Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 02:08 am GMT

PDB ID	:	6GEJ
EMDB ID	:	EMD-4395
Title	:	Chromatin remodeller-nucleosome complex at 3.6 A resolution.
Authors	:	Willhoft, O.; Chua, E.Y.D.; Wilkinson, M.; Wigley, D.B.
Deposited on	:	2018-04-26
Resolution	:	3.60 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 (i) 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 (1)) were used in the production of this report:

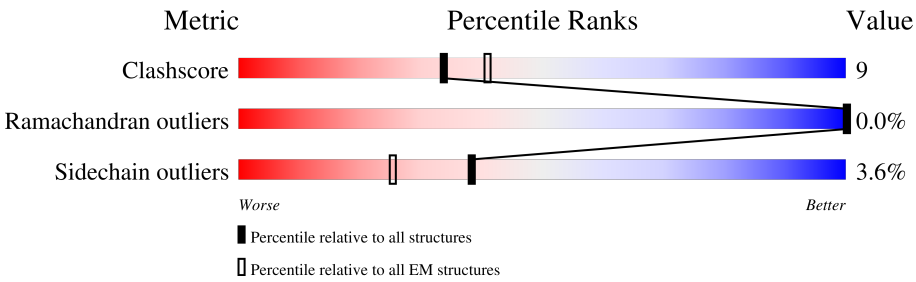
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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

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	Z	131	95% 5%
2	A	136	60% 11% 29%
2	B	136	60% 12% 29%
3	C	103	62% 16% • 20%
3	D	103	63% 14% • 22%
4	E	132	65% 11% • 22%
4	F	132	66% 9% • 23%
5	G	131	61% 12% 27%

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Mol	Chain	Length	Quality of chain
5	H	131	60% 10% 31%
6	I	154	39% 60%
7	J	154	47% 53%
8	M	1514	34% 11% 55%
9	R	438	73% 19% 6%
10	S	280	58% 16% 26%
11	T	463	75% 20%
11	V	463	70% 23% 6%
11	X	463	70% 24% 5%
12	U	471	67% 23% 9%
12	W	471	70% 21% 8%
12	Y	471	75% 19% 5%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 43702 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 Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	Z	131	655	393	131	131	0	0

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	97	796	506	152	138	0	0
2	B	97	796	506	152	138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	ASP	conflict	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	82	651	410	126	115	0	0
3	D	80	638	401	124	113	0	0

- Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	103	795	499	156	140	0	0
4	F	101	779	489	153	137	0	0

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	96	746	468	131	146	1	0	0
5	H	91	712	449	125	137	1	0	0

- Molecule 6 is a DNA chain called DNA (154-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	I	154	3137	1489	569	925	154	0	0

- Molecule 7 is a DNA chain called DNA (154-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	J	154	3177	1502	598	923	154	0	0

- Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	688	5398	3438	960	974	26	0	0

- Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	R	411	3335	2156	544	619	16	0	0

- Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	S	208	1695	1071	302	312	10	0	0

- Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	T	443	3391	2140	584	657	10	0	0

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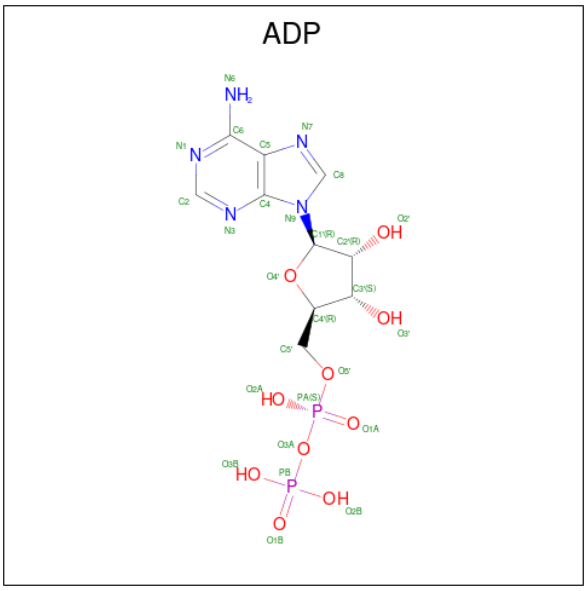
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	V	434	3336	2107	574	645	10	0	0
11	X	442	3397	2144	584	659	10	0	0

- Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	430	3299	2063	570	655	11	0	0
12	W	433	3325	2085	572	657	11	0	0
12	Y	447	3410	2133	590	675	12	0	0

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	M	1	27	10	5	10	2	0
13	R	1	27	10	5	10	2	0
13	T	1	27	10	5	10	2	0
13	U	1	27	10	5	10	2	0

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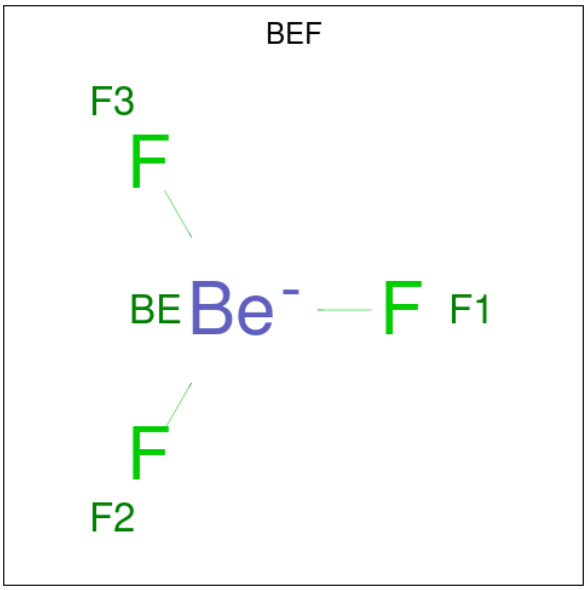
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	V	1	27	10	5	10	2	0
13	W	1	27	10	5	10	2	0
13	X	1	27	10	5	10	2	0
13	Y	1	27	10	5	10	2	0

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
14	M	1	4	1	3	0
14	R	1	4	1	3	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	M	1	1	1	0
15	R	1	1	1	0
15	U	2	2	2	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	V	1	1	1	0
			Total	Mg	
15	W	1	1	1	0
			Total	Mg	
15	X	1	1	1	0
			Total	Mg	
15	Y	1	1	1	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

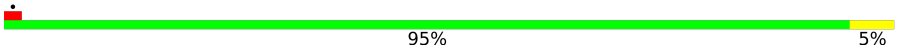
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	S	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

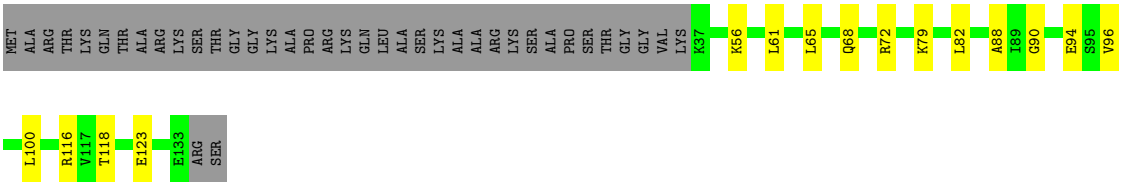
• Molecule 1: Vacuolar protein sorting-associated protein 72

Chain Z:



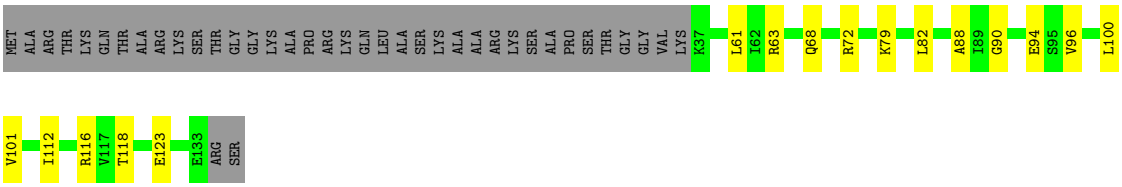
• Molecule 2: Histone H3

Chain A:



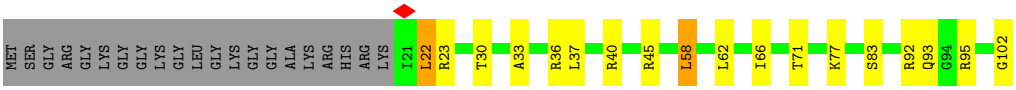
• Molecule 2: Histone H3

Chain B:



• Molecule 3: Histone H4

Chain C:



• Molecule 3: Histone H4

Chain D: 63% 14% • 22%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS ILE LEU R23 T30 K31 P32 A33 R36 L37 R45 L58 L62 I66 T71 K77 S83 R92 Q93 G94 R95 G102

• Molecule 4: Histone H2A.1

Chain E: 65% 11% • 22%

MET SER GLY GLY LYS GLY GLY LYS ALA GLY SER ALA ALA LYS ALA SER Q16 S17 R18 S19 A20 P27 R30 V31 L34 Q42 R43 R78 I88 L94 L98 V101 V108 H113 Q114 N115 P118 LYS LYS SER ALA LYS ALA THR LYS ALA SER GLN

GLU LEU

• Molecule 4: Histone H2A.1

Chain F: 66% 9% • 23%

MET SER GLY GLY LYS GLY GLY LYS ALA GLY SER ALA ALA LYS ALA SER GLN S17 R18 R30 L34 N39 R72 D73 R78 I79 R82 I88 L94 L98 V101 H113 Q114 N115 L116 L117 PRO LYS LYS SER ALA LYS ALA THR LYS ALA SER GLN GLU

LEU

• Molecule 5: Histone H2B.1

Chain G: 61% 12% 27%

MET SER ALA LYS ALA GLU LYS LYS PRO ALA SER LYS ALA PRO ALA GLU LYS LYS PRO ALA ALA LYS LYS THR SER THR SER THR ASP GLY LYS LYS ARG S33 R36 K37 Y43 D54 T55 S67 F73 I76 T91 R95 V101 R102 L103 I104 L105 A110

T128 GLN ALA

• Molecule 5: Histone H2B.1

Chain H: 60% 10% 31%

MET SER ALA LYS ALA GLU LYS LYS PRO ALA SER LYS ALA PRO ALA GLU LYS LYS PRO ALA ALA LYS LYS THR SER THR SER THR ASP GLY LYS LYS ARG SER LYS A35 D54 T55 G56 I57 I76 R95 V101 R102 L103 I104 L105 E108 L109 A110 Y124 S125 SER SER

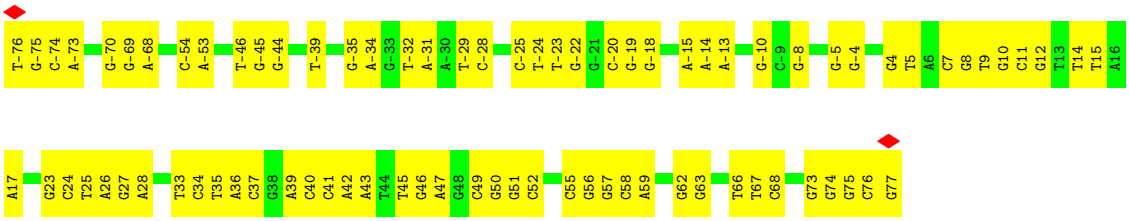
THR GLN ALA

• Molecule 6: DNA (154-MER)

Chain I: 39% 60% •

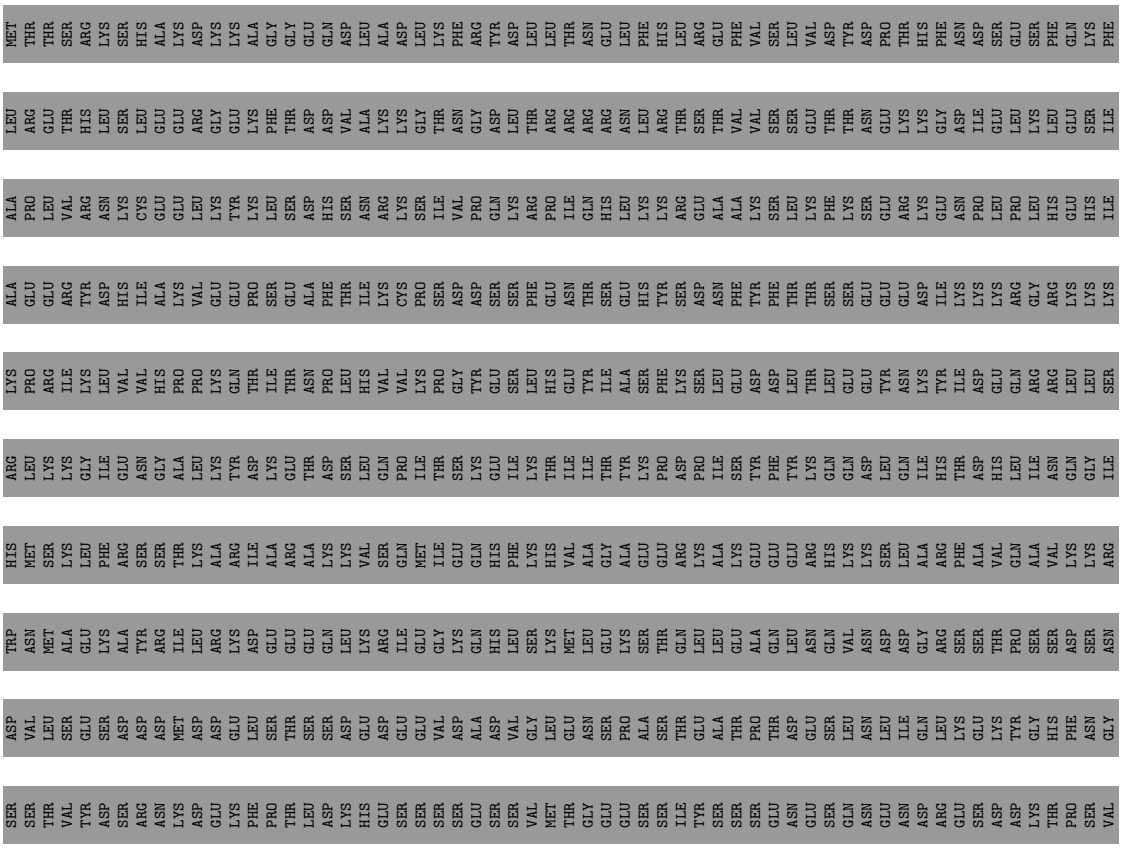
- Molecule 7: DNA (154-MER)

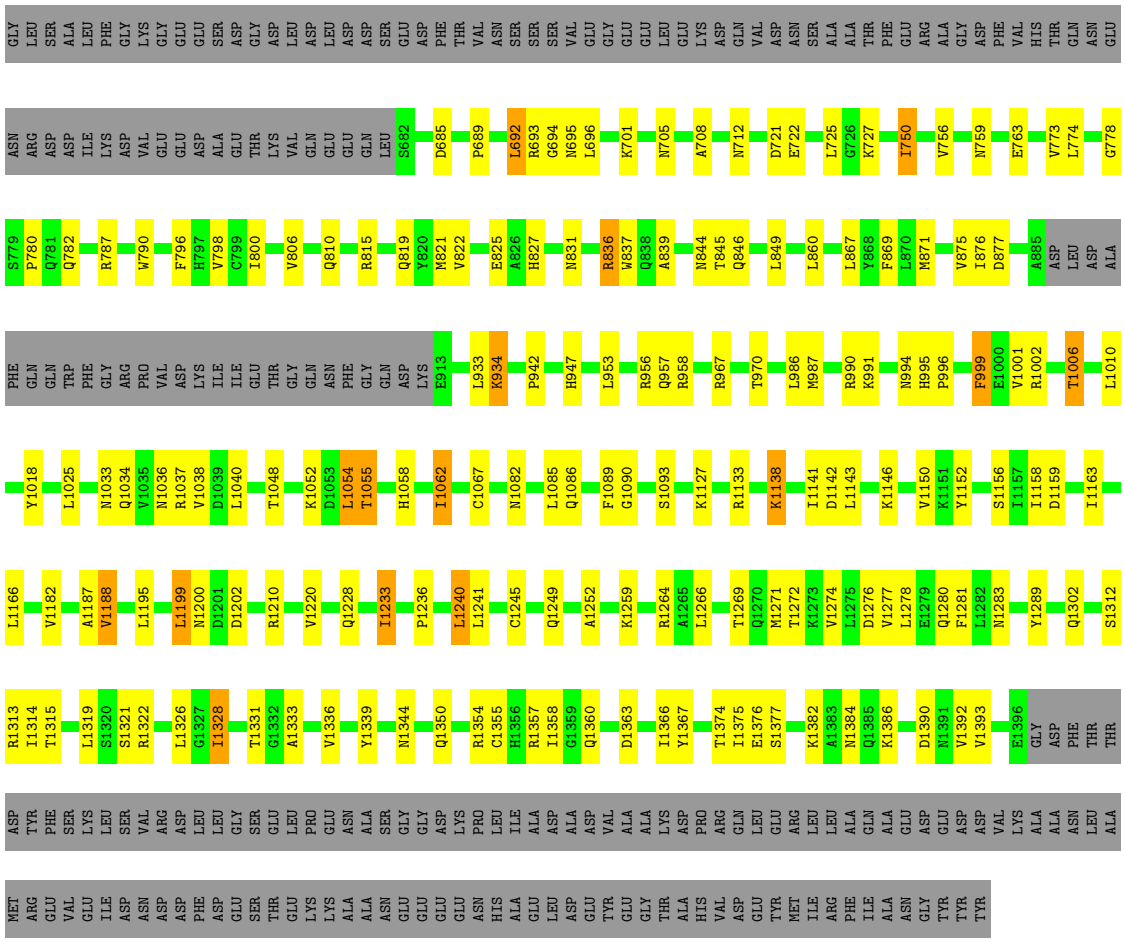
Chain J: 47% 53%



- Molecule 8: Helicase SWR1

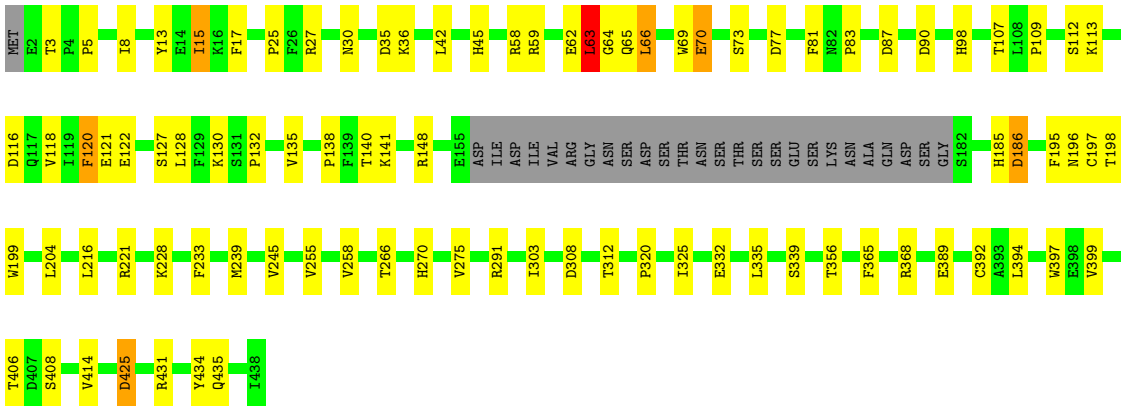
Chain M: 34% 11% 55%





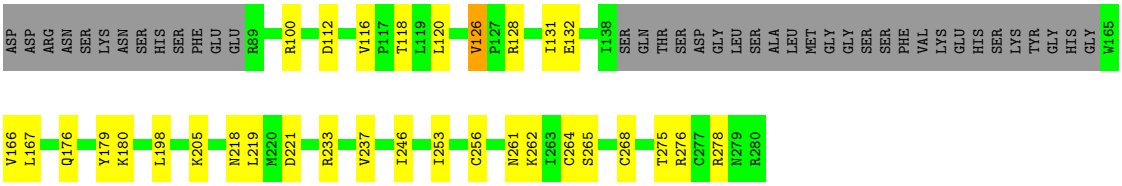
- Molecule 9: Actin-like protein ARP6

Chain R: 73% 19% • 6%



- Molecule 10: Vacuolar protein sorting-associated protein 71

Chain S: 58% 16% 26%

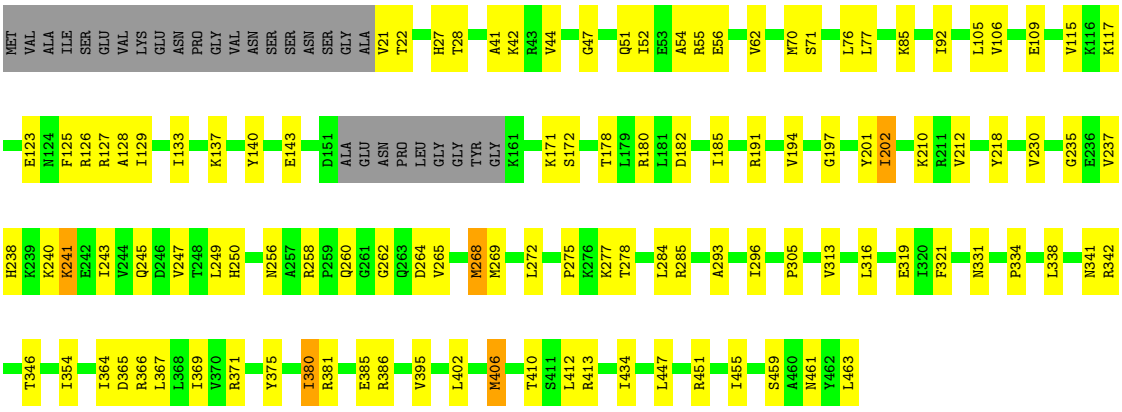


• Molecule 11: RuvB-like protein 1

Chain T:

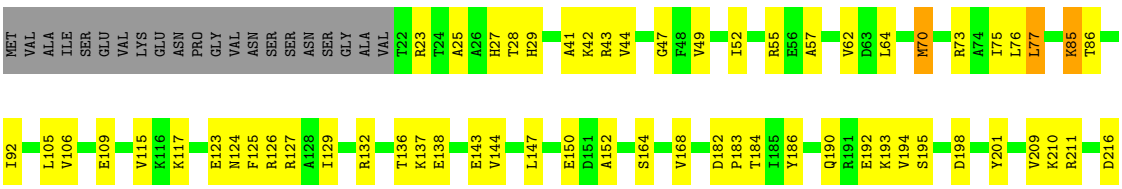
• Molecule 11: RuvB-like protein 1

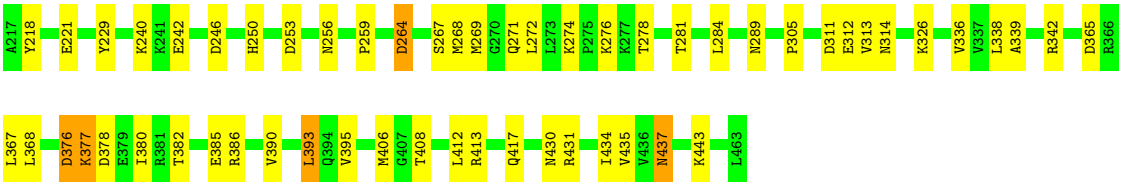
Chain V:



• Molecule 11: RuvB-like protein 1

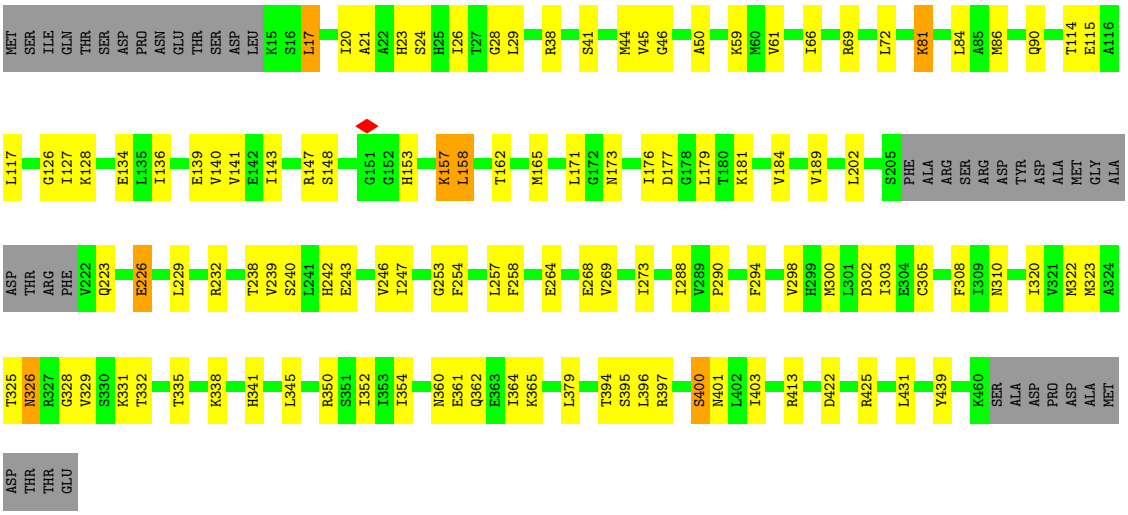
Chain X:





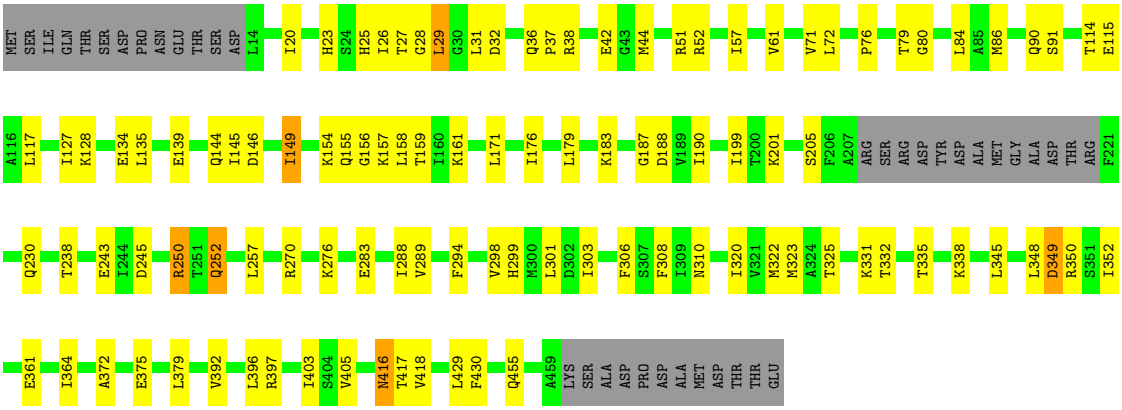
- Molecule 12: RuvB-like protein 2

Chain U:



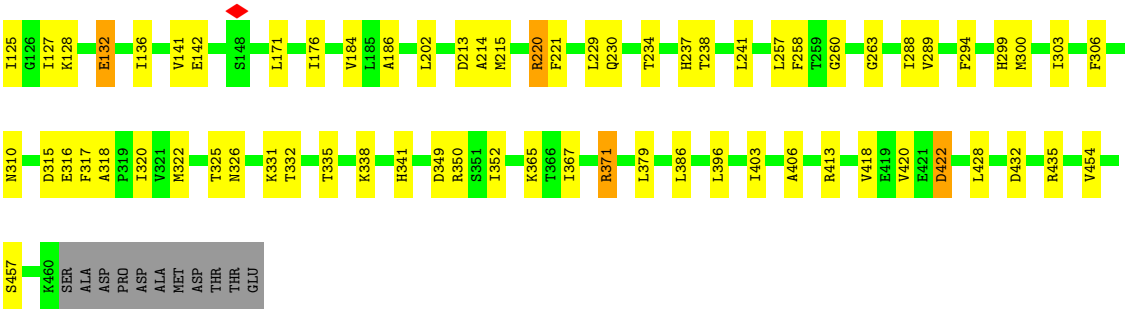
- Molecule 12: RuvB-like protein 2

Chain W:



- Molecule 12: RuvB-like protein 2

Chain Y:


I125
G126
I127
K128
E132
I136
V141
E142
S148
L171
I176
V184
L185
A186
L202
D213
A214
M215
R220
F221
L229
Q230
T234
H237
T238
L241
L257
F258
T259
G260
G263
I288
V289
F294
H299
M300
I303
F306
N310
D315
E316
F317
A318
P319
I320
V321
M322
T325
N326
K331
T332
T335
K338
H341
D349
R350
S351
I352
K365
T366
I367
R371
L379
L386
L396
I403
A406
R413
V418
E419
V420
E421
D422
L428
D432
R435
V454
S457
K460
SER
ALA
ASP
PRO
ASP
ALA
MET
ASP
THR
THR
GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98529	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 ($e^-/Å^2$)	1.71794871794872	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	0.358	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0295	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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: BEF, ADP, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
2	A	0.23	0/807	0.37	0/1081
2	B	0.23	0/807	0.37	0/1081
3	C	0.23	0/658	0.39	0/880
3	D	0.23	0/645	0.39	0/862
4	E	0.23	0/806	0.38	0/1091
4	F	0.23	0/789	0.38	0/1067
5	G	0.23	0/756	0.36	0/1017
5	H	0.23	0/722	0.36	0/972
6	I	0.52	0/3514	0.93	1/5416 (0.0%)
7	J	0.49	0/3568	0.89	0/5510
8	M	0.23	0/5495	0.42	0/7442
9	R	0.24	0/3429	0.40	2/4650 (0.0%)
10	S	0.23	0/1722	0.37	0/2320
11	T	0.24	0/3433	0.42	0/4646
11	V	0.24	0/3375	0.43	0/4565
11	X	0.24	0/3439	0.44	0/4652
12	U	0.24	0/3333	0.43	0/4492
12	W	0.24	0/3361	0.43	0/4530
12	Y	0.24	0/3447	0.43	0/4649
All	All	0.30	0/44106	0.54	3/60923 (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	Z	0	1
8	M	0	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	48	DG	O4'-C4'-C3'	-6.96	101.72	104.50
9	R	66	LEU	CA-CB-CG	5.47	127.89	115.30
9	R	63	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	M	1344	ASN	Peptide
8	M	692	LEU	Peptide
1	Z	188	UNK	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	Z	655	0	144	3	0
2	A	796	0	841	14	0
2	B	796	0	841	12	0
3	C	651	0	690	14	0
3	D	638	0	677	14	0
4	E	795	0	834	16	0
4	F	779	0	819	12	0
5	G	746	0	771	14	0
5	H	712	0	736	10	0
6	I	3137	0	1728	81	0
7	J	3177	0	1727	80	0
8	M	5398	0	5352	118	0
9	R	3335	0	3256	61	0
10	S	1695	0	1746	36	0
11	T	3391	0	3513	64	0
11	V	3336	0	3475	76	0
11	X	3397	0	3533	68	0
12	U	3299	0	3387	77	0
12	W	3325	0	3413	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	3410	0	3465	63	0
13	M	27	0	12	3	0
13	R	27	0	12	1	0
13	T	27	0	12	2	0
13	U	27	0	12	2	0
13	V	27	0	12	0	0
13	W	27	0	12	0	0
13	X	27	0	12	1	0
13	Y	27	0	12	4	0
14	M	4	0	0	1	0
14	R	4	0	0	1	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
16	S	2	0	0	0	0
All	All	43702	0	41044	760	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (760) 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)
11:T:406:MET:SD	11:T:443:LYS:NZ	2.29	1.06
9:R:77:ASP:O	9:R:81:PHE:HB2	1.68	0.93
11:X:406:MET:SD	11:X:443:LYS:HD2	2.08	0.93
10:S:176:GLN:O	10:S:180:LYS:HB2	1.72	0.89
11:V:406:MET:HE1	11:V:410:THR:HG21	1.58	0.85
11:X:406:MET:SD	11:X:443:LYS:CD	2.67	0.83
12:U:177:ASP:O	12:U:181:LYS:HB2	1.80	0.81
6:I:-68:DG:N2	7:J:68:DC:O2	2.13	0.81
6:I:-51:DC:N3	7:J:51:DG:N1	2.28	0.80
6:I:-52:DG:N2	7:J:52:DC:O2	2.14	0.80
11:X:377:LYS:HG2	11:X:408:THR:HG21	1.62	0.80
8:M:1058:HIS:O	8:M:1062:ILE:HB	1.83	0.79
6:I:-51:DC:O2	7:J:51:DG:N2	2.16	0.78
11:V:406:MET:HE1	11:V:410:THR:CG2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-46:DC:N3	7:J:46:DG:N1	2.29	0.76
12:U:173:ASN:O	12:U:176:ILE:N	2.19	0.75
11:T:68:LYS:HD2	11:T:305:PRO:HD2	1.66	0.75
6:I:-68:DG:N1	7:J:68:DC:N3	2.34	0.75
6:I:-46:DC:O2	7:J:46:DG:N2	2.16	0.75
6:I:-52:DG:N1	7:J:52:DC:N3	2.35	0.74
6:I:10:DC:O2	7:J:-10:DG:N2	2.16	0.74
11:X:43:ARG:HG3	11:X:44:VAL:HG23	1.70	0.74
11:X:274:LYS:NZ	12:Y:110:GLU:OE2	2.20	0.74
11:T:41:ALA:HB3	11:T:52:ILE:HG23	1.69	0.73
9:R:148:ARG:HG3	9:R:389:GLU:CG	2.19	0.73
8:M:1236:PRO:HB3	8:M:1240:LEU:HD21	1.71	0.72
8:M:875:VAL:HG13	8:M:877:ASP:H	1.54	0.72
2:A:56:LYS:HG2	10:S:53:LEU:HD21	1.71	0.72
12:W:38:ARG:O	12:W:51:ARG:NH2	2.22	0.72
12:U:397:ARG:O	12:U:401:ASN:ND2	2.23	0.71
8:M:1228:GLN:NE2	11:V:262:GLY:O	2.22	0.71
8:M:1163:ILE:O	11:X:256:ASN:ND2	2.23	0.71
11:V:313:VAL:HG21	11:V:338:LEU:HB3	1.73	0.71
12:W:298:VAL:HG21	12:W:323:MET:HB3	1.72	0.71
11:X:192:GLU:HG3	11:X:209:VAL:HB	1.73	0.70
8:M:1034:GLN:HA	8:M:1037:ARG:HB2	1.72	0.70
9:R:228:LYS:HD2	9:R:239:MET:HA	1.74	0.69
11:X:49:VAL:H	13:X:501:ADP:HN62	1.39	0.69
11:X:380:ILE:HD12	11:X:412:LEU:HD13	1.74	0.69
11:X:406:MET:SD	11:X:443:LYS:CE	2.80	0.69
12:Y:379:LEU:HD11	12:Y:403:ILE:HD11	1.73	0.69
6:I:10:DC:N3	7:J:-10:DG:N1	2.30	0.69
12:U:126:GLY:HA2	12:U:240:SER:HA	1.74	0.69
8:M:689:PRO:O	8:M:692:LEU:HB2	1.91	0.69
12:U:143:ILE:HG12	12:U:158:LEU:HB2	1.75	0.69
7:J:-25:DC:H2"	7:J:-24:DT:H5"	1.73	0.69
12:W:361:GLU:HG3	12:W:392:VAL:HG21	1.75	0.69
11:X:62:VAL:HG22	11:X:92:ILE:HG13	1.75	0.69
11:X:42:LYS:O	11:X:55:ARG:NH2	2.25	0.69
11:X:382:THR:HA	11:X:385:GLU:HG2	1.75	0.69
11:V:258:ARG:HH11	11:V:278:THR:H	1.40	0.68
8:M:1326:LEU:O	8:M:1354:ARG:NH1	2.27	0.68
11:X:132:ARG:HG2	11:X:246:ASP:HB3	1.76	0.68
9:R:148:ARG:HG3	9:R:389:GLU:HG2	1.76	0.68
12:W:156:GLY:HA3	12:W:176:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-75:DC:H2"	6:I:-74:DC:C5	2.29	0.67
11:V:41:ALA:HB3	11:V:52:ILE:HG23	1.74	0.67
12:U:128:LYS:HG2	12:U:238:THR:HG22	1.77	0.67
8:M:995:HIS:ND1	8:M:1245:CYS:SG	2.68	0.67
12:Y:184:VAL:HG12	12:Y:186:ALA:H	1.60	0.67
11:V:126:ARG:HH12	11:V:285:ARG:HB3	1.61	0.66
12:Y:22:ALA:O	12:Y:371:ARG:NH2	2.26	0.66
11:T:42:LYS:O	11:T:55:ARG:NH2	2.28	0.66
11:V:380:ILE:HG13	11:V:412:LEU:HD13	1.76	0.66
11:X:313:VAL:HG21	11:X:338:LEU:HB3	1.78	0.66
12:W:416:ASN:H	12:W:416:ASN:HD22	1.43	0.66
3:D:77:LYS:HG2	5:G:95:ARG:HH12	1.60	0.65
11:X:126:ARG:NH1	11:X:289:ASN:OD1	2.28	0.65
9:R:116:ASP:O	9:R:120:PHE:HB2	1.97	0.65
12:Y:127:ILE:HG12	12:Y:288:ILE:HG22	1.78	0.65
5:H:108:GLU:HG2	10:S:44:ARG:HH11	1.60	0.64
8:M:778:GLY:HA3	8:M:782:GLN:HB2	1.79	0.64
8:M:1386:LYS:NZ	8:M:1390:ASP:O	2.27	0.64
12:U:21:ALA:HB2	11:V:331:ASN:HB3	1.79	0.64
8:M:806:VAL:O	8:M:810:GLN:HB3	1.97	0.64
11:V:109:GLU:HG2	12:W:114:THR:HG21	1.80	0.64
12:U:431:LEU:HD11	11:V:371:ARG:HE	1.63	0.64
11:X:431:ARG:HH11	11:X:435:VAL:HG21	1.62	0.64
8:M:1127:LYS:NZ	11:T:136:THR:OG1	2.31	0.64
8:M:1138:LYS:H	8:M:1138:LYS:HD3	1.63	0.64
11:V:62:VAL:HG22	11:V:92:ILE:HG13	1.80	0.64
6:I:-56:DC:H2"	6:I:-55:DG:N7	2.12	0.63
8:M:695:ASN:O	13:M:1601:ADP:N6	2.31	0.63
8:M:822:VAL:HG12	8:M:849:LEU:HB3	1.79	0.63
11:X:201:TYR:HB3	11:X:210:LYS:HB3	1.78	0.63
11:T:132:ARG:HA	11:T:246:ASP:HA	1.81	0.63
9:R:198:THR:HB	9:R:216:LEU:HB2	1.79	0.63
7:J:-19:DG:H5"	8:M:1272:THR:HG23	1.79	0.63
6:I:22:DC:H2"	6:I:23:DA:H5"	1.80	0.63
11:V:275:PRO:HB2	12:W:250:ARG:HH21	1.63	0.62
12:W:28:GLY:H	12:W:90:GLN:HB3	1.63	0.62
6:I:-31:DA:H2"	6:I:-30:DG:H5'	1.82	0.62
12:W:397:ARG:NH2	11:X:365:ASP:OD2	2.32	0.62
9:R:233:PHE:HB3	10:S:276:ARG:HH11	1.64	0.62
11:T:189:ILE:HG12	11:T:209:VAL:HG11	1.81	0.62
11:X:395:VAL:HG13	11:X:434:ILE:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:10:LYS:HE3	11:V:178:THR:HG21	1.81	0.62
11:V:42:LYS:O	11:V:55:ARG:NH2	2.33	0.62
12:Y:141:VAL:HG12	12:Y:142:GLU:HG3	1.82	0.61
4:F:79:ILE:HD12	5:H:57:ILE:HG12	1.82	0.61
12:U:162:THR:OG1	12:U:165:MET:O	2.14	0.61
12:W:127:ILE:HG12	12:W:288:ILE:HG22	1.82	0.61
8:M:1025:LEU:HD11	12:U:239:VAL:HG11	1.82	0.61
7:J:-19:DG:H2'	7:J:-18:DG:C8	2.35	0.61
12:Y:367:ILE:HG21	12:Y:396:LEU:HD21	1.82	0.61
8:M:1166:LEU:HD22	11:X:259:PRO:HB3	1.83	0.61
8:M:1220:VAL:O	11:V:191:ARG:NH1	2.33	0.61
9:R:258:VAL:O	9:R:368:ARG:NH1	2.33	0.61
11:T:42:LYS:HD2	11:T:45:GLU:HB2	1.82	0.61
11:X:129:ILE:HG22	11:X:305:PRO:HA	1.81	0.61
12:Y:299:HIS:HB3	12:Y:325:THR:HG23	1.82	0.61
6:I:21:DC:OP2	8:M:831:ASN:ND2	2.33	0.61
9:R:434:TYR:OH	10:S:221:ASP:OD1	2.19	0.61
11:V:51:GLN:HG3	11:V:54:ALA:HB3	1.83	0.61
11:V:172:SER:OG	11:V:235:GLY:O	2.19	0.60
9:R:58:ARG:NH1	10:S:112:ASP:OD1	2.33	0.60
6:I:66:DC:H2"	6:I:67:DA:H5'	1.82	0.60
6:I:67:DA:H2"	6:I:68:DT:H71	1.84	0.60
8:M:1200:ASN:O	8:M:1210:ARG:NH1	2.34	0.60
9:R:112:SER:OG	9:R:130:LYS:NZ	2.31	0.60
11:V:201:TYR:N	11:V:210:LYS:O	2.32	0.60
12:W:27:THR:HA	12:W:90:GLN:HG2	1.84	0.60
12:U:72:LEU:N	12:U:352:ILE:O	2.26	0.60
11:V:123:GLU:OE2	11:V:250:HIS:NE2	2.34	0.60
12:U:61:VAL:HG22	12:U:320:ILE:HG21	1.84	0.60
12:W:115:GLU:OE2	12:W:270:ARG:NH2	2.35	0.59
12:W:146:ASP:N	12:W:155:GLN:O	2.35	0.59
11:X:23:ARG:HH11	12:Y:317:PHE:HA	1.67	0.59
7:J:62:DG:OP1	8:M:787:ARG:NH2	2.36	0.59
8:M:1264:ARG:HB2	8:M:1333:ALA:HA	1.82	0.59
8:M:750:ILE:HD11	8:M:800:ILE:HG23	1.83	0.59
11:V:406:MET:CE	11:V:410:THR:CG2	2.81	0.59
11:T:344:MET:HA	11:T:356:PRO:HA	1.85	0.59
11:T:413:ARG:HD3	13:T:501:ADP:H5'1	1.83	0.59
12:U:127:ILE:HG12	12:U:288:ILE:HG22	1.84	0.59
12:W:364:ILE:HD12	12:W:392:VAL:HG22	1.85	0.59
8:M:1264:ARG:NH2	8:M:1312:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:395:VAL:HG22	11:V:434:ILE:HD12	1.84	0.59
12:W:80:GLY:O	12:W:84:LEU:N	2.33	0.59
8:M:778:GLY:HA3	8:M:782:GLN:HE21	1.68	0.59
3:C:30:THR:HG21	7:J:-13:DA:H5"	1.84	0.59
11:T:131:LEU:HD11	11:T:301:ALA:HB1	1.84	0.59
12:U:413:ARG:NH2	12:U:422:ASP:OD1	2.35	0.59
9:R:339:SER:OG	10:S:233:ARG:NH2	2.37	0.58
9:R:121:GLU:HB3	10:S:198:LEU:HD11	1.83	0.58
6:I:71:DT:H2"	6:I:72:DG:C8	2.38	0.58
8:M:1089:PHE:O	8:M:1093:SER:HB3	2.04	0.58
8:M:1241:LEU:HD11	8:M:1277:VAL:HG13	1.86	0.58
11:V:455:ILE:O	11:V:459:SER:OG	2.22	0.58
11:V:44:VAL:HG13	11:V:386:ARG:NH1	2.18	0.58
10:S:100:ARG:HH12	10:S:132:GLU:HA	1.69	0.57
11:X:138:GLU:HG2	11:X:240:LYS:HG2	1.84	0.57
11:X:281:THR:HG23	11:X:284:LEU:H	1.68	0.57
11:T:351:GLU:OE1	12:Y:331:LYS:NZ	2.36	0.57
12:U:396:LEU:O	12:U:400:SER:OG	2.22	0.57
12:U:397:ARG:NH1	13:U:502:ADP:O3B	2.38	0.57
12:W:190:ILE:HG22	12:W:201:LYS:HG2	1.84	0.57
8:M:727:LYS:NZ	13:M:1601:ADP:O3B	2.30	0.57
12:U:134:GLU:HG2	12:U:232:ARG:HG3	1.86	0.57
4:F:30:ARG:O	4:F:34:LEU:HB2	2.05	0.57
8:M:821:MET:HG2	8:M:845:THR:HG21	1.85	0.57
9:R:65:GLN:HE21	9:R:107:THR:HA	1.69	0.57
4:F:30:ARG:HE	7:J:-45:DG:H5'	1.69	0.57
7:J:-5:DG:H2"	7:J:-4:DG:C8	2.40	0.57
8:M:1264:ARG:NH1	8:M:1314:ILE:O	2.38	0.57
9:R:98:HIS:HD2	9:R:127:SER:HB2	1.68	0.57
12:U:425:ARG:NH1	11:V:56:GLU:OE2	2.36	0.57
3:C:40:ARG:HH21	4:E:108:VAL:HG13	1.70	0.57
8:M:1062:ILE:HG23	8:M:1133:ARG:HE	1.70	0.57
9:R:58:ARG:HB3	10:S:166:VAL:HG13	1.85	0.57
6:I:-51:DC:N4	7:J:51:DG:O6	2.33	0.57
9:R:5:PRO:HB3	9:R:98:HIS:HB2	1.86	0.57
11:T:62:VAL:HG22	11:T:92:ILE:HG13	1.87	0.57
11:V:47:GLY:H	11:V:386:ARG:NH2	2.03	0.57
2:B:100:LEU:HD23	3:C:37:LEU:HD13	1.86	0.56
11:T:109:GLU:HG2	12:U:114:THR:HG21	1.87	0.56
12:U:298:VAL:HG21	12:U:323:MET:HB2	1.87	0.56
11:V:125:PHE:HD1	11:V:334:PRO:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:171:LEU:HD21	12:U:179:LEU:HD22	1.87	0.56
4:E:30:ARG:O	4:E:34:LEU:HB2	2.05	0.56
4:E:98:LEU:HD13	4:E:101:VAL:HG21	1.87	0.56
6:I:-7:DG:H2"	6:I:-6:DT:C5	2.41	0.56
8:M:1350:GLN:HE21	8:M:1354:ARG:HH12	1.53	0.56
12:U:329:VAL:H	12:U:341:HIS:H	1.54	0.56
2:B:101:VAL:HG11	4:E:108:VAL:HG11	1.88	0.56
6:I:-46:DC:H2"	6:I:-45:DA:N7	2.22	0.56
8:M:1156:SER:O	11:X:137:LYS:NZ	2.38	0.56
8:M:1252:ALA:HB2	8:M:1281:PHE:HZ	1.71	0.56
11:V:126:ARG:HH21	11:V:249:LEU:HD21	1.71	0.56
8:M:942:PRO:HB2	8:M:1363:ASP:HA	1.88	0.55
12:W:429:LEU:HD22	11:X:57:ALA:HB2	1.88	0.55
6:I:-59:DT:H2"	6:I:-58:DG:C8	2.41	0.55
6:I:48:DG:H2"	6:I:49:DC:C5	2.41	0.55
12:W:158:LEU:HD23	12:W:171:LEU:HD11	1.88	0.55
12:W:310:ASN:O	12:W:350:ARG:NH1	2.38	0.55
11:X:126:ARG:NH2	11:X:253:ASP:OD2	2.40	0.55
2:A:100:LEU:HD23	3:D:37:LEU:HD13	1.87	0.55
8:M:1033:ASN:HB3	8:M:1037:ARG:HG3	1.89	0.55
11:T:130:GLY:HA2	11:T:248:THR:HA	1.88	0.55
12:W:128:LYS:HG2	12:W:238:THR:HG22	1.89	0.55
12:W:139:GLU:O	12:W:161:LYS:N	2.31	0.55
2:B:116:ARG:NH2	2:B:123:GLU:OE2	2.39	0.55
4:F:98:LEU:HD13	4:F:101:VAL:HG21	1.87	0.55
6:I:46:DA:H2"	6:I:47:DG:C8	2.41	0.55
8:M:956:ARG:HD2	8:M:1002:ARG:HH21	1.72	0.55
11:T:48:PHE:HB3	11:T:55:ARG:HH11	1.72	0.55
12:W:134:GLU:OE1	12:W:230:GLN:NE2	2.40	0.55
6:I:-58:DG:O4'	8:M:815:ARG:NH2	2.38	0.55
8:M:685:ASP:OD2	8:M:701:LYS:NZ	2.32	0.55
11:T:123:GLU:O	11:T:127:ARG:HG3	2.07	0.55
2:A:116:ARG:NH2	2:A:123:GLU:OE2	2.39	0.54
3:D:93:GLN:OE1	3:D:95:ARG:NH2	2.40	0.54
6:I:-59:DT:H1'	8:M:815:ARG:HH21	1.71	0.54
12:U:136:ILE:HG23	12:U:229:LEU:HB3	1.89	0.54
11:V:76:LEU:HD21	11:V:369:ILE:HG12	1.89	0.54
11:X:44:VAL:HG22	11:X:49:VAL:HG12	1.89	0.54
9:R:118:VAL:O	9:R:122:GLU:HB2	2.06	0.54
7:J:-46:DT:H2'	7:J:-45:DG:C8	2.42	0.54
11:X:109:GLU:HG2	12:Y:114:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:267:SER:O	11:X:271:GLN:NE2	2.39	0.54
9:R:275:VAL:HG22	9:R:303:ILE:HG12	1.89	0.54
11:X:77:LEU:HD12	11:X:85:LYS:HG2	1.90	0.54
3:C:93:GLN:OE1	3:C:95:ARG:NH2	2.41	0.54
11:X:29:HIS:HB3	11:X:390:VAL:HG21	1.90	0.54
8:M:825:GLU:HB2	8:M:827:HIS:CE1	2.42	0.54
7:J:23:DG:H2"	7:J:24:DC:H5"	1.90	0.54
7:J:25:DT:H2"	7:J:26:DA:C8	2.42	0.54
9:R:228:LYS:HG2	9:R:245:VAL:HG21	1.90	0.54
10:S:275:THR:O	10:S:278:ARG:NH1	2.39	0.54
12:W:379:LEU:HD23	12:W:418:VAL:HG21	1.89	0.54
8:M:1188:VAL:HG23	11:V:260:GLN:HB2	1.88	0.54
6:I:25:DG:H2"	6:I:26:DG:C8	2.43	0.54
12:U:81:LYS:HB3	13:U:502:ADP:O2B	2.08	0.54
4:F:73:ASP:OD2	10:S:51:TYR:N	2.41	0.53
8:M:756:VAL:HG13	8:M:759:ASN:HD22	1.73	0.53
12:U:17:LEU:HD23	11:V:296:ILE:HG21	1.90	0.53
11:V:212:VAL:HG12	11:V:230:VAL:HG11	1.89	0.53
6:I:-18:DC:H2"	6:I:-17:DT:H5'	1.91	0.53
12:Y:128:LYS:HG2	12:Y:238:THR:HG22	1.90	0.53
7:J:27:DG:H2"	7:J:28:DA:C8	2.43	0.53
12:Y:315:ASP:OD2	12:Y:316:GLU:N	2.37	0.53
6:I:1:DT:H2"	6:I:2:DG:C8	2.44	0.53
9:R:148:ARG:HG3	9:R:389:GLU:HG3	1.91	0.53
9:R:27:ARG:HE	9:R:394:LEU:HD21	1.74	0.53
11:X:264:ASP:O	11:X:268:MET:N	2.37	0.53
3:C:71:THR:HG21	5:H:103:LEU:HB3	1.91	0.53
7:J:76:DC:H2'	7:J:77:DG:C8	2.44	0.53
10:S:6:GLU:O	11:V:180:ARG:N	2.39	0.53
12:U:50:ALA:HB1	12:U:84:LEU:HD11	1.90	0.53
7:J:41:DC:N3	7:J:42:DA:N6	2.56	0.52
8:M:1054:LEU:HD22	8:M:1055:THR:H	1.74	0.52
9:R:435:GLN:NE2	10:S:221:ASP:OD2	2.42	0.52
8:M:953:LEU:HD23	8:M:958:ARG:HD2	1.91	0.52
12:W:25:HIS:CD2	12:W:26:ILE:HG23	2.44	0.52
3:C:33:ALA:HA	3:C:36:ARG:HE	1.75	0.52
4:E:43:ARG:HB3	5:G:91:THR:HA	1.90	0.52
4:F:72:ARG:NH1	5:H:54:ASP:OD2	2.41	0.52
7:J:-23:DT:H2"	7:J:-22:DG:H5'	1.91	0.52
12:Y:332:THR:OG1	12:Y:335:THR:OG1	2.28	0.52
10:S:246:ILE:HG13	10:S:268:CYS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:1150:VAL:HG12	8:M:1152:TYR:H	1.75	0.52
11:T:252:LEU:O	11:T:256:ASN:HB2	2.09	0.52
6:I:72:DG:H1'	6:I:73:DT:H5'	1.92	0.52
5:H:101:VAL:HG13	5:H:105:LEU:HD12	1.92	0.52
11:V:463:LEU:HG	12:W:76:PRO:HD3	1.92	0.52
3:C:22:LEU:HG	3:C:23:ARG:HG2	1.92	0.52
6:I:19:DC:H2"	6:I:20:DG:H8	1.75	0.52
11:T:147:LEU:HB2	11:T:168:VAL:HG22	1.91	0.52
11:V:346:THR:HG22	11:V:354:ILE:HG12	1.92	0.52
12:W:29:LEU:H	12:W:91:SER:HB3	1.74	0.52
10:S:167:LEU:HD23	10:S:205:LYS:HG2	1.92	0.52
5:G:101:VAL:HG13	5:G:105:LEU:HD12	1.92	0.51
8:M:759:ASN:O	8:M:763:GLU:HB2	2.08	0.51
8:M:1357:ARG:NH1	13:M:1601:ADP:O5'	2.42	0.51
12:U:202:LEU:O	12:U:223:GLN:NE2	2.43	0.51
3:D:33:ALA:HA	3:D:36:ARG:HE	1.75	0.51
3:D:71:THR:HG21	5:G:103:LEU:HB3	1.91	0.51
5:H:102:ARG:HA	5:H:110:ALA:HB1	1.92	0.51
9:R:356:THR:HA	9:R:392:CYS:HB3	1.92	0.51
11:V:406:MET:CE	11:V:410:THR:OG1	2.58	0.51
6:I:6:DC:H2"	6:I:7:DC:C5	2.45	0.51
6:I:8:DC:H2"	6:I:9:DG:C8	2.45	0.51
12:U:23:HIS:HB3	12:U:86:MET:HG2	1.93	0.51
11:V:41:ALA:HB1	11:V:55:ARG:HH21	1.75	0.51
12:Y:38:ARG:O	12:Y:51:ARG:NH2	2.39	0.51
8:M:1382:LYS:NZ	8:M:1393:VAL:O	2.43	0.51
9:R:196:ASN:OD1	9:R:221:ARG:NH1	2.44	0.51
8:M:1233:ILE:HD12	11:V:210:LYS:HB2	1.92	0.51
12:W:243:GLU:HG3	12:W:257:LEU:HD21	1.92	0.51
7:J:-20:DC:N4	7:J:-19:DG:O6	2.43	0.51
8:M:1331:THR:HG22	8:M:1357:ARG:HB2	1.93	0.51
12:U:72:LEU:HD21	12:U:341:HIS:HE2	1.75	0.51
5:G:102:ARG:HA	5:G:110:ALA:HB1	1.91	0.51
9:R:414:VAL:HG22	9:R:431:ARG:HH11	1.76	0.51
13:R:501:ADP:O1B	14:R:502:BEF:F3	2.19	0.51
12:Y:80:GLY:HA2	13:Y:501:ADP:C8	2.46	0.51
12:Y:80:GLY:HA2	13:Y:501:ADP:H8	1.75	0.51
9:R:35:ASP:OD1	9:R:36:LYS:N	2.43	0.50
6:I:-65:DT:H1'	6:I:-64:DC:H5'	1.94	0.50
8:M:1048:THR:OG1	11:T:256:ASN:ND2	2.44	0.50
9:R:58:ARG:HD2	10:S:166:VAL:HG22	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:27:HIS:O	11:X:28:THR:OG1	2.24	0.50
12:Y:213:ASP:OD1	12:Y:214:ALA:N	2.44	0.50
4:F:113:HIS:NE2	4:F:115:ASN:OD1	2.44	0.50
5:G:36:ARG:HE	7:J:49:DC:H4'	1.77	0.50
7:J:-24:DT:H2"	7:J:-23:DT:H5'	1.94	0.50
8:M:759:ASN:OD1	8:M:1302:GLN:NE2	2.33	0.50
10:S:8:ILE:HD12	11:V:180:ARG:HB2	1.93	0.50
11:T:106:VAL:HB	11:T:109:GLU:HG3	1.93	0.50
12:U:139:GLU:HG2	12:U:189:VAL:HG22	1.93	0.50
12:Y:26:ILE:HG22	12:Y:44:MET:HG2	1.92	0.50
2:A:68:GLN:HE21	2:A:72:ARG:HE	1.58	0.50
7:J:7:DC:H2"	7:J:8:DG:C8	2.46	0.50
9:R:140:THR:HG22	9:R:399:VAL:HG21	1.93	0.50
7:J:-69:DG:H2"	7:J:-68:DA:C8	2.47	0.50
12:W:245:ASP:OD2	12:W:270:ARG:NH1	2.44	0.50
4:E:78:ARG:HH11	7:J:58:DC:H5'	1.77	0.50
12:Y:331:LYS:HA	12:Y:338:LYS:HA	1.93	0.50
1:Z:153:UNK:CB	12:W:146:ASP:HA	2.42	0.50
2:B:68:GLN:HE21	2:B:72:ARG:HE	1.58	0.50
8:M:990:ARG:NH1	8:M:1376:GLU:OE2	2.43	0.50
11:X:41:ALA:HB3	11:X:52:ILE:HG23	1.93	0.50
7:J:9:DT:H2"	7:J:10:DG:H8	1.77	0.50
7:J:14:DT:H5'	7:J:14:DT:C6	2.47	0.49
12:U:28:GLY:H	12:U:90:GLN:HB3	1.77	0.49
12:Y:171:LEU:HD23	12:Y:176:ILE:HD13	1.94	0.49
12:Y:202:LEU:O	12:Y:220:ARG:NE	2.33	0.49
2:B:79:LYS:HB3	2:B:82:LEU:HD11	1.94	0.49
6:I:-27:DC:H2"	6:I:-26:DT:H71	1.94	0.49
9:R:270:HIS:HA	9:R:291:ARG:HH12	1.77	0.49
12:U:300:MET:HE1	11:V:319:GLU:HA	1.94	0.49
12:Y:68:GLY:HA2	12:Y:318:ALA:HB3	1.93	0.49
6:I:-2:DC:H2"	6:I:-1:DG:C8	2.47	0.49
7:J:-29:DT:H2"	7:J:-28:DC:C5	2.47	0.49
12:Y:61:VAL:HG22	12:Y:320:ILE:HG21	1.95	0.49
7:J:-15:DA:OP2	8:M:780:PRO:HD3	2.12	0.49
9:R:197:CYS:SG	9:R:199:TRP:NE1	2.86	0.49
10:S:16:ASP:HA	12:U:147:ARG:HD3	1.93	0.49
11:T:119:GLU:O	11:T:123:GLU:HB2	2.13	0.49
6:I:-40:DG:H2'	6:I:-39:DT:H71	1.95	0.49
7:J:-14:DA:H2"	7:J:-13:DA:H8	1.78	0.49
8:M:1336:VAL:HB	8:M:1366:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:48:DG:H1'	6:I:49:DC:C2	2.47	0.49
9:R:63:LEU:HD13	9:R:64:GLY:H	1.78	0.49
11:X:216:ASP:HA	11:X:229:TYR:HB3	1.95	0.49
6:I:40:DG:N2	7:J:-39:DT:O2	2.45	0.49
11:X:123:GLU:OE2	11:X:250:HIS:NE2	2.45	0.49
3:C:77:LYS:HG2	5:H:95:ARG:HH12	1.77	0.49
4:E:113:HIS:NE2	4:E:115:ASN:OD1	2.43	0.49
6:I:-66:DA:H1'	6:I:-65:DT:H5'	1.94	0.49
9:R:148:ARG:CG	9:R:389:GLU:HG2	2.42	0.49
10:S:100:ARG:HD2	10:S:120:LEU:HD23	1.94	0.49
11:V:76:LEU:HB3	11:V:367:LEU:HD22	1.95	0.49
11:X:406:MET:CE	11:X:443:LYS:HD2	2.42	0.49
12:Y:28:GLY:HA2	12:Y:91:SER:HB3	1.94	0.49
1:Z:203:UNK:O	1:Z:207:UNK:N	2.45	0.49
2:A:79:LYS:HB3	2:A:82:LEU:HD11	1.93	0.49
4:E:42:GLN:OE1	4:F:39:ASN:ND2	2.46	0.49
11:T:23:ARG:HH12	12:U:290:PRO:HB3	1.77	0.49
12:U:29:LEU:HA	12:U:44:MET:HG3	1.94	0.49
2:B:61:LEU:HD12	3:C:37:LEU:HD23	1.95	0.49
6:I:49:DC:H2"	6:I:50:DA:N7	2.28	0.49
12:W:332:THR:OG1	12:W:335:THR:OG1	2.30	0.49
6:I:-68:DG:H2"	6:I:-67:DA:C8	2.48	0.48
8:M:727:LYS:NZ	14:M:1602:BEF:F1	2.35	0.48
11:T:375:TYR:OH	13:T:501:ADP:N7	2.37	0.48
11:V:27:HIS:O	11:V:28:THR:OG1	2.30	0.48
12:W:372:ALA:HB2	12:W:403:ILE:HD11	1.95	0.48
12:Y:25:HIS:HD2	12:Y:26:ILE:HG23	1.77	0.48
12:Y:406:ALA:HB1	12:Y:418:VAL:HG11	1.94	0.48
6:I:20:DG:H1'	6:I:21:DC:H5'	1.94	0.48
12:Y:413:ARG:NH2	12:Y:422:ASP:OD1	2.43	0.48
2:B:88:ALA:HB2	3:C:83:SER:HA	1.95	0.48
8:M:1038:VAL:HG23	11:T:245:GLN:HB3	1.95	0.48
12:U:325:THR:OG1	12:U:341:HIS:NE2	2.46	0.48
8:M:967:ARG:O	8:M:970:THR:OG1	2.23	0.48
9:R:63:LEU:O	9:R:196:ASN:ND2	2.41	0.48
9:R:83:PRO:HB3	9:R:90:ASP:HB3	1.95	0.48
9:R:121:GLU:HB2	10:S:198:LEU:HD21	1.95	0.48
11:T:134:LYS:HA	11:T:243:ILE:O	2.14	0.48
4:F:88:ILE:HG23	4:F:94:LEU:HB3	1.95	0.48
4:E:88:ILE:HG23	4:E:94:LEU:HB3	1.95	0.48
7:J:-74:DC:H2"	7:J:-73:DA:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-35:DG:H2"	7:J:-34:DA:C8	2.48	0.48
7:J:55:DC:H2"	7:J:56:DG:N7	2.28	0.48
8:M:773:VAL:HG13	8:M:798:VAL:HG13	1.95	0.48
8:M:875:VAL:HG22	8:M:876:ILE:H	1.78	0.48
9:R:15:ILE:HG22	9:R:30:ASN:HB2	1.96	0.48
10:S:218:ASN:OD1	10:S:219:LEU:N	2.47	0.48
12:W:72:LEU:N	12:W:352:ILE:O	2.40	0.48
2:A:65:LEU:HD23	7:J:17:DA:H3'	1.95	0.48
4:E:27:PRO:HD3	5:G:43:TYR:CE1	2.49	0.48
4:F:82:ARG:HH12	10:S:53:LEU:HB2	1.79	0.48
6:I:-52:DG:O6	7:J:52:DC:N4	2.47	0.48
11:T:138:GLU:HB3	11:T:238:HIS:HE2	1.77	0.48
6:I:-10:DC:H2"	6:I:-9:DA:C8	2.49	0.48
9:R:255:VAL:HG21	9:R:365:PHE:HB2	1.95	0.48
11:X:105:LEU:HD22	11:X:106:VAL:H	1.79	0.47
11:X:124:ASN:HD22	11:X:127:ARG:HD3	1.78	0.47
8:M:956:ARG:NH1	8:M:1001:VAL:O	2.47	0.47
9:R:406:THR:HG22	9:R:408:SER:H	1.79	0.47
11:V:123:GLU:O	11:V:127:ARG:HG3	2.14	0.47
7:J:11:DC:H2'	7:J:12:DG:C8	2.49	0.47
12:U:328:GLY:HA2	12:U:341:HIS:HA	1.95	0.47
11:X:143:GLU:HG2	11:X:144:VAL:H	1.78	0.47
12:Y:125:ILE:HG23	12:Y:241:LEU:HD13	1.95	0.47
7:J:35:DT:H2"	7:J:36:DA:N7	2.30	0.47
11:T:174:LYS:HG2	11:T:236:GLU:HG2	1.97	0.47
11:T:424:ILE:HG23	12:U:59:LYS:HD3	1.96	0.47
12:U:394:THR:OG1	12:U:395:SER:N	2.46	0.47
11:X:406:MET:SD	11:X:443:LYS:HE2	2.54	0.47
12:Y:57:ILE:HD13	12:Y:71:VAL:HG11	1.97	0.47
6:I:-68:DG:O6	7:J:68:DC:N4	2.46	0.47
6:I:40:DG:H2'	6:I:41:DT:H71	1.96	0.47
12:U:269:VAL:O	12:U:273:ILE:HG12	2.13	0.47
11:V:140:TYR:HB2	11:V:202:ILE:HG23	1.96	0.47
12:Y:45:VAL:H	13:Y:501:ADP:HN62	1.62	0.47
12:Y:128:LYS:HE3	12:Y:289:VAL:HG21	1.97	0.47
12:U:66:ILE:HG21	12:U:69:ARG:HH11	1.79	0.47
12:U:326:ASN:OD1	12:U:326:ASN:N	2.48	0.47
8:M:692:LEU:O	8:M:694:GLY:N	2.47	0.47
8:M:1269:THR:O	8:M:1321:SER:OG	2.33	0.47
12:W:379:LEU:HD11	12:W:403:ILE:HD11	1.95	0.47
11:X:85:LYS:HD2	11:X:339:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:376:ASP:O	11:X:380:ILE:HG12	2.14	0.47
7:J:-54:DC:H2"	7:J:-53:DA:H8	1.80	0.47
8:M:774:LEU:HG	8:M:796:PHE:HB3	1.96	0.47
8:M:1055:THR:HA	8:M:1141:ILE:HG22	1.97	0.47
11:T:313:VAL:HG21	11:T:338:LEU:HB3	1.97	0.47
12:U:254:PHE:HA	12:U:257:LEU:HD13	1.96	0.47
12:U:422:ASP:OD1	12:U:422:ASP:N	2.48	0.47
11:V:197:GLY:HA3	11:V:218:TYR:HE2	1.79	0.47
12:Y:310:ASN:HB3	12:Y:350:ARG:NH2	2.29	0.47
6:I:37:DC:H2"	6:I:38:DT:H72	1.97	0.47
9:R:62:GLU:HG3	9:R:63:LEU:H	1.80	0.47
7:J:46:DG:H2"	7:J:47:DA:N7	2.30	0.47
10:S:256:CYS:N	10:S:261:ASN:O	2.41	0.47
11:V:21:VAL:HG12	11:V:22:THR:HG23	1.97	0.47
2:A:61:LEU:HD12	3:D:37:LEU:HD23	1.97	0.46
2:A:65:LEU:HB2	7:J:17:DA:H5"	1.97	0.46
9:R:13:TYR:HB2	9:R:195:PHE:CG	2.50	0.46
11:T:283:LYS:O	11:T:287:GLU:HG2	2.15	0.46
12:W:187:GLY:O	12:W:205:SER:OG	2.20	0.46
12:Y:422:ASP:OD1	12:Y:422:ASP:N	2.46	0.46
6:I:-37:DG:H2'	6:I:-37:DG:OP2	2.14	0.46
7:J:34:DC:H2"	7:J:35:DT:C5	2.49	0.46
8:M:947:HIS:HB2	8:M:1367:TYR:HA	1.97	0.46
11:V:76:LEU:HD22	11:V:367:LEU:HB3	1.97	0.46
6:I:-13:DA:C8	6:I:-13:DA:H5'	2.50	0.46
6:I:23:DA:N6	7:J:-23:DT:O4	2.48	0.46
11:T:177:LYS:HB3	11:T:237:VAL:HG21	1.97	0.46
12:W:27:THR:O	12:W:42:GLU:HB3	2.15	0.46
12:Y:132:GLU:HA	12:Y:234:THR:HA	1.96	0.46
9:R:335:LEU:HD12	10:S:237:VAL:HG21	1.97	0.46
12:U:360:ASN:OD1	12:U:361:GLU:N	2.43	0.46
12:W:149:ILE:H	12:W:149:ILE:HG13	1.46	0.46
11:T:126:ARG:HD2	11:T:285:ARG:HH11	1.80	0.46
12:U:247:ILE:HA	12:U:253:GLY:HA3	1.98	0.46
12:Y:303:ILE:HA	12:Y:306:PHE:HD2	1.79	0.46
5:G:54:ASP:OD1	5:G:55:THR:N	2.44	0.46
8:M:1182:VAL:HG11	12:W:276:LYS:HE3	1.98	0.46
6:I:4:DC:H2"	6:I:5:DC:C5	2.51	0.46
8:M:787:ARG:HA	8:M:790:TRP:HB2	1.98	0.46
9:R:42:LEU:HB3	9:R:45:HIS:HD2	1.81	0.46
11:T:322:THR:OG1	12:Y:300:MET:SD	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:73:DG:H2"	7:J:74:DG:H5'	1.96	0.46
11:T:138:GLU:HB3	11:T:238:HIS:NE2	2.30	0.46
11:T:281:THR:HG23	11:T:284:LEU:H	1.79	0.46
12:W:364:ILE:HG23	12:W:396:LEU:HD13	1.98	0.46
2:B:118:THR:HG22	3:C:45:ARG:HD2	1.98	0.46
7:J:-76:DT:H2"	7:J:-75:DG:C8	2.51	0.46
11:T:51:GLN:NE2	11:T:83:THR:O	2.38	0.46
12:W:31:LEU:HD21	12:W:52:ARG:HA	1.98	0.46
12:W:117:LEU:HD23	12:W:308:PHE:HD2	1.80	0.46
11:X:136:THR:HG22	11:X:242:GLU:HB3	1.97	0.46
12:Y:28:GLY:H	12:Y:90:GLN:HB3	1.80	0.46
7:J:-20:DC:H2'	7:J:-19:DG:C8	2.51	0.46
8:M:1374:THR:N	8:M:1377:SER:OG	2.49	0.46
11:V:413:ARG:HD2	12:W:349:ASP:HB3	1.98	0.46
5:H:76:ILE:HG12	5:H:104:ILE:HD11	1.98	0.45
11:V:85:LYS:HE2	11:V:341:ASN:HB3	1.98	0.45
12:Y:27:THR:HA	12:Y:90:GLN:HG2	1.98	0.45
2:B:96:VAL:HG13	3:C:58:LEU:HD21	1.98	0.45
6:I:-50:DC:H2"	6:I:-49:DG:C8	2.51	0.45
7:J:45:DT:H2"	7:J:46:DG:C8	2.51	0.45
11:T:456:LEU:HA	11:T:463:LEU:HB2	1.97	0.45
6:I:-46:DC:N4	7:J:46:DG:O6	2.38	0.45
7:J:56:DG:H2"	7:J:57:DG:C8	2.51	0.45
9:R:148:ARG:CD	9:R:389:GLU:HG2	2.45	0.45
11:T:21:VAL:HG12	11:T:22:THR:HG23	1.98	0.45
11:T:450:LYS:NZ	12:Y:457:SER:OG	2.39	0.45
12:Y:31:LEU:HD12	12:Y:55:GLY:HA3	1.98	0.45
5:G:76:ILE:HG12	5:G:104:ILE:HD11	1.98	0.45
6:I:-36:DT:H2"	6:I:-35:DA:N7	2.31	0.45
6:I:-16:DT:H2"	6:I:-15:DA:C8	2.51	0.45
6:I:-57:DC:H2"	6:I:-56:DC:C5	2.52	0.45
6:I:-47:DT:H2"	6:I:-46:DC:C5	2.51	0.45
11:T:27:HIS:O	11:T:28:THR:OG1	2.28	0.45
11:X:25:ALA:HB1	12:Y:68:GLY:HA3	1.99	0.45
8:M:721:ASP:HB3	8:M:727:LYS:HG2	1.97	0.45
11:T:439:VAL:O	11:T:443:LYS:HG3	2.17	0.45
12:U:38:ARG:HD2	12:U:41:SER:HB3	1.98	0.45
12:U:115:GLU:HG3	12:U:264:GLU:HA	1.98	0.45
11:V:238:HIS:CE1	11:V:240:LYS:HE3	2.51	0.45
12:W:331:LYS:HA	12:W:338:LYS:HA	1.99	0.45
7:J:4:DG:H2"	7:J:5:DT:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:721:ASP:H	8:M:727:LYS:HD3	1.82	0.45
12:U:302:ASP:OD1	12:U:303:ILE:N	2.47	0.45
12:W:128:LYS:HE3	12:W:289:VAL:HG21	1.99	0.45
12:Y:54:ALA:HB2	12:Y:84:LEU:HD21	1.99	0.45
11:T:128:ALA:HB3	11:T:334:PRO:HG3	1.99	0.45
11:T:174:LYS:HB3	11:T:236:GLU:HA	1.99	0.45
12:W:61:VAL:HG22	12:W:320:ILE:HG21	1.99	0.45
11:X:76:LEU:HB3	11:X:367:LEU:HD13	1.98	0.45
11:X:152:ALA:HB3	11:X:164:SER:HB2	1.99	0.45
12:Y:25:HIS:CD2	12:Y:26:ILE:HG23	2.51	0.45
12:Y:97:PRO:HB2	12:Y:124:SER:O	2.17	0.45
6:I:3:DT:H2"	6:I:4:DC:C6	2.53	0.44
7:J:74:DG:H1'	7:J:75:DG:C8	2.52	0.44
12:W:23:HIS:HB3	12:W:86:MET:HG2	1.99	0.44
8:M:995:HIS:HD1	8:M:1245:CYS:HG	1.61	0.44
8:M:1283:ASN:ND2	8:M:1289:TYR:OH	2.50	0.44
11:T:105:LEU:HD22	11:T:106:VAL:H	1.82	0.44
12:U:294:PHE:HD1	12:U:322:MET:HG3	1.81	0.44
6:I:26:DG:H2"	6:I:27:DG:C8	2.51	0.44
7:J:58:DC:H2"	7:J:59:DA:C8	2.52	0.44
9:R:69:TRP:O	9:R:73:SER:HB2	2.17	0.44
11:T:279:GLU:O	12:Y:260:GLY:HA3	2.16	0.44
11:X:393:LEU:HD13	11:X:434:ILE:HD11	1.99	0.44
2:B:63:ARG:HH12	7:J:-14:DA:H4'	1.82	0.44
2:B:90:GLY:O	2:B:94:GLU:HB2	2.18	0.44
8:M:722:GLU:HB3	8:M:725:LEU:HD13	1.99	0.44
8:M:1328:ILE:O	8:M:1354:ARG:NE	2.47	0.44
12:U:117:LEU:HD23	12:U:308:PHE:HD2	1.82	0.44
12:U:332:THR:OG1	12:U:335:THR:OG1	2.34	0.44
12:W:57:ILE:HD13	12:W:71:VAL:HG11	1.98	0.44
11:X:274:LYS:HE3	12:Y:263:GLY:HA2	1.98	0.44
5:G:37:LYS:O	7:J:49:DC:H5"	2.18	0.44
11:T:170:LEU:HD13	11:T:179:LEU:HD13	2.00	0.44
12:U:157:LYS:HE2	12:U:157:LYS:HB3	1.81	0.44
11:X:47:GLY:HA2	11:X:386:ARG:HE	1.83	0.44
12:Y:432:ASP:H	12:Y:435:ARG:HD3	1.82	0.44
2:A:96:VAL:HG13	3:D:58:LEU:HD21	1.99	0.44
11:T:127:ARG:HH21	12:U:268:GLU:HB2	1.82	0.44
2:A:61:LEU:O	3:D:36:ARG:NH1	2.49	0.44
6:I:58:DG:H2"	6:I:59:DA:C8	2.52	0.44
12:U:379:LEU:HD11	12:U:403:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:299:HIS:HB3	12:W:325:THR:HG23	2.00	0.44
11:X:314:ASN:HD22	11:X:342:ARG:HG3	1.81	0.44
6:I:-5:DA:H2"	6:I:-4:DC:C5	2.53	0.44
8:M:819:GLN:HG3	8:M:846:GLN:NE2	2.33	0.44
10:S:54:ALA:O	10:S:58:ALA:HB2	2.18	0.44
12:U:117:LEU:HD22	12:U:305:CYS:HB3	2.00	0.44
7:J:36:DA:H1'	7:J:37:DC:H5'	2.00	0.44
7:J:39:DA:C4	7:J:40:DC:C5	3.06	0.44
8:M:1018:TYR:OH	12:U:243:GLU:OE1	2.32	0.44
8:M:1386:LYS:NZ	8:M:1390:ASP:H	2.16	0.44
9:R:69:TRP:O	9:R:73:SER:CB	2.66	0.44
9:R:308:ASP:O	9:R:312:THR:OG1	2.26	0.44
11:T:131:LEU:O	11:T:247:VAL:N	2.42	0.44
11:T:139:VAL:HG11	11:T:201:TYR:CZ	2.53	0.44
12:U:38:ARG:HB2	12:U:41:SER:HB3	1.99	0.44
12:U:345:LEU:HD12	12:Y:454:VAL:HG12	1.99	0.44
8:M:957:GLN:HE21	8:M:996:PRO:HD3	1.82	0.43
11:X:147:LEU:HD22	11:X:168:VAL:HG22	1.99	0.43
2:A:88:ALA:HB2	3:D:83:SER:HA	2.00	0.43
6:I:-10:DC:H2"	6:I:-9:DA:H8	1.81	0.43
6:I:5:DC:H2"	6:I:6:DC:C5	2.53	0.43
6:I:10:DC:H2"	6:I:11:DG:C8	2.53	0.43
8:M:1006:THR:HG22	11:V:137:LYS:NZ	2.34	0.43
8:M:1276:ASP:OD1	8:M:1276:ASP:N	2.44	0.43
11:V:264:ASP:OD1	11:V:265:VAL:N	2.51	0.43
11:X:70:MET:HB3	11:X:73:ARG:HG3	2.00	0.43
11:X:413:ARG:NH2	12:Y:349:ASP:OD2	2.50	0.43
12:Y:386:LEU:HD23	12:Y:386:LEU:HA	1.85	0.43
6:I:-23:DC:H2"	6:I:-22:DA:C8	2.53	0.43
7:J:15:DT:H5'	7:J:15:DT:C6	2.54	0.43
8:M:1138:LYS:HG3	12:Y:258:PHE:CZ	2.53	0.43
4:F:18:ARG:H	4:F:18:ARG:HD3	1.84	0.43
8:M:1249:GLN:NE2	12:W:283:GLU:O	2.50	0.43
11:X:70:MET:SD	11:X:70:MET:N	2.91	0.43
6:I:62:DT:H2"	6:I:63:DA:N7	2.33	0.43
8:M:987:MET:O	8:M:991:LYS:HB2	2.18	0.43
9:R:141:LYS:HG3	9:R:185:HIS:CE1	2.53	0.43
11:T:154:ASN:OD1	11:T:154:ASN:N	2.51	0.43
11:T:211:ARG:HE	11:T:213:GLY:HA2	1.83	0.43
11:V:268:MET:HE1	12:W:252:GLN:HB3	2.01	0.43
2:A:118:THR:HG22	3:D:45:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:LYS:HZ3	5:G:95:ARG:HH22	1.66	0.43
6:I:-34:DG:H2"	6:I:-33:DA:C8	2.54	0.43
7:J:33:DT:H6	7:J:33:DT:H2'	1.69	0.43
12:W:144:GLN:O	12:W:157:LYS:N	2.44	0.43
12:W:345:LEU:HD23	12:W:348:LEU:HD12	2.00	0.43
12:W:405:VAL:HG11	12:W:430:PHE:HE2	1.84	0.43
4:E:16:GLN:HE21	4:E:20:ALA:HB3	1.83	0.43
6:I:45:DC:H2"	6:I:46:DA:H8	1.83	0.43
7:J:62:DG:H2"	7:J:63:DG:C8	2.54	0.43
11:T:188:SER:O	11:T:192:GLU:HG2	2.19	0.43
11:T:219:ALA:HA	11:T:229:TYR:CZ	2.53	0.43
11:V:241:LYS:HB2	11:V:241:LYS:HE2	1.71	0.43
12:Y:294:PHE:HD1	12:Y:322:MET:HG3	1.83	0.43
2:A:90:GLY:O	2:A:94:GLU:HB2	2.18	0.43
4:E:18:ARG:H	4:E:18:ARG:HD3	1.84	0.43
5:H:54:ASP:OD1	5:H:55:THR:N	2.44	0.43
11:X:75:ILE:HG22	11:X:368:LEU:HB2	2.01	0.43
11:V:128:ALA:HB3	11:V:334:PRO:HG3	2.00	0.43
11:V:243:ILE:HG22	11:V:245:GLN:H	1.82	0.43
12:W:145:ILE:HA	12:W:156:GLY:HA2	2.00	0.43
7:J:-32:DT:H2"	7:J:-31:DA:C8	2.54	0.42
7:J:42:DA:H2"	7:J:43:DA:C8	2.54	0.42
8:M:708:ALA:O	8:M:712:ASN:ND2	2.52	0.42
12:U:148:SER:HA	12:U:153:HIS:O	2.19	0.42
11:V:129:ILE:HG22	11:V:305:PRO:HA	2.02	0.42
11:V:316:LEU:HB2	11:V:321:PHE:CZ	2.54	0.42
11:V:381:ARG:NH1	11:V:385:GLU:OE2	2.52	0.42
7:J:55:DC:H2"	7:J:56:DG:C8	2.53	0.42
8:M:819:GLN:HG3	8:M:846:GLN:HE22	1.84	0.42
12:U:362:GLN:HA	12:U:365:LYS:HE2	2.01	0.42
2:A:61:LEU:HD13	3:D:36:ARG:HB3	2.00	0.42
8:M:722:GLU:HG2	8:M:934:LYS:HE3	1.99	0.42
11:T:23:ARG:HH22	12:U:290:PRO:HB3	1.84	0.42
11:V:182:ASP:HB3	11:V:185:ILE:HG22	2.00	0.42
12:W:36:GLN:HA	12:W:37:PRO:HD3	1.91	0.42
11:X:376:ASP:N	11:X:376:ASP:OD1	2.52	0.42
4:E:31:VAL:HG13	5:G:73:PHE:HE1	1.83	0.42
8:M:722:GLU:HB2	8:M:933:LEU:HA	2.01	0.42
8:M:750:ILE:HG13	8:M:800:ILE:HA	2.02	0.42
8:M:1086:GLN:O	8:M:1090:GLY:HA3	2.19	0.42
11:T:129:ILE:HG23	11:T:334:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:375:TYR:HB2	11:V:380:ILE:HD12	2.01	0.42
4:E:78:ARG:NH1	7:J:58:DC:H5'	2.35	0.42
7:J:-70:DG:H2"	7:J:-69:DG:C8	2.53	0.42
9:R:320:PRO:HB3	9:R:325:ILE:HG13	2.02	0.42
11:V:406:MET:HE2	11:V:410:THR:OG1	2.19	0.42
11:X:198:ASP:CG	11:X:211:ARG:HE	2.23	0.42
11:X:201:TYR:N	11:X:210:LYS:O	2.52	0.42
6:I:64:DT:H2"	6:I:65:DA:N7	2.34	0.42
8:M:837:TRP:CZ3	8:M:869:PHE:HB2	2.54	0.42
8:M:1202:ASP:N	8:M:1202:ASP:OD1	2.52	0.42
11:V:143:GLU:O	11:V:171:LYS:N	2.46	0.42
7:J:9:DT:H2"	7:J:10:DG:C8	2.54	0.42
8:M:692:LEU:HD21	8:M:696:LEU:HD21	2.01	0.42
8:M:1266:LEU:HD22	8:M:1319:LEU:HD11	2.00	0.42
9:R:13:TYR:HA	9:R:59:ARG:HH22	1.84	0.42
9:R:135:VAL:O	9:R:138:PRO:HD2	2.20	0.42
10:S:1:MET:HG2	10:S:2:LYS:H	1.83	0.42
11:V:105:LEU:HD22	11:V:106:VAL:H	1.84	0.42
11:V:115:VAL:HG21	11:V:277:LYS:HE2	2.02	0.42
12:Y:23:HIS:CD2	13:Y:501:ADP:H3'	2.55	0.42
9:R:98:HIS:CD2	9:R:127:SER:HB2	2.52	0.42
11:T:202:ILE:HG12	11:T:209:VAL:HG22	2.02	0.42
11:T:418:LEU:HD23	11:T:418:LEU:HA	1.92	0.42
12:W:301:LEU:HB3	12:W:306:PHE:CZ	2.55	0.42
6:I:38:DT:H6	6:I:38:DT:H2'	1.69	0.42
7:J:-45:DG:H2"	7:J:-44:DG:C8	2.55	0.42
8:M:836:ARG:HA	8:M:839:ALA:HB3	2.01	0.42
8:M:986:LEU:HD22	8:M:1375:ILE:HD13	2.01	0.42
8:M:1142:ASP:O	8:M:1146:LYS:HB2	2.20	0.42
9:R:332:GLU:HG3	10:S:237:VAL:HG23	2.02	0.42
10:S:253:ILE:HG23	10:S:262:LYS:HD3	2.01	0.42
6:I:-29:DC:H2"	6:I:-28:DT:OP2	2.20	0.42
6:I:18:DC:H2'	6:I:19:DC:C6	2.55	0.42
7:J:-8:DG:C8	7:J:-8:DG:H5'	2.54	0.42
7:J:66:DT:H2"	7:J:67:DT:C6	2.54	0.42
9:R:425:ASP:N	9:R:425:ASP:OD1	2.52	0.42
11:X:193:LYS:O	11:X:211:ARG:NH1	2.53	0.42
12:Y:76:PRO:O	12:Y:79:THR:OG1	2.27	0.42
7:J:-44:DG:C8	7:J:-44:DG:H5'	2.55	0.41
8:M:1159:ASP:O	8:M:1163:ILE:HG12	2.20	0.41
9:R:186:ASP:N	9:R:186:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:258:PHE:HD1	11:V:284:LEU:HB2	1.85	0.41
11:V:117:LYS:HE3	11:V:117:LYS:HB2	1.91	0.41
11:V:269:MET:HE3	11:V:269:MET:HB2	1.61	0.41
12:W:20:ILE:HG21	12:W:375:GLU:HG2	2.02	0.41
12:W:179:LEU:HD12	12:W:199:ILE:HD11	2.02	0.41
8:M:1010:LEU:HD23	11:V:256:ASN:HD21	1.85	0.41
8:M:1200:ASN:OD1	8:M:1200:ASN:N	2.53	0.41
9:R:109:PRO:O	9:R:113:LYS:HG3	2.20	0.41
11:T:70:MET:HB3	11:T:73:ARG:HG3	2.01	0.41
11:X:437:ASN:N	11:X:437:ASN:OD1	2.53	0.41
3:C:102:GLY:HA3	5:G:67:SER:OG	2.20	0.41
8:M:1143:LEU:HD21	12:Y:237:HIS:CG	2.55	0.41
8:M:1199:LEU:H	8:M:1199:LEU:HG	1.75	0.41
9:R:25:PRO:HB3	9:R:397:TRP:CE2	2.55	0.41
12:U:331:LYS:HB2	12:U:338:LYS:HG2	2.02	0.41
12:W:294:PHE:HD1	12:W:322:MET:HG3	1.85	0.41
12:Y:215:MET:HE1	12:Y:221:PHE:HZ	1.85	0.41
12:Y:386:LEU:HD12	12:Y:420:VAL:HG13	2.03	0.41
8:M:1187:ALA:HB2	11:V:247:VAL:HG21	2.01	0.41
10:S:18:TYR:OH	12:U:184:VAL:O	2.38	0.41
11:T:72:GLY:N	11:T:333:ALA:O	2.53	0.41
4:F:18:ARG:HB2	5:H:124:TYR:HE1	1.85	0.41
6:I:-59:DT:H1'	8:M:815:ARG:NH2	2.34	0.41
6:I:19:DC:H2"	6:I:20:DG:C8	2.55	0.41
11:T:29:HIS:HB3	11:T:390:VAL:HG21	2.03	0.41
11:V:402:LEU:HD23	11:V:402:LEU:HA	1.89	0.41
11:X:218:TYR:O	11:X:221:GLU:HG2	2.20	0.41
6:I:-37:DG:C8	6:I:-36:DT:H72	2.56	0.41
7:J:49:DC:H2"	7:J:50:DG:C8	2.56	0.41
8:M:1350:GLN:HE21	8:M:1354:ARG:NH1	2.19	0.41
12:U:127:ILE:N	12:U:239:VAL:O	2.53	0.41
12:U:158:LEU:HB3	12:U:171:LEU:HD11	2.03	0.41
12:Y:57:ILE:HD11	12:Y:71:VAL:HG21	2.03	0.41
8:M:994:ASN:OD1	8:M:995:HIS:N	2.48	0.41
8:M:1355:CYS:O	8:M:1360:GLN:NE2	2.53	0.41
12:U:310:ASN:HB3	12:U:350:ARG:NH2	2.36	0.41
2:B:112:ILE:HD13	4:E:113:HIS:CE1	2.55	0.41
9:R:8:ILE:HG12	9:R:17:PHE:HB2	2.03	0.41
12:U:21:ALA:HB3	12:U:24:SER:HB2	2.02	0.41
12:U:45:VAL:HG12	12:U:46:GLY:H	1.86	0.41
12:U:364:ILE:HG23	12:U:396:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:447:LEU:HD22	11:V:451:ARG:HD2	2.02	0.41
12:W:158:LEU:HD12	12:W:159:THR:N	2.36	0.41
12:Y:136:ILE:HG23	12:Y:229:LEU:HG	2.02	0.41
3:C:62:LEU:O	3:C:66:ILE:HB	2.21	0.41
6:I:-73:DC:O2	7:J:74:DG:N2	2.54	0.41
6:I:-26:DT:H2"	6:I:-25:DA:N7	2.36	0.41
6:I:11:DG:C8	6:I:12:DT:H72	2.55	0.41
8:M:1259:LYS:HE2	8:M:1315:THR:HG21	2.02	0.41
10:S:112:ASP:O	10:S:116:VAL:HG23	2.21	0.41
10:S:126:VAL:HG23	10:S:131:ILE:HD13	2.03	0.41
10:S:264:CYS:SG	10:S:265:SER:N	2.94	0.41
11:T:48:PHE:HB3	11:T:55:ARG:NH1	2.36	0.41
12:U:20:ILE:O	11:V:71:SER:HB3	2.21	0.41
12:U:72:LEU:O	12:U:354:ILE:N	2.49	0.41
12:U:242:HIS:O	12:U:246:VAL:HG23	2.21	0.41
8:M:685:ASP:HB2	8:M:705:ASN:OD1	2.20	0.41
11:T:315:MET:HA	11:T:348:ARG:HD3	2.03	0.41
11:V:272:LEU:HD23	11:X:269:MET:HG3	2.02	0.41
6:I:58:DG:H2"	6:I:59:DA:H8	1.86	0.40
9:R:132:PRO:HG2	9:R:135:VAL:HG23	2.02	0.40
12:U:147:ARG:HD2	12:U:148:SER:H	1.86	0.40
11:V:293:ALA:O	11:V:296:ILE:HG22	2.21	0.40
3:D:30:THR:HB	3:D:32:PRO:HD2	2.03	0.40
8:M:1036:ASN:O	11:T:245:GLN:HB2	2.21	0.40
8:M:1062:ILE:HG13	12:Y:202:LEU:HD22	2.03	0.40
1:Z:159:UNK:O	1:Z:160:UNK:C	2.69	0.40
8:M:1054:LEU:HD13	8:M:1055:THR:O	2.21	0.40
8:M:1158:ILE:H	8:M:1158:ILE:HG13	1.70	0.40
12:W:303:ILE:HD13	12:W:335:THR:HG23	2.02	0.40
11:X:182:ASP:OD2	11:X:184:THR:OG1	2.39	0.40
12:Y:136:ILE:HG12	12:Y:230:GLN:HB3	2.03	0.40
3:D:62:LEU:O	3:D:66:ILE:HB	2.21	0.40
4:E:27:PRO:HD3	5:G:43:TYR:CZ	2.57	0.40
8:M:1271:MET:HG3	8:M:1274:VAL:HG23	2.02	0.40
9:R:70:GLU:H	9:R:70:GLU:HG2	1.53	0.40
12:W:32:ASP:OD1	12:W:38:ARG:HG3	2.22	0.40
11:X:183:PRO:O	11:X:186:TYR:HD2	2.05	0.40
12:Y:171:LEU:HD12	12:Y:171:LEU:HA	1.92	0.40
6:I:-71:DG:H2"	6:I:-70:DG:C8	2.55	0.40
7:J:-70:DG:H2"	7:J:-69:DG:H8	1.86	0.40
7:J:40:DC:C2	7:J:41:DC:C5	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:846:GLN:OE1	8:M:846:GLN:N	2.54	0.40
9:R:120:PHE:CD2	9:R:128:LEU:HD21	2.57	0.40
10:S:9:ASP:O	10:S:13:TYR:HB3	2.20	0.40
10:S:118:THR:HG22	10:S:128:ARG:HD3	2.02	0.40
12:U:226:GLU:H	12:U:226:GLU:CD	2.24	0.40
12:U:439:TYR:CE2	11:V:371:ARG:HD2	2.57	0.40
12:W:44:MET:HB2	12:W:51:ARG:HH11	1.87	0.40
11:X:117:LYS:HE3	11:X:117:LYS:HB2	1.94	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	
2	A	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
2	B	95/136 (70%)	90 (95%)	5 (5%)	0	100	100
3	C	80/103 (78%)	75 (94%)	5 (6%)	0	100	100
3	D	78/103 (76%)	73 (94%)	5 (6%)	0	100	100
4	E	101/132 (76%)	99 (98%)	2 (2%)	0	100	100
4	F	99/132 (75%)	97 (98%)	2 (2%)	0	100	100
5	G	94/131 (72%)	87 (93%)	7 (7%)	0	100	100
5	H	89/131 (68%)	84 (94%)	5 (6%)	0	100	100
8	M	684/1514 (45%)	621 (91%)	62 (9%)	1 (0%)	51	83
9	R	407/438 (93%)	396 (97%)	11 (3%)	0	100	100
10	S	200/280 (71%)	195 (98%)	5 (2%)	0	100	100
11	T	441/463 (95%)	423 (96%)	17 (4%)	1 (0%)	47	79
11	V	430/463 (93%)	414 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	440/463 (95%)	422 (96%)	18 (4%)	0	100	100
12	U	426/471 (90%)	405 (95%)	21 (5%)	0	100	100
12	W	429/471 (91%)	420 (98%)	9 (2%)	0	100	100
12	Y	445/471 (94%)	427 (96%)	18 (4%)	0	100	100
All	All	4633/6038 (77%)	4418 (95%)	213 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	999	PHE
11	T	236	GLU

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	
2	A	84/113 (74%)	84 (100%)	0	100	100
2	B	84/113 (74%)	84 (100%)	0	100	100
3	C	68/81 (84%)	65 (96%)	3 (4%)	28	63
3	D	67/81 (83%)	65 (97%)	2 (3%)	41	71
4	E	82/99 (83%)	80 (98%)	2 (2%)	49	75
4	F	80/99 (81%)	78 (98%)	2 (2%)	47	75
5	G	83/109 (76%)	83 (100%)	0	100	100
5	H	78/109 (72%)	78 (100%)	0	100	100
8	M	574/1376 (42%)	541 (94%)	33 (6%)	20	55
9	R	372/396 (94%)	361 (97%)	11 (3%)	41	71
10	S	199/261 (76%)	197 (99%)	2 (1%)	76	88
11	T	371/391 (95%)	360 (97%)	11 (3%)	41	71
11	V	368/391 (94%)	353 (96%)	15 (4%)	30	64
11	X	374/391 (96%)	348 (93%)	26 (7%)	15	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	U	367/403 (91%)	357 (97%)	10 (3%)	44	73
12	W	369/403 (92%)	356 (96%)	13 (4%)	36	68
12	Y	372/403 (92%)	360 (97%)	12 (3%)	39	70
All	All	3992/5219 (76%)	3850 (96%)	142 (4%)	38	67

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	22	LEU
3	C	58	LEU
3	C	92	ARG
3	D	58	LEU
3	D	92	ARG
4	E	18	ARG
4	E	34	LEU
4	F	18	ARG
4	F	34	LEU
8	M	693	ARG
8	M	750	ILE
8	M	836	ARG
8	M	844	ASN
8	M	860	LEU
8	M	867	LEU
8	M	871	MET
8	M	934	LYS
8	M	999	PHE
8	M	1006	THR
8	M	1040	LEU
8	M	1052	LYS
8	M	1054	LEU
8	M	1055	THR
8	M	1062	ILE
8	M	1067	CYS
8	M	1082	ASN
8	M	1085	LEU
8	M	1138	LYS
8	M	1188	VAL
8	M	1195	LEU
8	M	1199	LEU
8	M	1233	ILE
8	M	1240	LEU

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Mol	Chain	Res	Type
8	M	1278	LEU
8	M	1280	GLN
8	M	1313	ARG
8	M	1322	ARG
8	M	1328	ILE
8	M	1339	TYR
8	M	1358	ILE
8	M	1384	ASN
8	M	1392	VAL
9	R	3	THR
9	R	15	ILE
9	R	63	LEU
9	R	66	LEU
9	R	70	GLU
9	R	87	ASP
9	R	120	PHE
9	R	186	ASP
9	R	204	LEU
9	R	266	THR
9	R	425	ASP
10	S	126	VAL
10	S	179	TYR
11	T	48	PHE
11	T	70	MET
11	T	77	LEU
11	T	125	PHE
11	T	154	ASN
11	T	211	ARG
11	T	256	ASN
11	T	268	MET
11	T	312	GLU
11	T	326	LYS
11	T	462	TYR
12	U	17	LEU
12	U	26	ILE
12	U	81	LYS
12	U	140	VAL
12	U	141	VAL
12	U	157	LYS
12	U	158	LEU
12	U	226	GLU
12	U	326	ASN

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Mol	Chain	Res	Type
12	U	400	SER
11	V	70	MET
11	V	77	LEU
11	V	133	ILE
11	V	194	VAL
11	V	202	ILE
11	V	237	VAL
11	V	241	LYS
11	V	268	MET
11	V	342	ARG
11	V	364	ILE
11	V	365	ASP
11	V	366	ARG
11	V	380	ILE
11	V	406	MET
11	V	461	ASN
12	W	29	LEU
12	W	79	THR
12	W	135	LEU
12	W	149	ILE
12	W	154	LYS
12	W	183	LYS
12	W	188	ASP
12	W	250	ARG
12	W	252	GLN
12	W	349	ASP
12	W	416	ASN
12	W	417	THR
12	W	455	GLN
11	X	64	LEU
11	X	70	MET
11	X	77	LEU
11	X	85	LYS
11	X	86	THR
11	X	115	VAL
11	X	125	PHE
11	X	150	GLU
11	X	190	GLN
11	X	194	VAL
11	X	195	SER
11	X	264	ASP
11	X	272	LEU

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Mol	Chain	Res	Type
11	X	276	LYS
11	X	278	THR
11	X	311	ASP
11	X	312	GLU
11	X	326	LYS
11	X	336	VAL
11	X	376	ASP
11	X	377	LYS
11	X	378	ASP
11	X	393	LEU
11	X	417	GLN
11	X	430	ASN
11	X	437	ASN
12	Y	23	HIS
12	Y	79	THR
12	Y	132	GLU
12	Y	220	ARG
12	Y	257	LEU
12	Y	326	ASN
12	Y	341	HIS
12	Y	352	ILE
12	Y	365	LYS
12	Y	371	ARG
12	Y	422	ASP
12	Y	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	16	GLN
4	E	39	ASN
4	E	42	GLN
4	F	39	ASN
4	F	42	GLN
5	G	52	HIS
5	H	52	HIS
8	M	782	GLN
8	M	844	ASN
8	M	857	GLN
8	M	1058	HIS
8	M	1173	ASN
8	M	1226	GLN

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Mol	Chain	Res	Type
8	M	1283	ASN
8	M	1350	GLN
8	M	1384	ASN
9	R	45	HIS
9	R	98	HIS
9	R	251	GLN
9	R	374	GLN
11	T	27	HIS
11	T	256	ASN
11	T	271	GLN
12	U	119	GLN
12	U	252	GLN
12	U	401	ASN
12	U	443	ASN
12	U	451	GLN
11	V	124	ASN
11	V	205	ASN
11	V	238	HIS
11	V	256	ASN
11	V	357	HIS
12	W	63	ASN
12	W	153	HIS
12	W	252	GLN
12	W	407	GLN
12	W	416	ASN
12	W	455	GLN
11	X	124	ASN
11	X	256	ASN
11	X	271	GLN
12	Y	25	HIS
12	Y	36	GLN
12	Y	63	ASN
12	Y	144	GLN
12	Y	299	HIS
12	Y	451	GLN
12	Y	455	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
14	BEF	M	1602	13	0,3,3	-	-	-		
13	ADP	T	501	15	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	W	501	15	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	X	501	15	24,29,29	0.98	1 (4%)	29,45,45	1.52	4 (13%)
13	ADP	Y	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
14	BEF	R	502	13	0,3,3	-	-	-		
13	ADP	V	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
13	ADP	U	502	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	4 (13%)
13	ADP	M	1601	14	24,29,29	0.95	1 (4%)	29,45,45	1.38	4 (13%)
13	ADP	R	501	14,15	24,29,29	0.96	1 (4%)	29,45,45	1.36	3 (10%)

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
13	ADP	T	501	15	-	4/12/32/32	0/3/3/3
13	ADP	W	501	15	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	X	501	15	-	2/12/32/32	0/3/3/3
13	ADP	Y	501	-	-	2/12/32/32	0/3/3/3
13	ADP	V	501	15	-	3/12/32/32	0/3/3/3
13	ADP	U	502	-	-	4/12/32/32	0/3/3/3
13	ADP	M	1601	14	-	6/12/32/32	0/3/3/3
13	ADP	R	501	14,15	-	6/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	501	ADP	C5-C4	2.54	1.47	1.40
13	Y	501	ADP	C5-C4	2.54	1.47	1.40
13	W	501	ADP	C5-C4	2.50	1.47	1.40
13	R	501	ADP	C5-C4	2.49	1.47	1.40
13	M	1601	ADP	C5-C4	2.46	1.47	1.40
13	U	502	ADP	C5-C4	2.45	1.47	1.40
13	V	501	ADP	C5-C4	2.44	1.47	1.40
13	T	501	ADP	C5-C4	2.43	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	501	ADP	PA-O3A-PB	-4.05	118.94	132.83
13	U	502	ADP	PA-O3A-PB	-3.91	119.40	132.83
13	Y	501	ADP	PA-O3A-PB	-3.86	119.59	132.83
13	W	501	ADP	PA-O3A-PB	-3.78	119.84	132.83
13	V	501	ADP	PA-O3A-PB	-3.57	120.57	132.83
13	X	501	ADP	C3'-C2'-C1'	3.47	106.21	100.98
13	T	501	ADP	PA-O3A-PB	-3.44	121.01	132.83
13	M	1601	ADP	C3'-C2'-C1'	3.37	106.06	100.98
13	V	501	ADP	N3-C2-N1	-3.24	123.61	128.68
13	R	501	ADP	C3'-C2'-C1'	3.24	105.86	100.98
13	U	502	ADP	C3'-C2'-C1'	3.21	105.81	100.98
13	Y	501	ADP	C3'-C2'-C1'	3.20	105.79	100.98
13	R	501	ADP	N3-C2-N1	-3.19	123.69	128.68
13	W	501	ADP	N3-C2-N1	-3.17	123.72	128.68
13	M	1601	ADP	N3-C2-N1	-3.16	123.74	128.68
13	U	502	ADP	N3-C2-N1	-3.16	123.74	128.68
13	T	501	ADP	N3-C2-N1	-3.14	123.76	128.68
13	V	501	ADP	C3'-C2'-C1'	3.11	105.66	100.98
13	Y	501	ADP	N3-C2-N1	-3.09	123.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	501	ADP	N3-C2-N1	-3.09	123.85	128.68
13	W	501	ADP	C3'-C2'-C1'	3.06	105.58	100.98
13	T	501	ADP	C3'-C2'-C1'	3.05	105.57	100.98
13	T	501	ADP	C4-C5-N7	-2.85	106.43	109.40
13	V	501	ADP	C4-C5-N7	-2.77	106.52	109.40
13	W	501	ADP	C4-C5-N7	-2.74	106.54	109.40
13	Y	501	ADP	C4-C5-N7	-2.64	106.65	109.40
13	R	501	ADP	C4-C5-N7	-2.63	106.66	109.40
13	X	501	ADP	C4-C5-N7	-2.61	106.68	109.40
13	M	1601	ADP	C4-C5-N7	-2.60	106.69	109.40
13	U	502	ADP	C4-C5-N7	-2.56	106.73	109.40
13	M	1601	ADP	PA-O3A-PB	-2.52	124.19	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PA-O3A-PB-O2B
13	M	1601	ADP	C5'-O5'-PA-O1A
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	PA-O3A-PB-O2B
13	R	501	ADP	PA-O3A-PB-O3B
13	R	501	ADP	C5'-O5'-PA-O3A
13	T	501	ADP	C5'-O5'-PA-O1A
13	T	501	ADP	C5'-O5'-PA-O2A
13	U	502	ADP	C5'-O5'-PA-O3A
13	U	502	ADP	O4'-C4'-C5'-O5'
13	U	502	ADP	C3'-C4'-C5'-O5'
13	V	501	ADP	C5'-O5'-PA-O1A
13	W	501	ADP	C5'-O5'-PA-O1A
13	W	501	ADP	C5'-O5'-PA-O2A
13	W	501	ADP	O4'-C4'-C5'-O5'
13	W	501	ADP	C3'-C4'-C5'-O5'
13	X	501	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C5'-O5'-PA-O1A
13	U	502	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	M	1601	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	PA-O3A-PB-O1B

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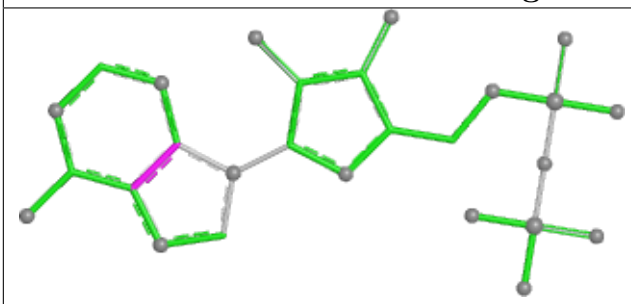
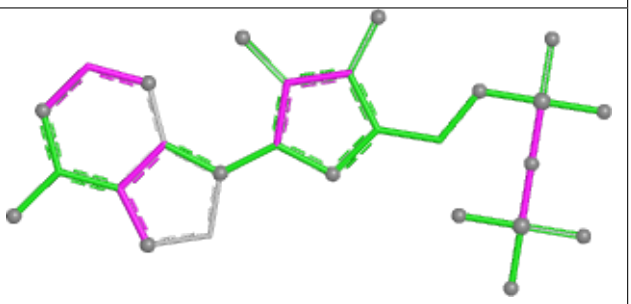
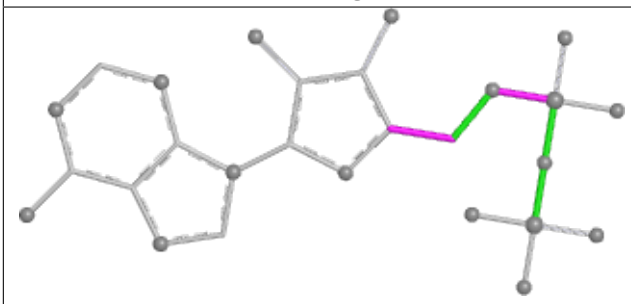
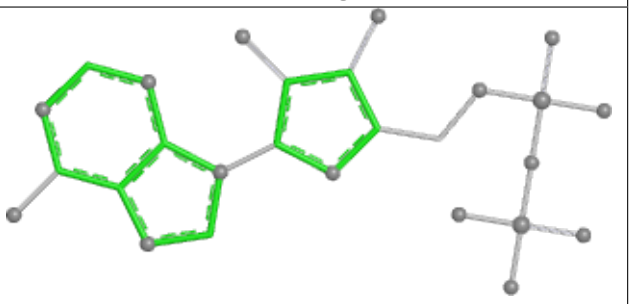
Mol	Chain	Res	Type	Atoms
13	R	501	ADP	PB-O3A-PA-O2A
13	T	501	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O3A
13	T	501	ADP	C5'-O5'-PA-O3A
13	V	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O3A
13	X	501	ADP	C5'-O5'-PA-O3A

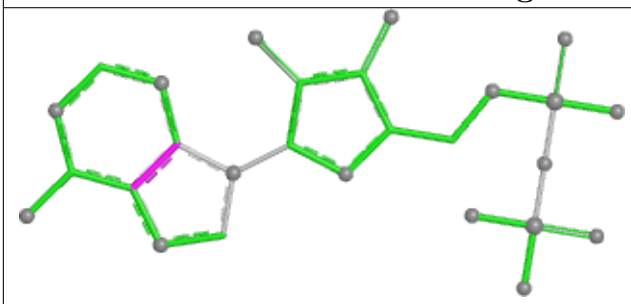
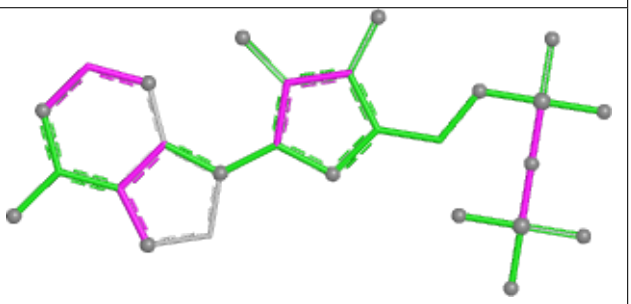
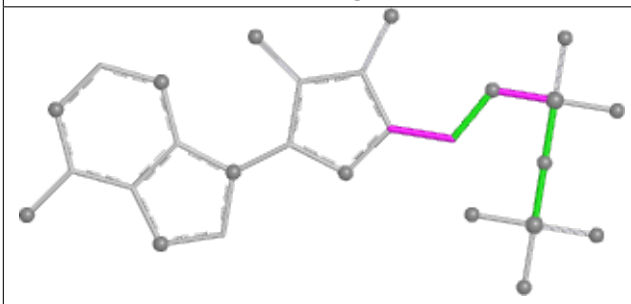
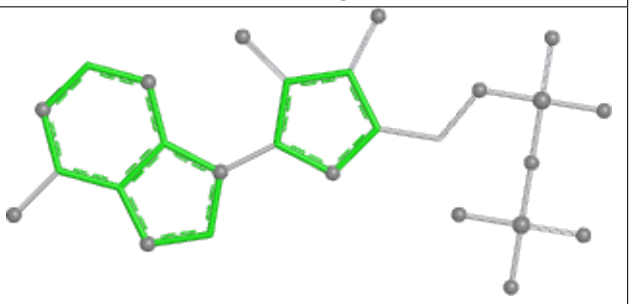
There are no ring outliers.

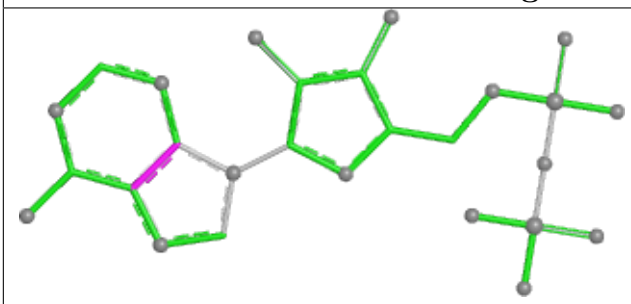
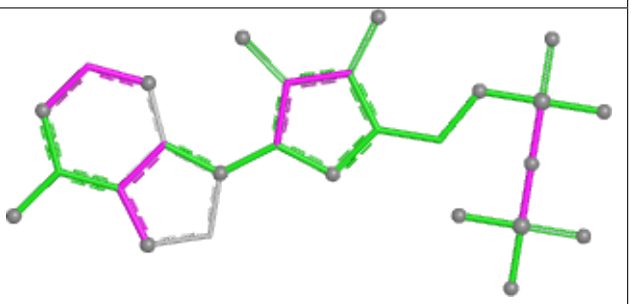
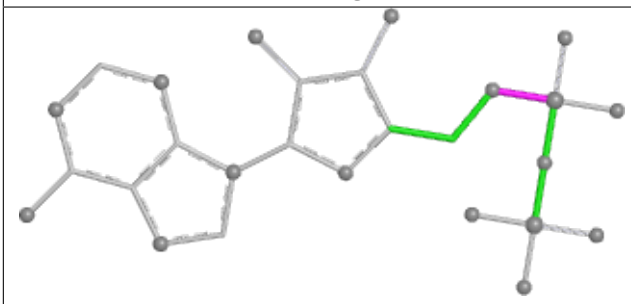
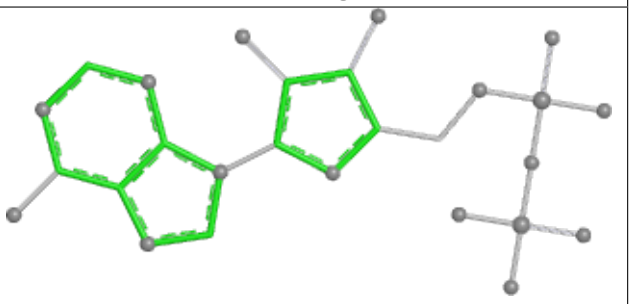
8 monomers are involved in 14 short contacts:

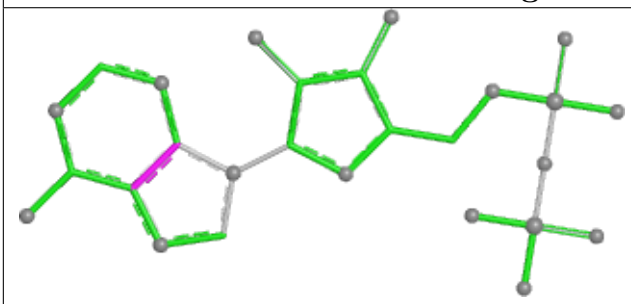
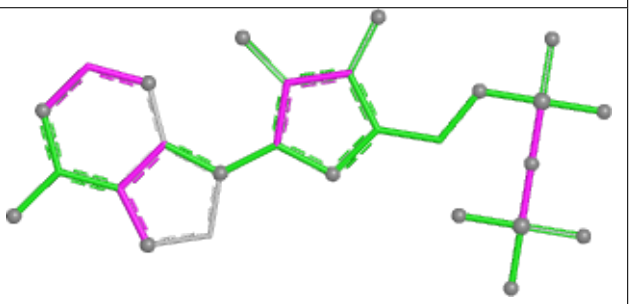
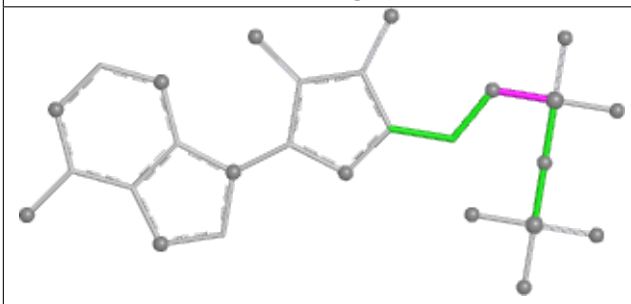
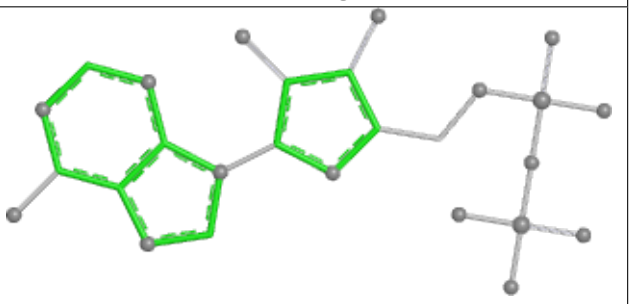
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	1602	BEF	1	0
13	T	501	ADP	2	0
13	X	501	ADP	1	0
13	Y	501	ADP	4	0
14	R	502	BEF	1	0
13	U	502	ADP	2	0
13	M	1601	ADP	3	0
13	R	501	ADP	1	0

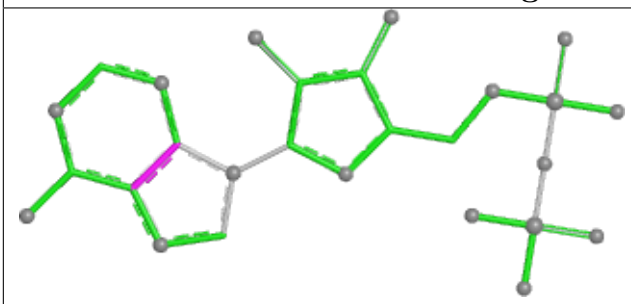
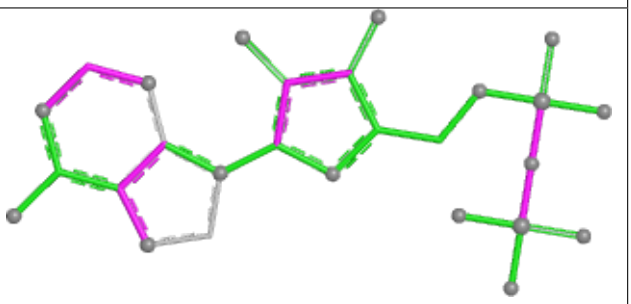
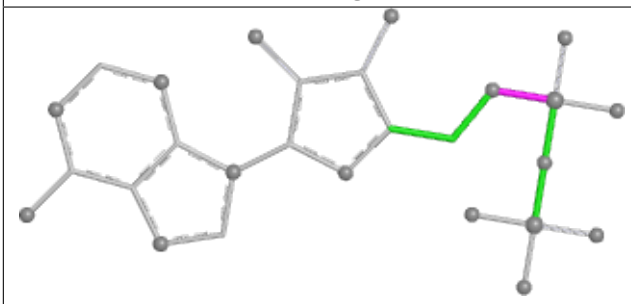
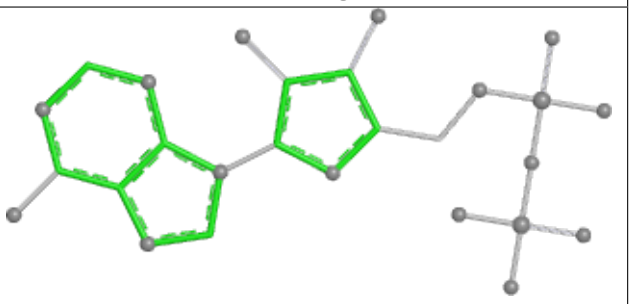
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

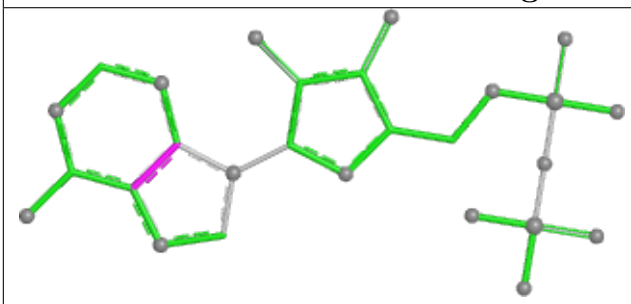
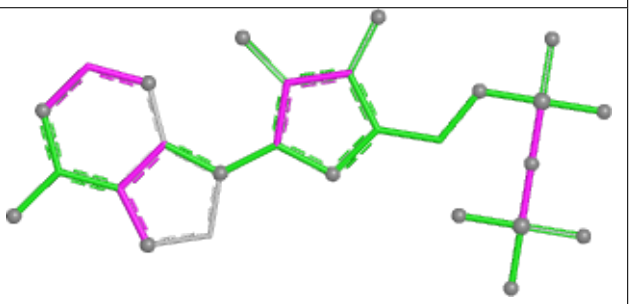
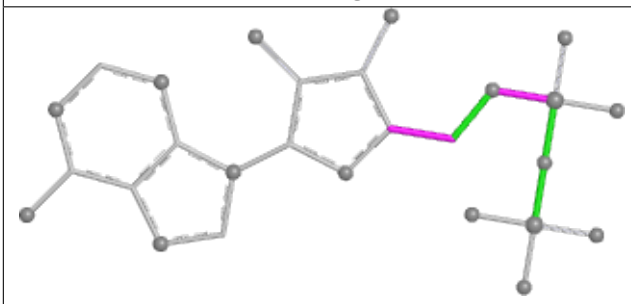
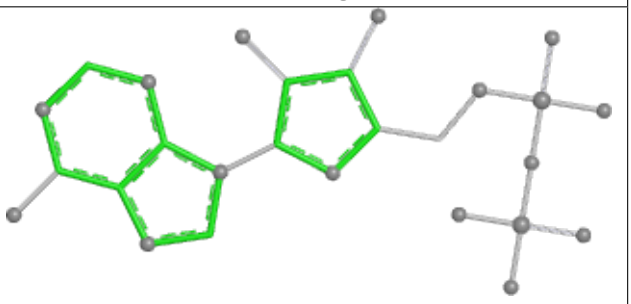
Ligand ADP T 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

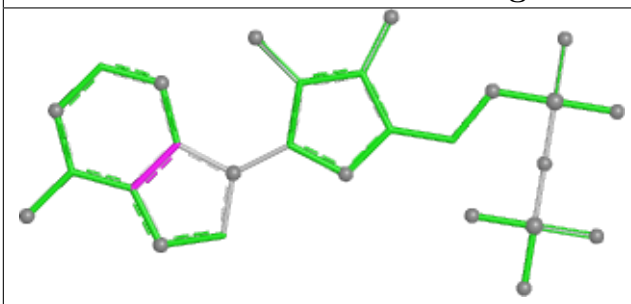
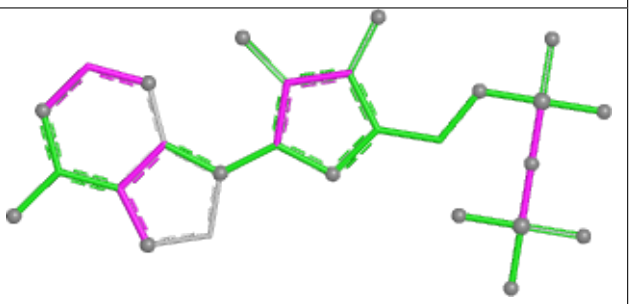
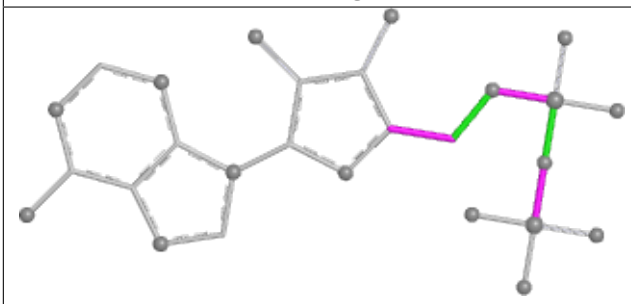
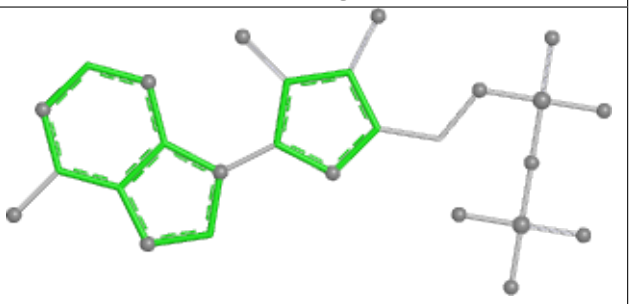
Ligand ADP W 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

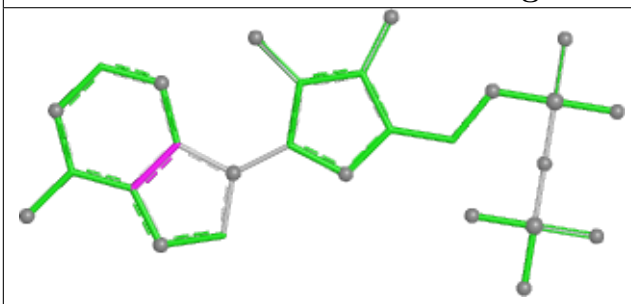
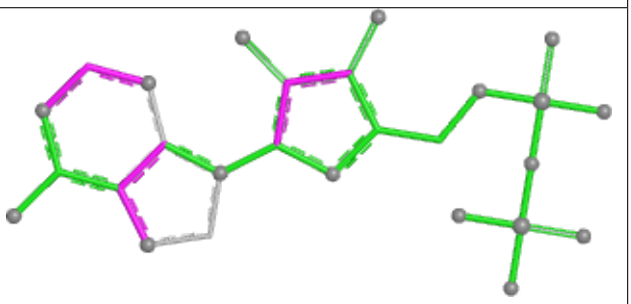
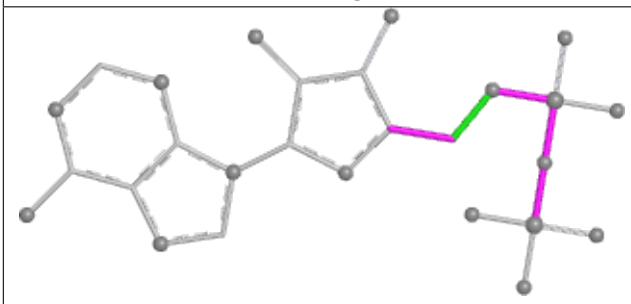
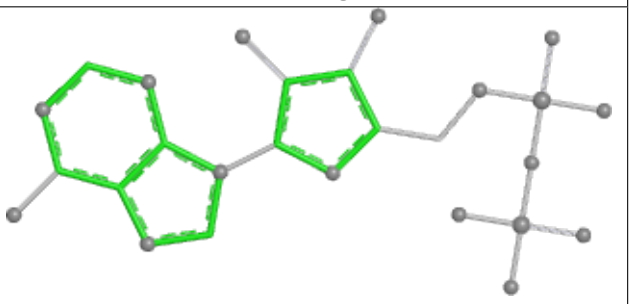
Ligand ADP X 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP Y 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP V 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP U 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP M 1601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP R 501	
 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)

There are no chain breaks in this entry.

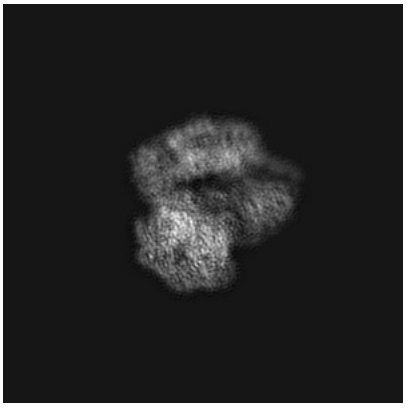
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4395. These allow visual inspection of the internal detail of the map and identification of artifacts.

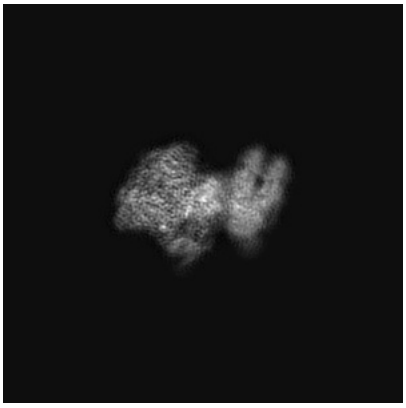
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

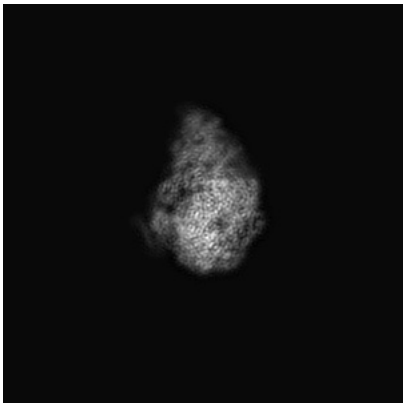
6.1.1 Primary map



X



Y

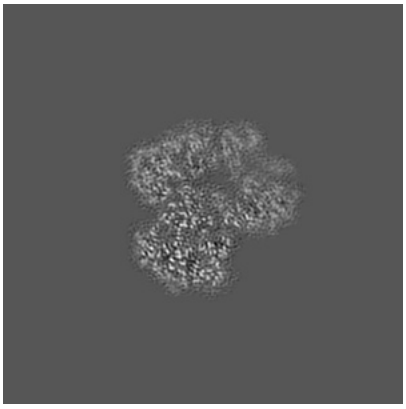


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

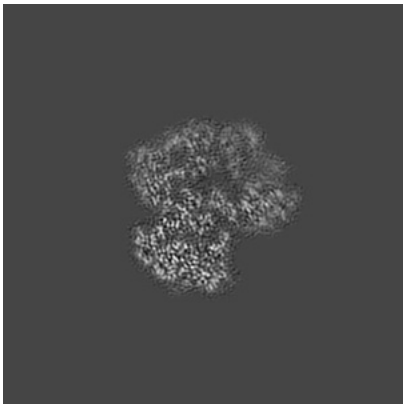
Y Index: 192

Z Index: 192

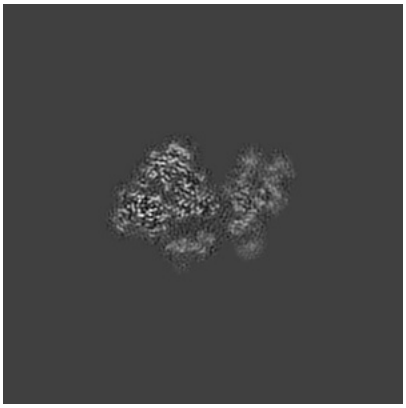
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

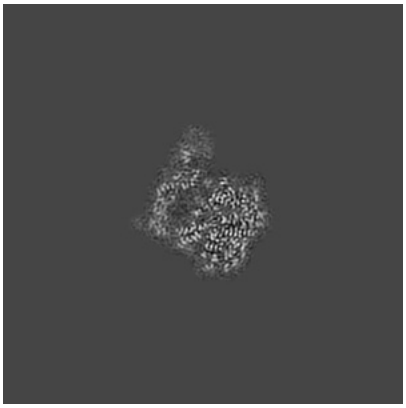
6.3.1 Primary map



X Index: 195



Y Index: 181

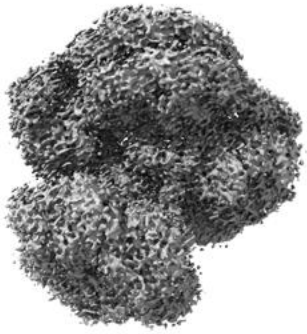


Z Index: 164

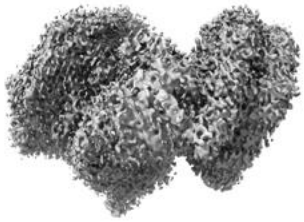
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0295. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

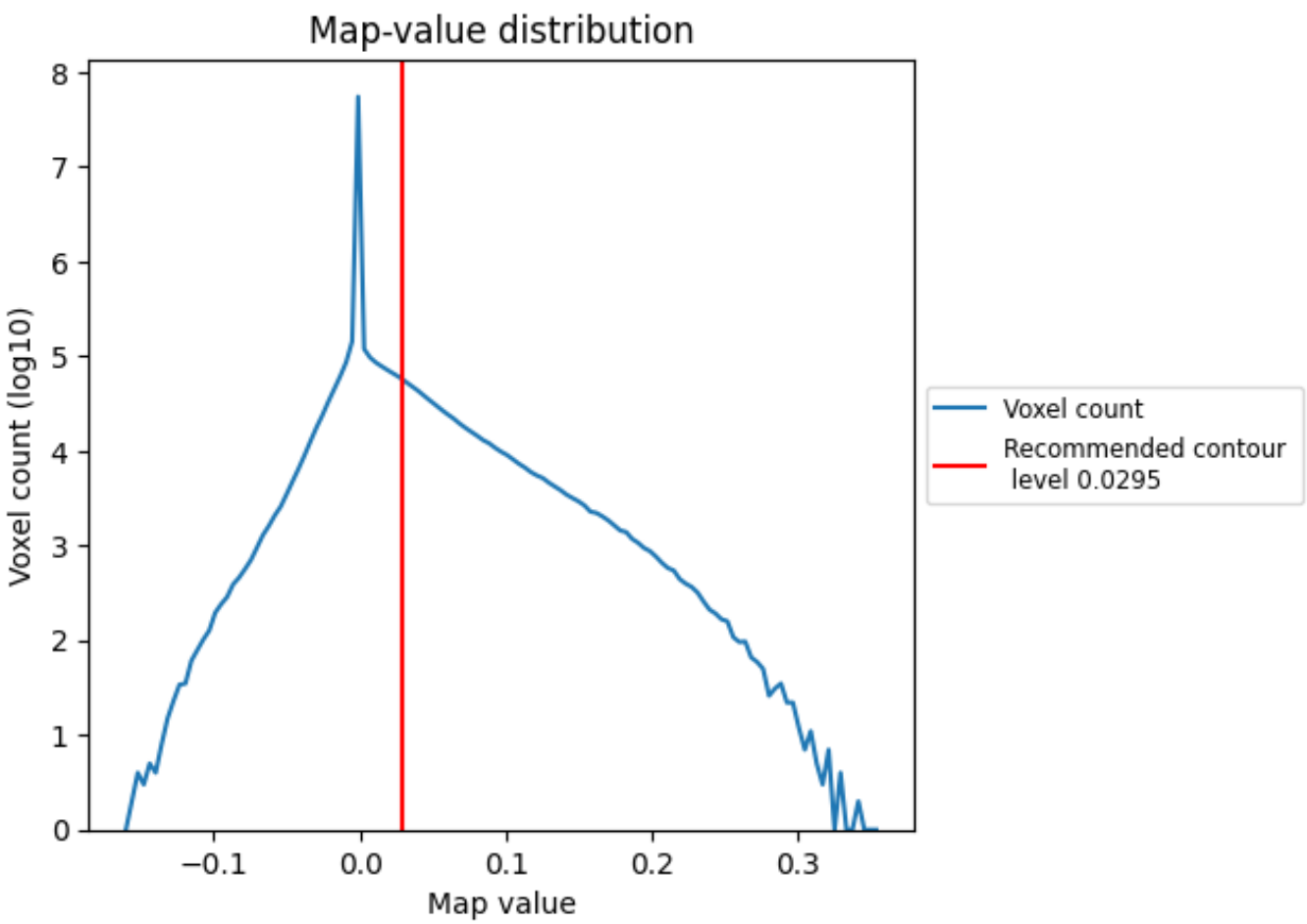
6.5 Mask visualisation (i)

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

7 Map analysis (i)

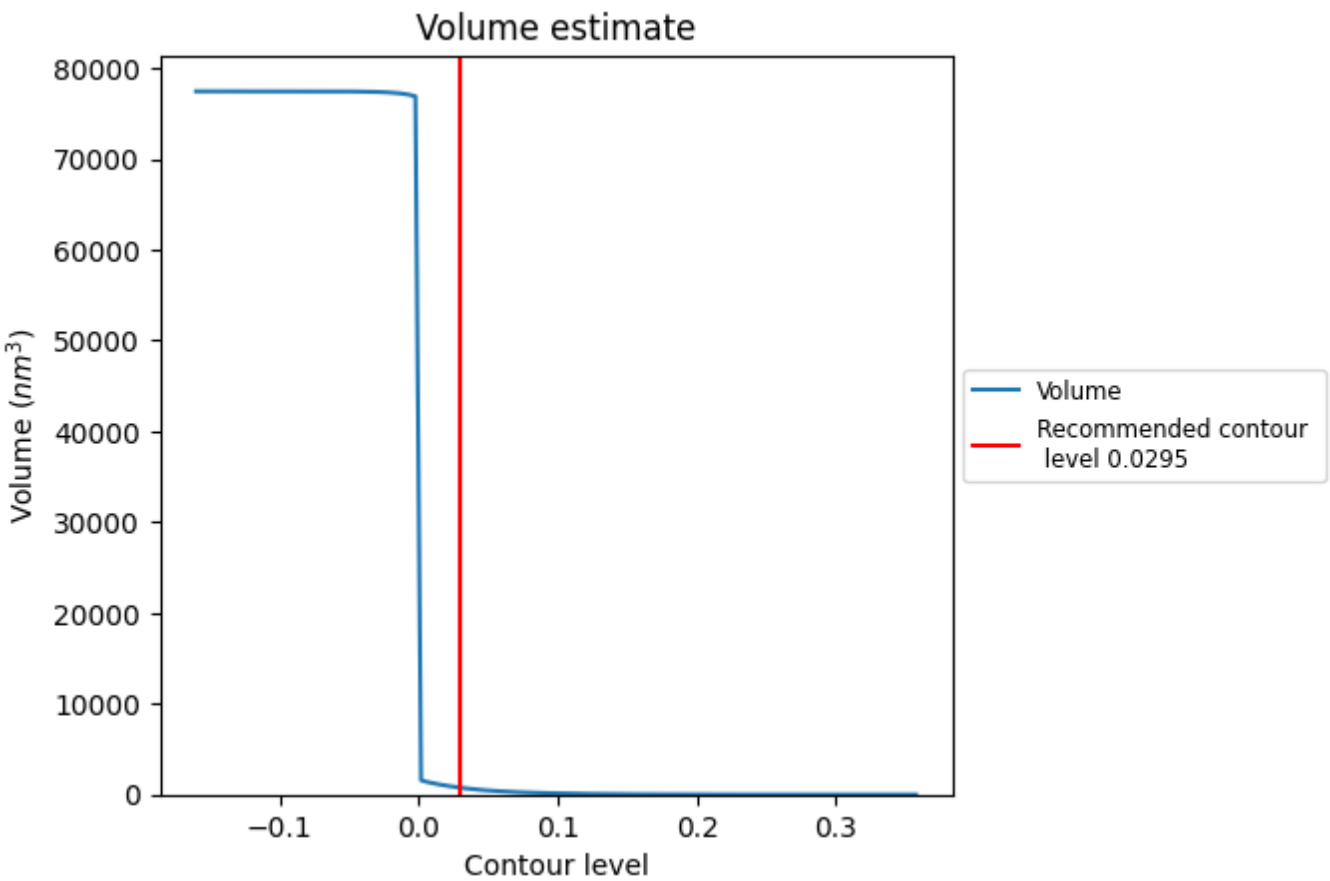
This section contains the results of statistical analysis of the map.

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.

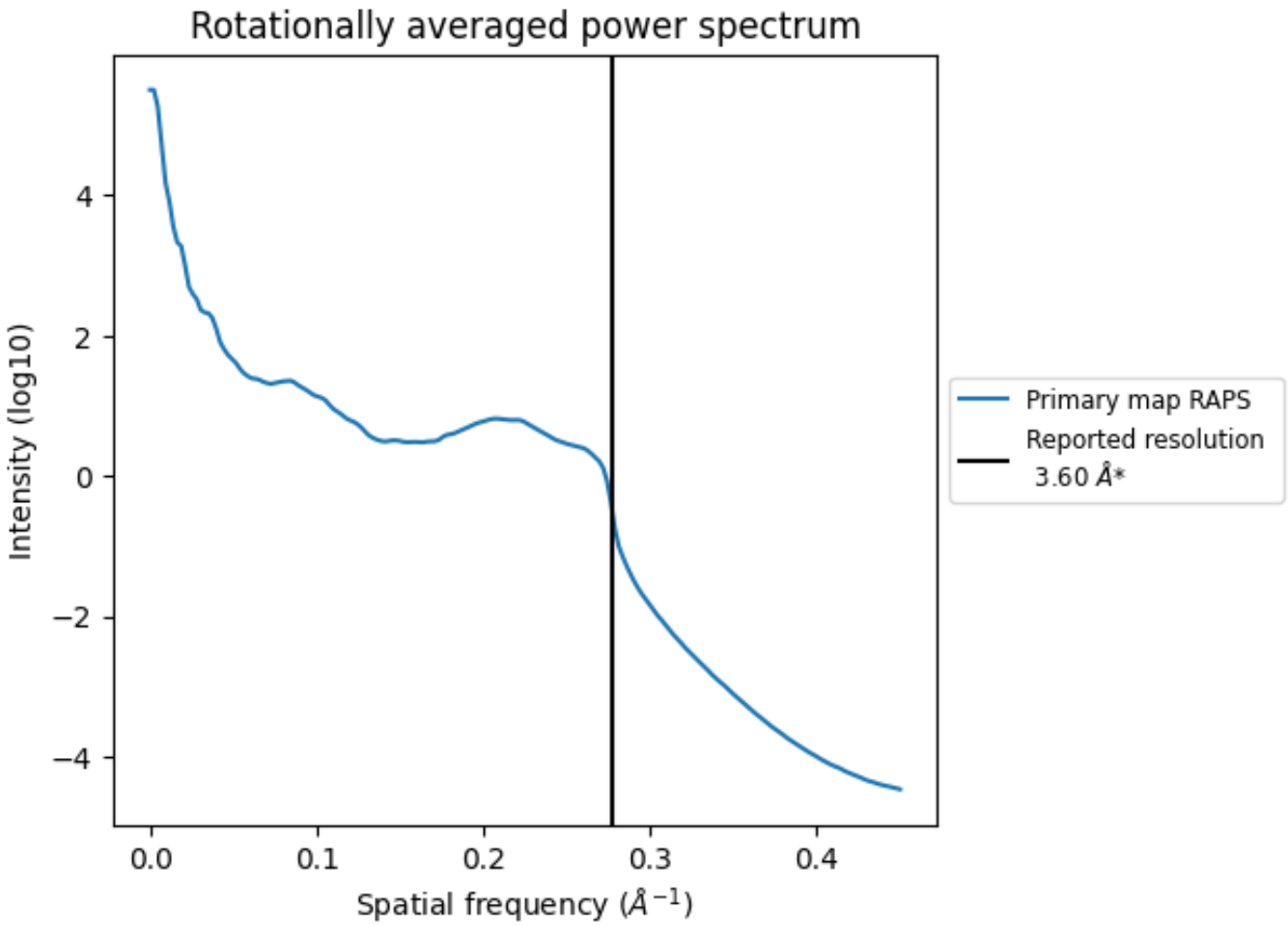
7.2 Volume estimate (i)



The volume at the recommended contour level is 765 nm^3; this corresponds to an approximate mass of 691 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 0.278 Å^{-1}

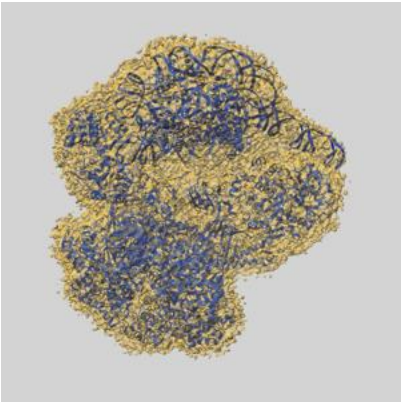
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

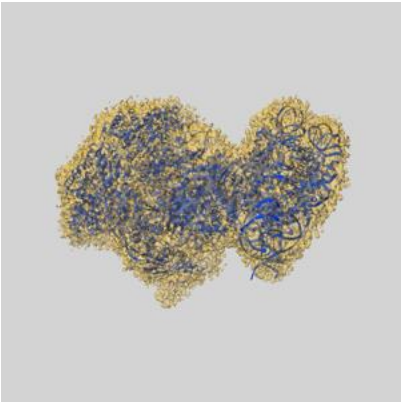
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4395 and PDB model 6GEJ. Per-residue inclusion information can be found in section 3 on page 9.

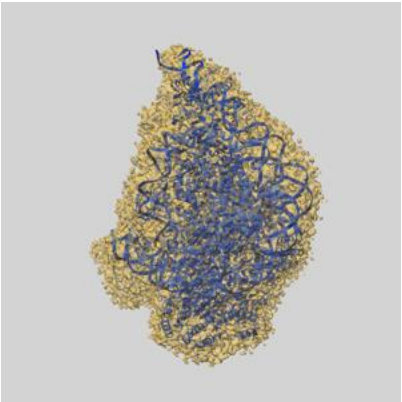
9.1 Map-model overlay (i)



X



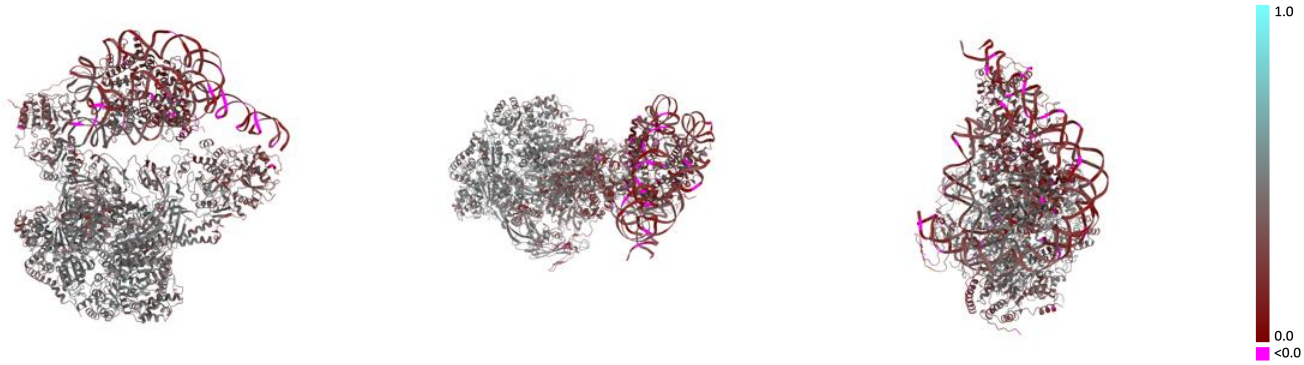
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0295 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.

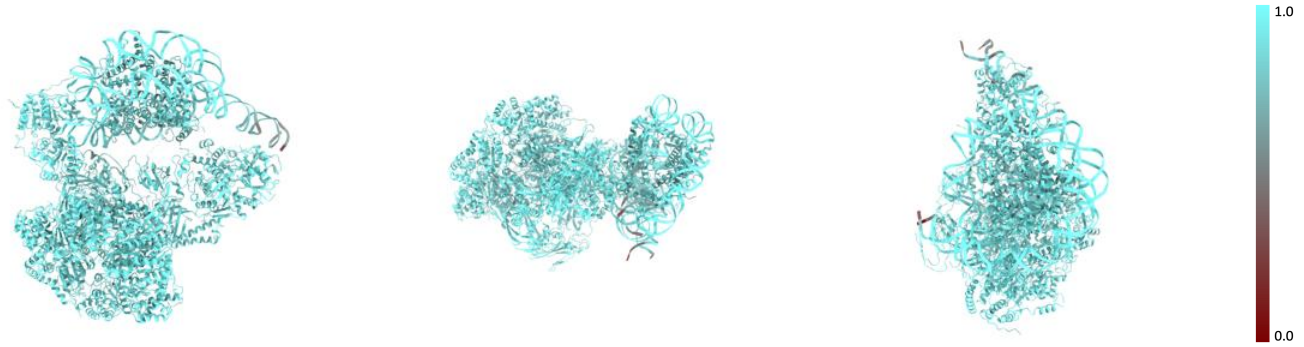
9.2 Q-score mapped to coordinate model (i)



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.

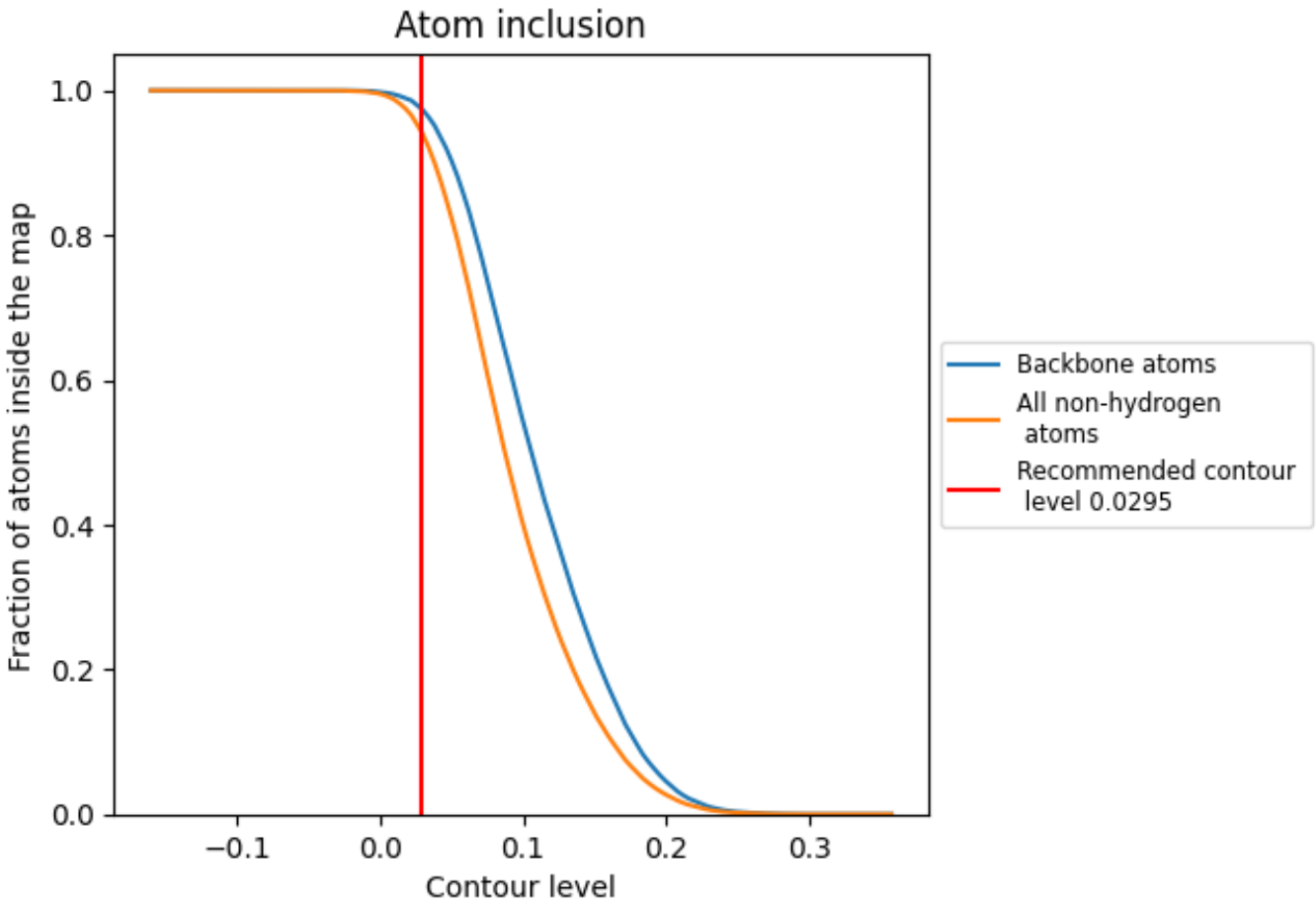
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0295).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9412	0.3720
A	0.9052	0.2700
B	0.9221	0.3700
C	0.9088	0.3840
D	0.8938	0.2810
E	0.9339	0.3170
F	0.8796	0.2370
G	0.9166	0.2980
H	0.8795	0.2390
I	0.9216	0.2000
J	0.9342	0.2240
M	0.9559	0.3960
R	0.9421	0.3640
S	0.8894	0.3130
T	0.9562	0.4520
U	0.9470	0.4380
V	0.9522	0.4460
W	0.9601	0.4570
X	0.9581	0.4440
Y	0.9654	0.4540
Z	0.9206	0.2110