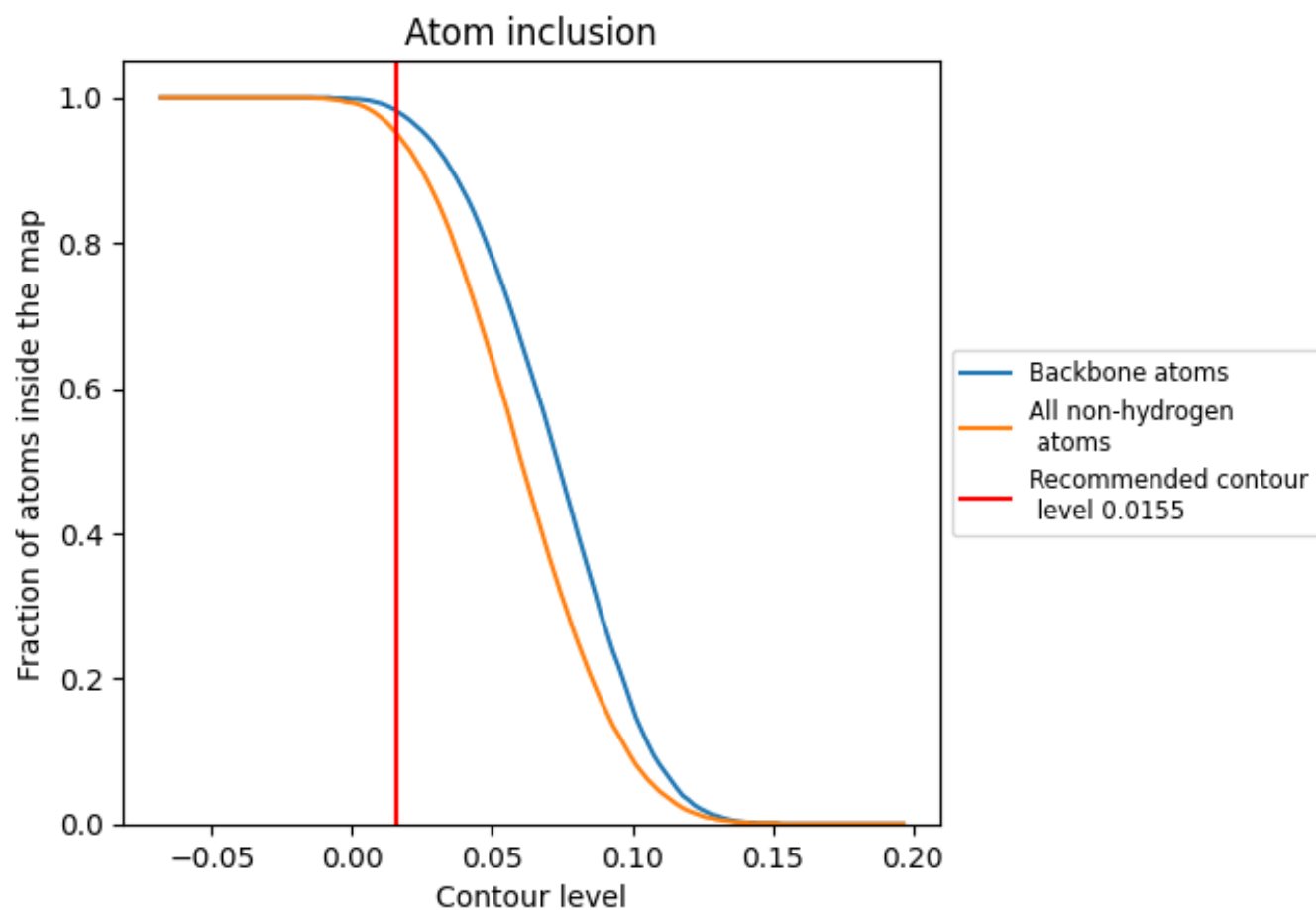
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0155).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.1810
A	 0.9740	 0.2190
B	 0.9560	 0.2070
C	 0.9470	 0.2250
D	 0.9610	 0.2110
E	 0.9690	 0.2130
F	 0.9680	 0.2120
G	 0.9740	 0.2020
H	 0.9980	 0.2470
I	 0.9080	 0.0820
J	 0.9460	 0.1120
K	 0.8970	 0.0910
L	 0.8930	 0.0710
M	 0.8700	 0.0710
N	 0.8610	 0.0420
O	 0.8450	 0.1050
P	 0.8050	 0.0950
R	 0.9880	 0.2190
X	 0.9690	 0.1290
Y	 0.9670	 0.1340

