Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:00 PM BST

PDB ID	:	5OT2
Title	:	RNA polymerase II elongation complex in the presence of 3d-Napht-A
Authors	:	Malvezzi, S.; Farnung, L.; Aloisi, C.; Angelov, T.; Cramer, P.; Sturla, S.J.
Deposited on	:	2017-08-19
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

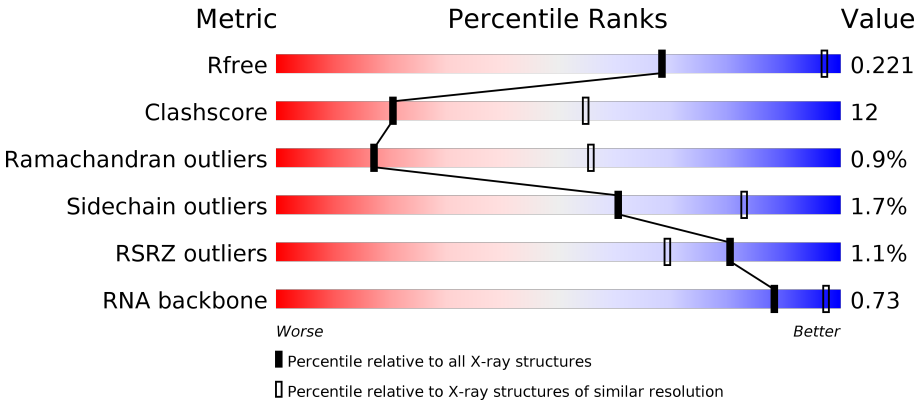
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	59% 22% • 19%
2	B	1224	2% 61% 28% • 10%
3	C	318	60% 22% • 17%
4	D	221	62% 16% 21%

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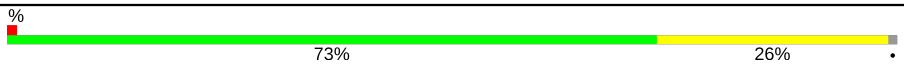
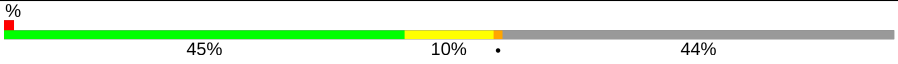
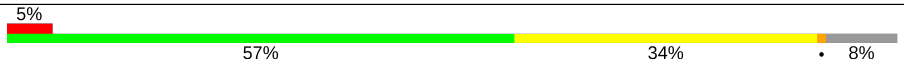
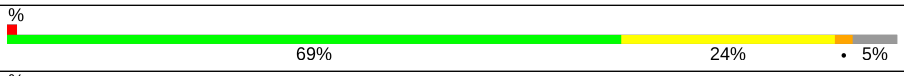
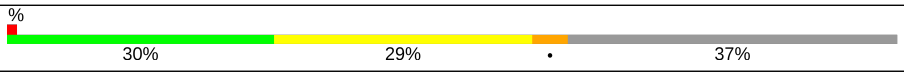
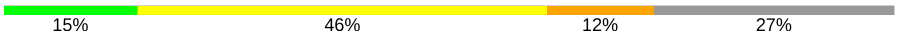
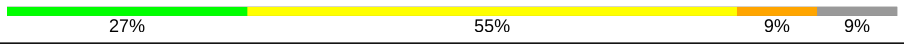
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	14	
15	P	11	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31711 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1412	Total	C	N	O	S	0	0	0
			11110	6998	1943	2107	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8769	5551	1537	1626	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2087	1313	347	414	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	175	Total	C	N	O	S	0	0	0
			1393	863	243	285	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			927	571	168	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 13 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	19	Total	Br	C	N	O	P	0	0	0
			378	1	182	60	116	19			

- Molecule 14 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			144	70	29	39	6			

- Molecule 15 is a RNA chain called RNA product strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			222	98	45	69	10			

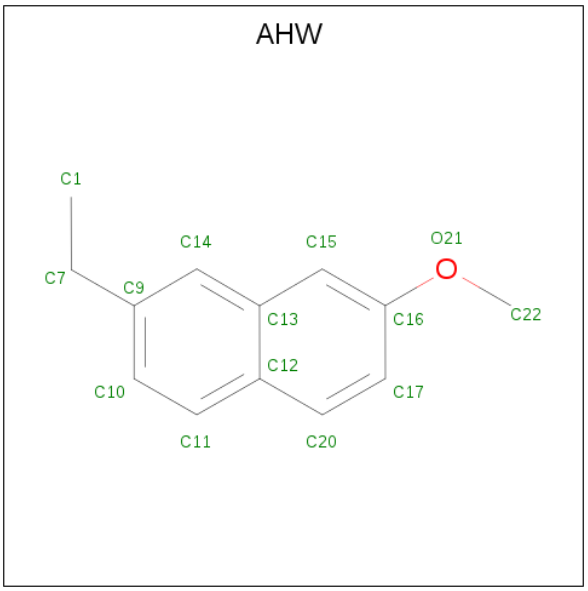
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is 2-ethyl-7-methoxy-naphthalene (three-letter code: AHW) (formula: $C_{13}H_{14}O$).



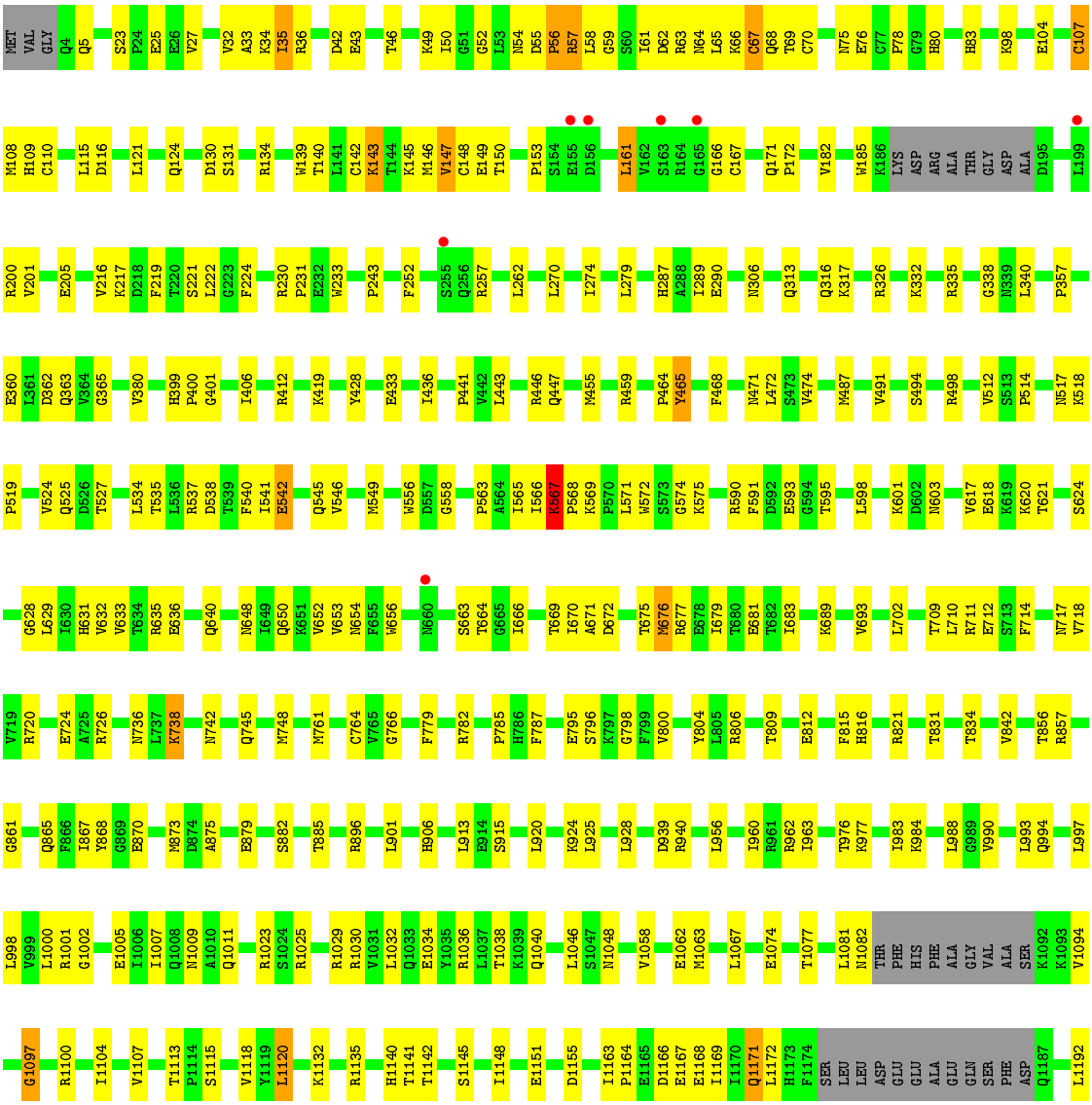
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	T	1	Total C O 14 13 1	0	0

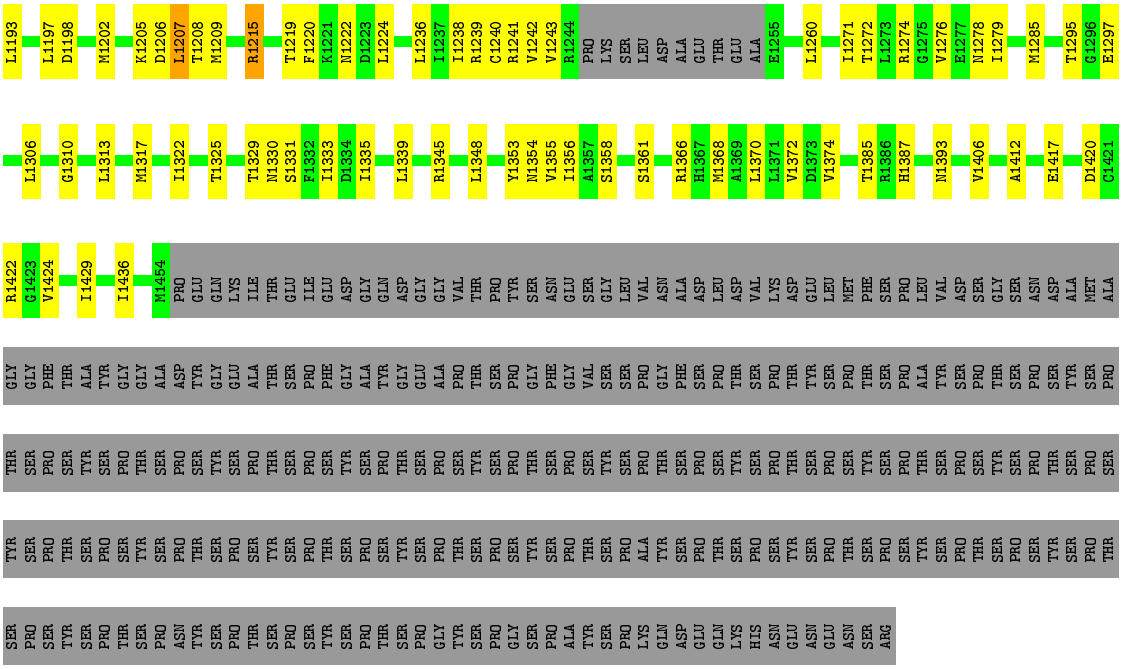
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: DNA-directed RNA polymerase II subunit RPB1

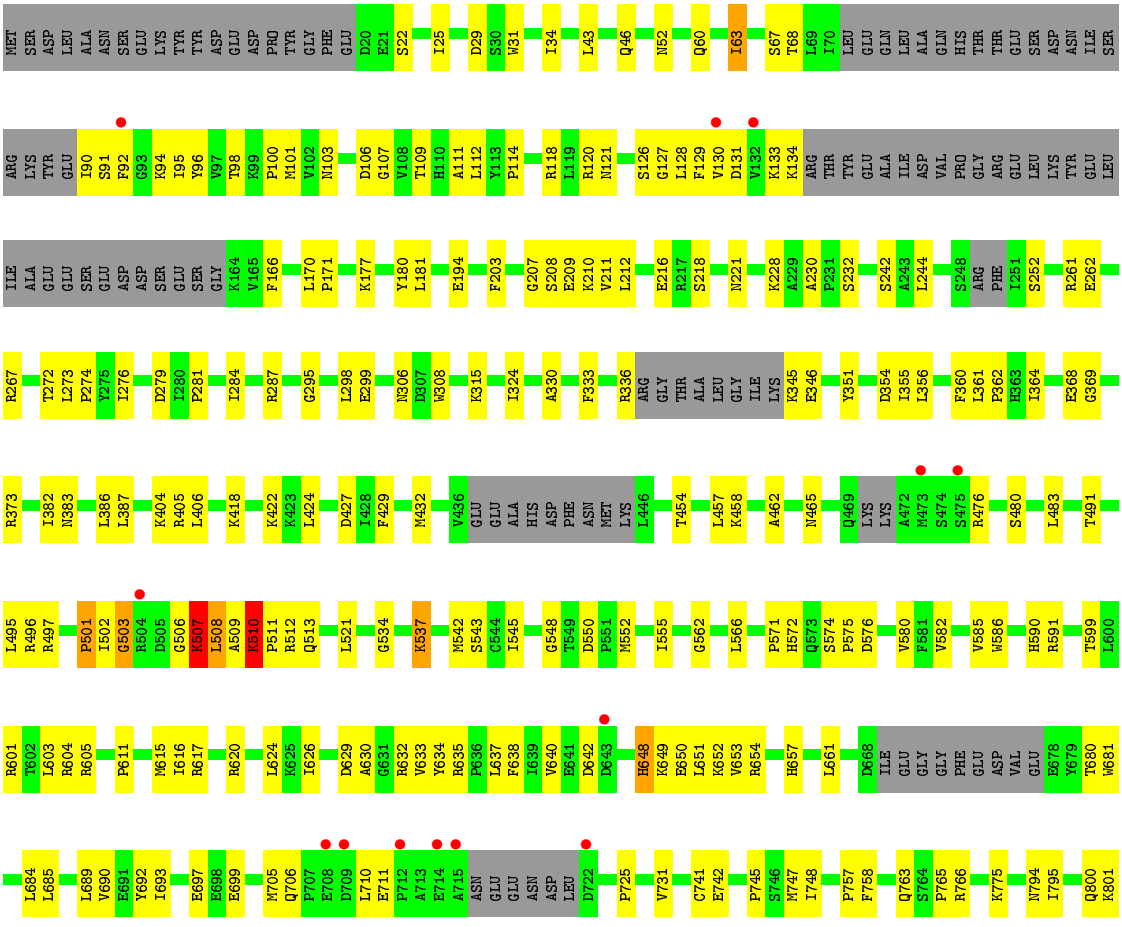
Chain A:

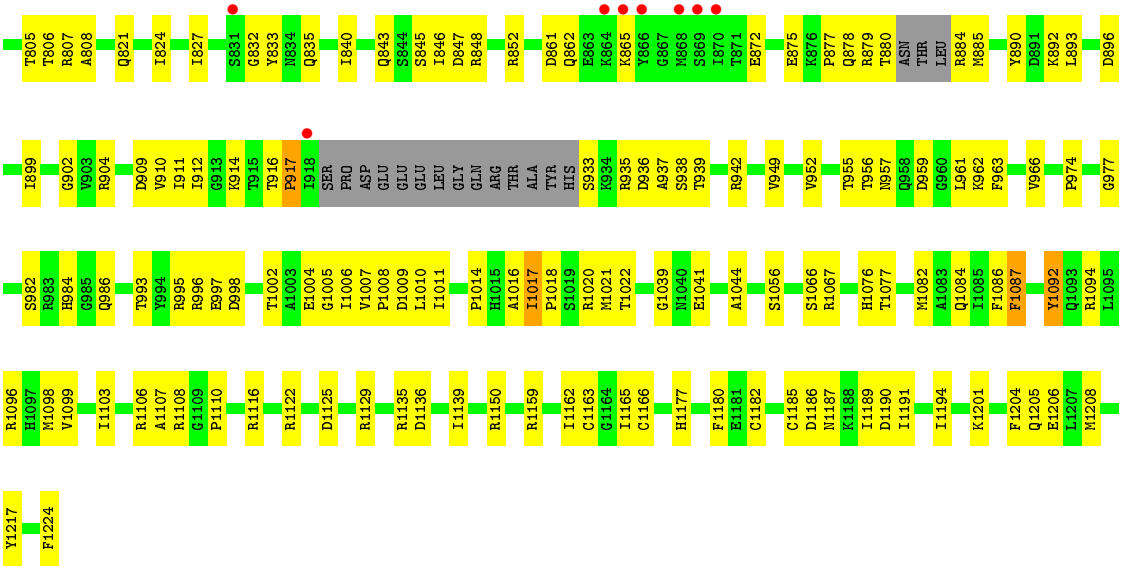




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

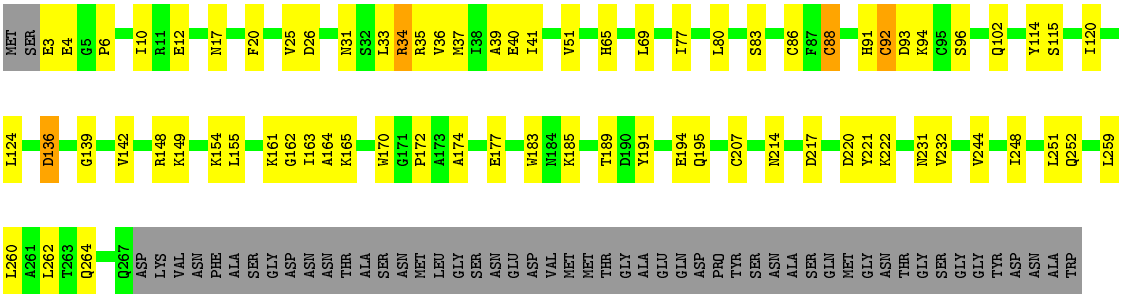
Chain B:





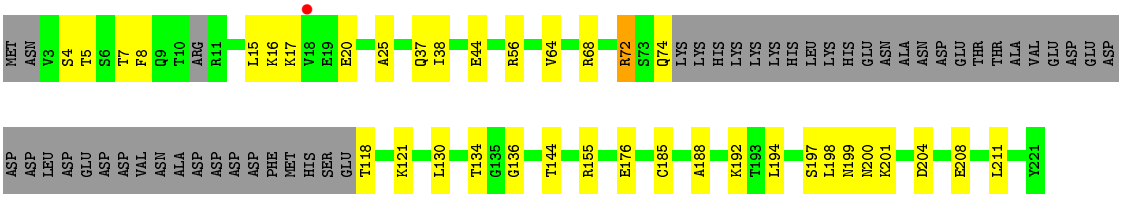
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



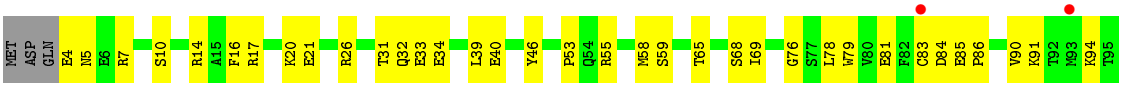
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

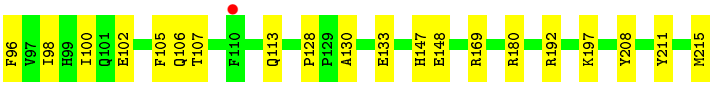
Chain D:



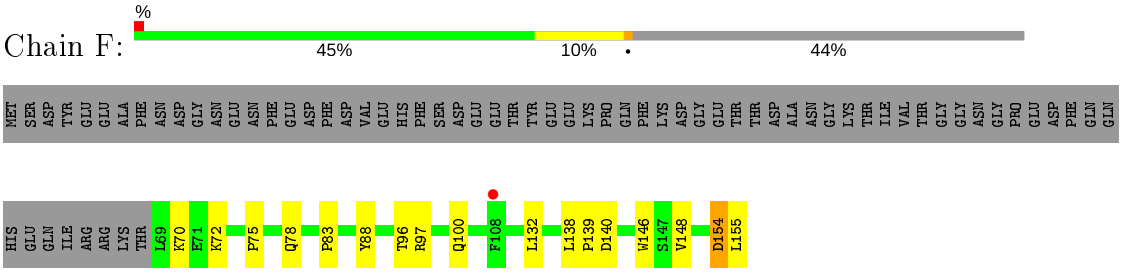
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

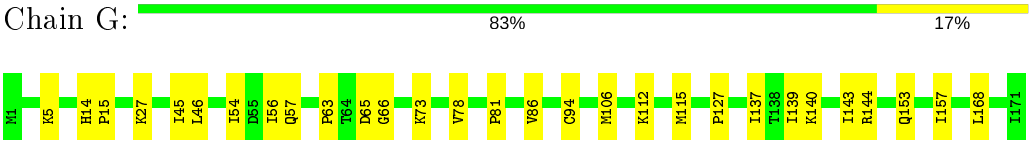




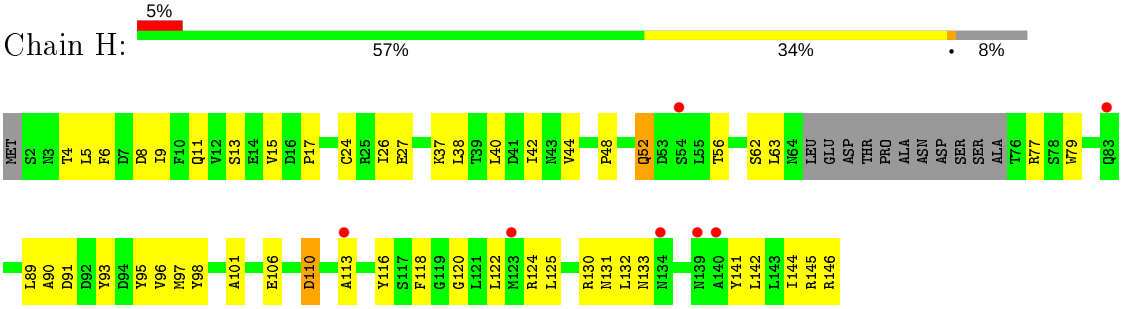
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



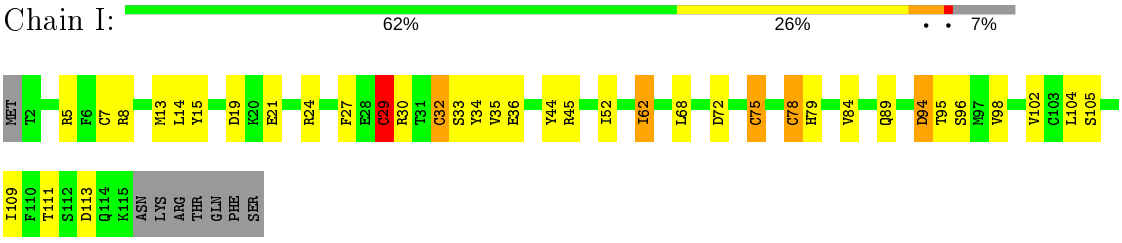
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



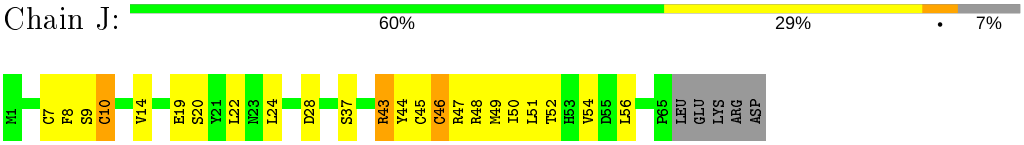
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

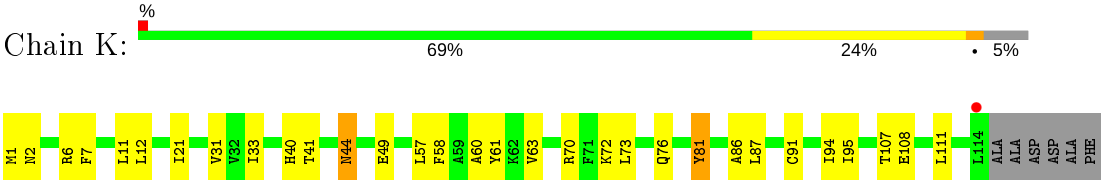


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



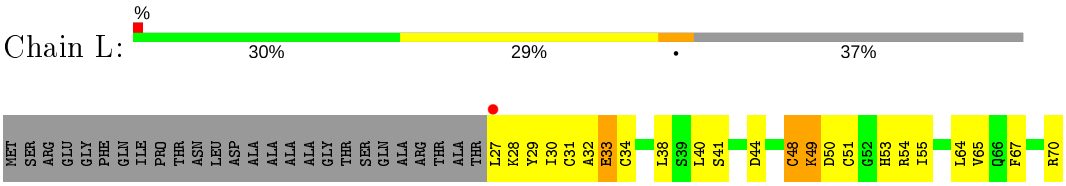
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



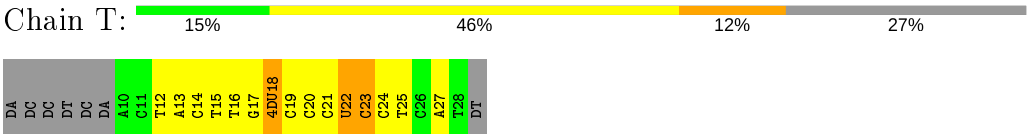
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



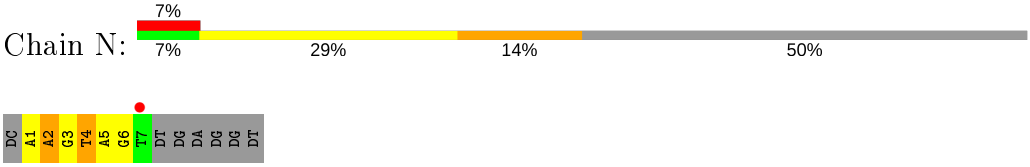
- Molecule 13: DNA template strand

Chain T:



- Molecule 14: DNA non-template strand

Chain N:



- Molecule 15: RNA product strand

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	221.35Å 394.93Å 283.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 3.20 49.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.88-3.20) 99.9 (49.88-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.178 , 0.222 0.178 , 0.221	Depositor DCC
R_{free} test set	1679 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å^2)	123.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 99.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	31711	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU, 4DU, AHW

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	0.37	0/11308	0.58	1/15294 (0.0%)
2	B	0.36	0/8938	0.58	0/12050
3	C	0.52	3/2125 (0.1%)	0.60	2/2880 (0.1%)
4	D	0.34	0/1403	0.55	0/1885
5	E	0.34	0/1771	0.50	0/2383
6	F	0.41	0/717	0.61	0/967
7	G	0.34	0/1368	0.58	0/1844
8	H	0.33	0/1094	0.57	0/1481
9	I	0.64	3/945 (0.3%)	0.65	2/1273 (0.2%)
10	J	0.50	1/541 (0.2%)	0.66	1/727 (0.1%)
11	K	0.35	0/937	0.56	1/1265 (0.1%)
12	L	0.42	0/353	0.87	1/468 (0.2%)
13	T	0.89	0/372	1.15	1/564 (0.2%)
14	N	0.72	0/162	1.28	2/249 (0.8%)
15	P	0.61	0/249	1.37	0/388
All	All	0.40	7/32283 (0.0%)	0.61	11/43718 (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
4	D	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	92	CYS	CB-SG	-14.74	1.57	1.82
9	I	32	CYS	CB-SG	-9.92	1.65	1.82
9	I	78	CYS	CB-SG	-8.77	1.67	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	86	CYS	CB-SG	-8.16	1.68	1.82
10	J	10	CYS	CB-SG	-6.90	1.70	1.82
3	C	88	CYS	CB-SG	-6.47	1.71	1.82
9	I	7	CYS	CB-SG	-6.10	1.71	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	86	CYS	CA-CB-SG	-8.45	98.80	114.00
3	C	92	CYS	N-CA-CB	-6.62	98.69	110.60
9	I	29	CYS	CA-CB-SG	6.42	125.55	114.00
14	N	2	DA	OP1-P-O3'	6.29	119.05	105.20
1	A	1207	LEU	CA-CB-CG	5.99	129.08	115.30
10	J	43	ARG	NE-CZ-NH1	-5.39	117.60	120.30
13	T	23	DC	OP1-P-OP2	-5.37	111.55	119.60
11	K	81	TYR	C-N-CA	-5.27	108.53	121.70
12	L	48	CYS	CA-CB-SG	-5.20	104.65	114.00
14	N	4	DT	N3-C4-O4	5.12	122.97	119.90
9	I	75	CYS	CA-CB-SG	5.11	123.20	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	25	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11110	0	11161	282	1
2	B	8769	0	8799	257	0
3	C	2087	0	2047	51	1
4	D	1393	0	1399	20	0
5	E	1735	0	1764	43	0
6	F	705	0	731	13	0
7	G	1340	0	1357	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1076	0	1046	47	0
9	I	927	0	880	27	0
10	J	532	0	542	19	0
11	K	919	0	929	24	0
12	L	351	0	374	21	0
13	T	378	0	213	20	0
14	N	144	0	81	7	0
15	P	222	0	109	12	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	T	14	0	0	1	0
All	All	31711	0	31432	776	1

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 (776) 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:J:10:CYS:SG	10:J:43:ARG:NH1	2.29	1.05
1:A:252:PHE:HA	15:P:1:U:H3	1.31	0.94
1:A:1209:MET:HE3	1:A:1236:LEU:HB3	1.48	0.93
12:L:34:CYS:SG	12:L:48:CYS:HB2	2.10	0.92
9:I:78:CYS:SG	9:I:105:SER:OG	2.29	0.91
1:A:1385:THR:HG22	1:A:1387:HIS:H	1.36	0.91
2:B:510:LYS:HD3	2:B:511:PRO:HD3	1.53	0.90
2:B:1163:CYS:SG	2:B:1187:ASN:ND2	2.48	0.87
1:A:70:CYS:SG	1:A:80:HIS:HE1	1.95	0.86
2:B:232:SER:O	2:B:261:ARG:NH2	2.08	0.85
2:B:942:ARG:NH2	13:T:24:DC:OP2	2.10	0.85
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.58	0.84
1:A:720:ARG:O	1:A:724:GLU:HB3	1.78	0.83
3:C:260:LEU:O	3:C:264:GLN:NE2	2.12	0.82
1:A:1081:LEU:HB3	1:A:1082:ASN:HA	1.60	0.82
1:A:107:CYS:CB	1:A:148:CYS:SG	2.68	0.82
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:63:LEU:HD23	8:H:90:ALA:H	1.45	0.81
12:L:31:CYS:SG	12:L:34:CYS:N	2.52	0.80
1:A:1329:THR:HG22	1:A:1331:SER:H	1.47	0.80
13:T:15:DT:O4	14:N:1:DA:N6	2.14	0.80
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.62	0.79
9:I:111:THR:HG22	9:I:113:ASP:H	1.45	0.79
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.16	0.78
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.65	0.78
1:A:925:LEU:HD22	1:A:983:ILE:HD11	1.64	0.78
1:A:32:VAL:HG21	1:A:69:THR:HG21	1.64	0.78
3:C:88:CYS:SG	3:C:92:CYS:N	2.56	0.77
2:B:287:ARG:NH1	2:B:324:ILE:O	2.16	0.77
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.66	0.77
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.67	0.76
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.18	0.76
5:E:31:THR:HG23	5:E:34:GLU:H	1.51	0.76
1:A:107:CYS:HB2	1:A:148:CYS:SG	2.25	0.75
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.18	0.75
8:H:5:LEU:HA	8:H:133:ASN:HD22	1.51	0.75
4:D:134:THR:HG23	4:D:136:GLY:H	1.51	0.75
12:L:31:CYS:SG	12:L:48:CYS:HB3	2.26	0.74
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.20	0.74
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.68	0.74
1:A:67:CYS:SG	1:A:80:HIS:CD2	2.58	0.74
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.70	0.74
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.69	0.73
1:A:140:THR:HA	1:A:143:LYS:HD3	1.70	0.73
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.21	0.73
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.71	0.73
7:G:139:ILE:HG23	7:G:140:LYS:HG2	1.71	0.73
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.21	0.72
2:B:996:ARG:NH2	3:C:174:ALA:O	2.21	0.72
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.71	0.72
2:B:501:PRO:O	2:B:503:GLY:N	2.22	0.72
1:A:67:CYS:O	1:A:70:CYS:N	2.20	0.72
12:L:32:ALA:HB3	12:L:55:ILE:HD13	1.72	0.72
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.72	0.71
2:B:232:SER:H	2:B:261:ARG:HH22	1.38	0.71
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.73	0.71
3:C:92:CYS:SG	3:C:93:ASP:N	2.64	0.70
2:B:101:MET:HG2	2:B:111:ALA:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:O	2:B:261:ARG:NH2	2.24	0.70
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.23	0.70
4:D:176:GLU:OE2	4:D:197:SER:OG	2.10	0.70
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.25	0.69
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.72	0.69
9:I:19:ASP:OD1	9:I:24:ARG:HG2	1.93	0.69
3:C:92:CYS:O	3:C:96:SER:OG	2.10	0.69
9:I:32:CYS:SG	9:I:33:SER:N	2.66	0.69
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.73	0.69
1:A:567:LYS:CE	8:H:97:MET:HG3	2.21	0.69
2:B:208:SER:OG	2:B:210:LYS:NZ	2.26	0.68
1:A:42:ASP:OD2	1:A:46:THR:OG1	2.11	0.68
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.76	0.68
2:B:103:ASN:HB3	2:B:109:THR:HG22	1.76	0.68
1:A:67:CYS:O	1:A:69:THR:N	2.26	0.68
2:B:599:THR:O	2:B:603:LEU:HB2	1.94	0.68
1:A:150:THR:HA	1:A:166:GLY:HA3	1.75	0.67
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.27	0.67
9:I:84:VAL:HG13	9:I:104:LEU:HD11	1.76	0.67
13:T:16:DT:H2"	13:T:17:DG:C8	2.29	0.67
1:A:542:GLU:OE2	1:A:569:LYS:NZ	2.27	0.67
1:A:1030:ARG:HA	1:A:1034:GLU:HG3	1.77	0.67
2:B:506:GLY:O	2:B:512:ARG:NH2	2.28	0.66
3:C:115:SER:HB3	3:C:142:VAL:H	1.59	0.66
1:A:67:CYS:HB3	1:A:70:CYS:HB2	1.77	0.66
2:B:368:GLU:OE2	2:B:369:GLY:N	2.22	0.65
2:B:982:SER:HB3	2:B:1092:TYR:CE1	2.31	0.65
12:L:34:CYS:SG	12:L:48:CYS:CB	2.79	0.65
15:P:3:G:H2'	15:P:4:A:C8	2.31	0.65
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.28	0.65
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.77	0.65
2:B:936:ASP:OD1	2:B:938:SER:N	2.28	0.65
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.21	0.65
12:L:33:GLU:HG2	12:L:51:CYS:SG	2.37	0.65
1:A:567:LYS:HE3	8:H:97:MET:HG3	1.77	0.65
13:T:20:DC:H42	15:P:9:G:H1	1.44	0.65
2:B:497:ARG:HH22	2:B:775:LYS:HD3	1.62	0.65
1:A:567:LYS:NZ	8:H:97:MET:HG3	2.12	0.65
2:B:1165:ILE:O	2:B:1217:TYR:OH	2.12	0.64
12:L:28:LYS:NZ	12:L:40:LEU:O	2.26	0.64
2:B:912:ILE:HB	2:B:939:THR:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.31	0.64
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.80	0.64
1:A:362:ASP:OD1	1:A:459:ARG:NH1	2.30	0.64
1:A:567:LYS:HZ1	8:H:97:MET:HG3	1.63	0.64
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.10	0.64
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.80	0.64
3:C:214:ASN:ND2	3:C:217:ASP:OD2	2.31	0.64
5:E:91:LYS:HA	5:E:94:LYS:HE3	1.79	0.64
13:T:24:DC:H42	15:P:5:G:H1	1.46	0.64
3:C:33:LEU:HD11	3:C:248:ILE:HG12	1.79	0.63
1:A:1132:LYS:HG2	1:A:1135:ARG:HH21	1.64	0.63
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.80	0.63
7:G:144:ARG:HG2	7:G:168:LEU:HD23	1.81	0.63
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.34	0.63
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.81	0.63
10:J:20:SER:O	10:J:24:LEU:HB2	1.99	0.63
15:P:3:G:H2'	15:P:4:A:H8	1.64	0.62
8:H:15:VAL:HG12	8:H:26:ILE:HG22	1.81	0.62
1:A:1171:GLN:HG2	1:A:1172:LEU:HD12	1.80	0.62
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.80	0.62
15:P:4:A:H2'	15:P:5:G:H8	1.64	0.62
5:E:128:PRO:HA	5:E:130:ALA:H	1.64	0.62
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.35	0.62
8:H:89:LEU:HG	8:H:91:ASP:HB3	1.82	0.62
2:B:959:ASP:OD1	2:B:961:LEU:HB2	2.00	0.62
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.81	0.61
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.81	0.61
3:C:31:ASN:O	3:C:35:ARG:HG3	2.00	0.61
1:A:664:THR:HG22	2:B:1014:PRO:HB3	1.82	0.61
1:A:115:LEU:HD11	1:A:145:LYS:HG3	1.83	0.61
2:B:1189:ILE:HG13	2:B:1190:ASP:N	2.15	0.61
1:A:738:LYS:H	1:A:738:LYS:HE3	1.65	0.61
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.82	0.61
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.81	0.61
2:B:295:GLY:H	2:B:298:LEU:HD13	1.66	0.61
1:A:831:THR:HA	18:T:101:AHW:C15	2.30	0.61
1:A:1132:LYS:HG2	1:A:1135:ARG:NH2	2.17	0.60
1:A:76:GLU:OE2	2:B:1159:ARG:NH2	2.33	0.60
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.31	0.60
1:A:64:ASN:O	1:A:66:LYS:N	2.34	0.60
10:J:9:SER:OG	10:J:48:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:4:GLU:HG2	5:E:5:ASN:H	1.65	0.60
2:B:862:GLN:O	2:B:914:LYS:NZ	2.34	0.60
1:A:1038:THR:HG22	1:A:1040:GLN:H	1.66	0.60
1:A:882:SER:O	1:A:1025:ARG:NH2	2.33	0.60
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.82	0.60
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.66	0.60
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.83	0.60
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.65	0.60
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.17	0.60
2:B:507:LYS:HG2	2:B:508:LEU:H	1.66	0.60
2:B:936:ASP:OD1	2:B:937:ALA:N	2.35	0.60
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.82	0.60
15:P:4:A:H2'	15:P:5:G:C8	2.36	0.60
2:B:43:LEU:O	2:B:496:ARG:NH1	2.34	0.59
2:B:801:LYS:O	10:J:52:THR:HG23	2.01	0.59
2:B:806:THR:HG22	2:B:808:ALA:H	1.67	0.59
1:A:538:ASP:HA	1:A:540:PHE:HE1	1.68	0.59
1:A:1120:LEU:HA	1:A:1322:ILE:HA	1.84	0.59
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.83	0.59
1:A:1424:VAL:HG21	2:B:1139:ILE:HD13	1.83	0.59
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.85	0.59
5:E:76:GLY:N	5:E:106:GLN:OE1	2.31	0.59
1:A:406:ILE:HG13	1:A:412:ARG:HG3	1.85	0.59
2:B:507:LYS:HG2	2:B:508:LEU:N	2.17	0.59
9:I:21:GLU:N	9:I:21:GLU:OE1	2.28	0.59
2:B:902:GLY:O	12:L:65:VAL:HG11	2.03	0.59
2:B:555:ILE:HD11	2:B:582:VAL:HG21	1.85	0.59
10:J:14:VAL:HG22	10:J:50:ILE:HD11	1.85	0.59
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.37	0.59
1:A:537:ARG:NH1	8:H:120:GLY:O	2.36	0.59
1:A:834:THR:HG21	1:A:1077:THR:HA	1.85	0.58
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.33	0.58
2:B:1166:CYS:CA	2:B:1185:CYS:SG	2.79	0.58
2:B:31:TRP:CD2	2:B:807:ARG:HG2	2.38	0.58
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.86	0.58
1:A:640:GLN:CD	1:A:640:GLN:H	2.05	0.58
2:B:843:GLN:HB2	2:B:993:THR:HB	1.85	0.58
1:A:78:PRO:O	2:B:1201:LYS:NZ	2.33	0.58
5:E:197:LYS:HD2	5:E:211:TYR:CE1	2.38	0.58
1:A:465:TYR:H	11:K:2:ASN:HB3	1.69	0.58
1:A:5:GLN:O	2:B:1159:ARG:NH1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG21	1:A:617:VAL:H	1.69	0.58
2:B:130:VAL:HG12	2:B:131:ASP:H	1.69	0.58
2:B:648:HIS:ND1	2:B:649:LYS:O	2.37	0.58
14:N:4:DT:H2"	14:N:5:DA:C8	2.38	0.57
5:E:197:LYS:HD2	5:E:211:TYR:HE1	1.68	0.57
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.86	0.57
1:A:671:ALA:HB3	1:A:676:MET:HG2	1.87	0.57
1:A:782:ARG:NH2	2:B:699:GLU:O	2.36	0.57
10:J:7:CYS:SG	10:J:10:CYS:N	2.74	0.57
1:A:795:GLU:HG3	2:B:731:VAL:HG11	1.87	0.57
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.85	0.57
14:N:3:DG:H2'	14:N:4:DT:H71	1.87	0.57
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.77	0.57
4:D:198:LEU:O	4:D:200:ASN:N	2.37	0.57
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.40	0.57
1:A:709:THR:HB	1:A:712:GLU:H	1.70	0.57
3:C:88:CYS:HB3	3:C:92:CYS:HB2	1.86	0.57
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.53	0.57
1:A:146:MET:HA	1:A:171:GLN:HB2	1.86	0.56
1:A:494:SER:O	1:A:498:ARG:HG3	2.05	0.56
2:B:861:ASP:OD1	2:B:862:GLN:N	2.38	0.56
7:G:81:PRO:HG3	7:G:106:MET:SD	2.45	0.56
1:A:1151:GLU:OE2	9:I:45:ARG:NH1	2.38	0.56
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.37	0.56
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.39	0.56
1:A:182:VAL:HG22	1:A:201:VAL:HG12	1.86	0.56
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.41	0.56
1:A:717:ASN:OD1	1:A:720:ARG:NH2	2.38	0.56
9:I:32:CYS:SG	9:I:34:TYR:N	2.78	0.56
9:I:29:CYS:SG	9:I:32:CYS:N	2.72	0.56
9:I:75:CYS:SG	9:I:78:CYS:N	2.74	0.56
13:T:13:DA:H2"	13:T:14:DC:H5"	1.88	0.56
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.87	0.56
12:L:41:SER:N	12:L:44:ASP:OD2	2.39	0.56
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.37	0.56
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.36	0.56
3:C:91:HIS:O	3:C:91:HIS:ND1	2.37	0.56
1:A:1002:GLY:H	1:A:1007:ILE:HG21	1.71	0.55
2:B:1067:ARG:NH2	3:C:194:GLU:OE2	2.38	0.55
2:B:1182:CYS:O	2:B:1186:ASP:N	2.39	0.55
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.88	0.55
1:A:121:LEU:HD12	1:A:121:LEU:H	1.71	0.55
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.89	0.55
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.88	0.55
12:L:53:HIS:ND1	12:L:55:ILE:HD11	2.21	0.55
1:A:663:SER:O	1:A:742:ASN:ND2	2.34	0.55
10:J:8:PHE:HD2	10:J:48:ARG:HH12	1.55	0.55
1:A:131:SER:HA	1:A:134:ARG:HH21	1.72	0.55
2:B:497:ARG:NH2	2:B:775:LYS:HD3	2.22	0.55
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.89	0.55
3:C:120:ILE:HG21	3:C:124:LEU:HD11	1.88	0.55
5:E:33:GLU:OE1	5:E:33:GLU:N	2.40	0.55
13:T:24:DC:N4	15:P:5:G:H1	2.04	0.55
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.42	0.55
4:D:15:LEU:HD12	4:D:16:LYS:H	1.71	0.55
1:A:110:CYS:SG	1:A:167:CYS:HB2	2.46	0.54
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.88	0.54
2:B:31:TRP:CE2	2:B:807:ARG:HG2	2.42	0.54
4:D:4:SER:OG	4:D:5:THR:N	2.40	0.54
5:E:65:THR:OG1	5:E:68:SER:OG	2.26	0.54
13:T:24:DC:H2"	13:T:25:DT:H5'	1.89	0.54
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.21	0.54
1:A:567:LYS:HG2	8:H:96:VAL:O	2.07	0.54
2:B:507:LYS:HD2	2:B:507:LYS:H	1.72	0.54
1:A:205:GLU:CD	1:A:205:GLU:H	2.10	0.54
1:A:443:LEU:HD21	1:A:455:MET:HE2	1.89	0.54
13:T:20:DC:N4	15:P:9:G:H1	2.04	0.54
1:A:1142:THR:O	1:A:1145:SER:OG	2.24	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:O	2.07	0.54
2:B:574:SER:HB3	2:B:591:ARG:CZ	2.38	0.54
2:B:957:ASN:ND2	2:B:959:ASP:OD2	2.41	0.54
3:C:244:VAL:O	3:C:248:ILE:HG13	2.08	0.54
8:H:63:LEU:HD23	8:H:90:ALA:N	2.20	0.54
2:B:640:VAL:HG12	2:B:651:LEU:HA	1.89	0.54
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.72	0.53
2:B:875:GLU:O	2:B:877:PRO:HD3	2.08	0.53
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.89	0.53
14:N:1:DA:H1'	14:N:2:DA:H5'	1.90	0.53
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.74	0.53
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.44	0.53
2:B:576:ASP:N	2:B:576:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:CD	2.86	0.53
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.73	0.53
2:B:67:SER:HB3	2:B:92:PHE:HB2	1.90	0.53
12:L:30:ILE:HG22	12:L:31:CYS:H	1.73	0.53
1:A:1222:ASN:N	1:A:1222:ASN:OD1	2.42	0.53
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.89	0.53
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.43	0.53
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.90	0.53
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.43	0.53
1:A:806:ARG:NH2	2:B:725:PRO:O	2.42	0.53
5:E:4:GLU:N	5:E:4:GLU:OE2	2.41	0.53
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.74	0.53
1:A:62:ASP:O	1:A:63:ARG:HD2	2.09	0.53
3:C:65:HIS:O	3:C:69:LEU:HD12	2.09	0.53
1:A:471:ASN:O	1:A:474:VAL:HG12	2.09	0.53
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.91	0.53
4:D:64:VAL:O	4:D:68:ARG:HG2	2.09	0.53
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.43	0.52
5:E:180:ARG:NH2	5:E:215:MET:SD	2.80	0.52
8:H:26:ILE:HD11	8:H:40:LEU:HB3	1.89	0.52
1:A:108:MET:O	1:A:109:HIS:HB3	2.09	0.52
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.34	0.52
1:A:569:LYS:HG3	1:A:571:LEU:HD13	1.90	0.52
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.43	0.52
2:B:261:ARG:C	2:B:267:ARG:HH12	2.12	0.52
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.90	0.52
1:A:50:ILE:HG23	1:A:52:GLY:H	1.73	0.52
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	1.92	0.52
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.91	0.52
2:B:60:GLN:NE2	2:B:63:ILE:HD11	2.25	0.52
2:B:642:ASP:HB2	2:B:649:LYS:HA	1.90	0.52
12:L:55:ILE:O	12:L:55:ILE:HD12	2.10	0.52
1:A:224:PHE:CE2	1:A:231:PRO:HB3	2.45	0.52
2:B:127:GLY:O	2:B:128:LEU:HD23	2.09	0.52
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.92	0.52
2:B:852:ARG:HH22	12:L:70:ARG:C	2.12	0.52
11:K:91:CYS:O	11:K:95:ILE:HG13	2.10	0.52
1:A:1219:THR:HG21	1:A:1271:ILE:HG21	1.92	0.52
5:E:90:VAL:O	5:E:94:LYS:HG2	2.10	0.52
9:I:62:ILE:HD11	9:I:102:VAL:HG11	1.91	0.52
7:G:65:ASP:OD1	7:G:66:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:MET:HA	3:C:189:THR:HA	1.91	0.52
1:A:1215:ARG:NH2	1:A:1272:THR:OG1	2.41	0.51
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.92	0.51
2:B:982:SER:HB3	2:B:1092:TYR:HE1	1.74	0.51
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.92	0.51
1:A:270:LEU:O	1:A:274:ILE:HG13	2.10	0.51
1:A:598:LEU:O	8:H:122:LEU:HD12	2.09	0.51
1:A:567:LYS:HE2	8:H:95:TYR:CD2	2.45	0.51
2:B:914:LYS:HG2	2:B:937:ALA:O	2.11	0.51
2:B:824:ILE:HG12	10:J:48:ARG:HH21	1.75	0.51
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.45	0.51
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.42	0.51
2:B:22:SER:HA	2:B:654:ARG:HB3	1.93	0.51
3:C:3:GLU:HG3	3:C:4:GLU:H	1.75	0.51
4:D:8:PHE:HZ	4:D:37:GLN:HB3	1.76	0.51
1:A:787:PHE:CE2	1:A:796:SER:HA	2.46	0.51
2:B:101:MET:HA	2:B:112:LEU:H	1.76	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	1.93	0.51
2:B:562:GLY:O	2:B:590:HIS:ND1	2.36	0.51
1:A:1215:ARG:O	1:A:1219:THR:OG1	2.16	0.51
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.76	0.51
1:A:1356:ILE:HG23	1:A:1361:SER:HB2	1.93	0.51
1:A:1097:GLY:HA2	1:A:1355:VAL:HG13	1.92	0.51
2:B:100:PRO:HG2	2:B:180:TYR:CE2	2.46	0.51
2:B:106:ASP:OD1	2:B:107:GLY:N	2.44	0.51
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.38	0.50
5:E:59:SER:HB3	5:E:81:GLU:HA	1.92	0.50
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.11	0.50
7:G:57:GLN:NE2	7:G:73:LYS:HD2	2.25	0.50
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.94	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
13:T:18:4DU:H8	13:T:19:DC:H6	1.77	0.50
1:A:56:PRO:C	1:A:57:ARG:HD3	2.31	0.50
2:B:680:THR:OG1	2:B:681:TRP:N	2.44	0.50
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.43	0.50
5:E:192:ARG:HB2	5:E:215:MET:SD	2.52	0.50
9:I:96:SER:HB3	9:I:98:VAL:HG23	1.93	0.50
2:B:638:PHE:HA	2:B:690:VAL:HG12	1.94	0.50
6:F:96:THR:O	6:F:100:GLN:HG3	2.12	0.50
15:P:5:G:H2'	15:P:6:G:H8	1.77	0.50
1:A:23:SER:O	1:A:27:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.94	0.49
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.45	0.49
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.48	0.49
3:C:183:TRP:O	3:C:185:LYS:N	2.44	0.49
10:J:7:CYS:SG	10:J:46:CYS:HB3	2.52	0.49
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.94	0.49
1:A:567:LYS:HZ1	8:H:97:MET:CG	2.25	0.49
1:A:650:GLN:O	1:A:654:ASN:ND2	2.45	0.49
2:B:315:LYS:HG2	9:I:13:MET:SD	2.52	0.49
2:B:550:ASP:OD2	2:B:552:MET:HG2	2.12	0.49
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.94	0.49
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.49
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.95	0.49
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.94	0.49
1:A:1202:MET:O	1:A:1207:LEU:N	2.27	0.49
1:A:518:LYS:HD2	1:A:624:SER:O	2.13	0.49
2:B:418:LYS:HE3	2:B:422:LYS:NZ	2.28	0.49
2:B:571:PRO:O	2:B:575:PRO:HA	2.13	0.49
8:H:6:PHE:HD1	8:H:130:ARG:HG3	1.78	0.49
2:B:766:ARG:HH22	2:B:1020:ARG:HH21	1.61	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
5:E:26:ARG:NH1	5:E:133:GLU:OE2	2.43	0.49
1:A:316:GLN:HG3	1:A:317:LYS:H	1.78	0.48
6:F:138:LEU:O	6:F:140:ASP:N	2.46	0.48
8:H:110:ASP:N	8:H:110:ASP:OD1	2.46	0.48
2:B:345:LYS:HG3	2:B:346:GLU:H	1.78	0.48
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.94	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.78	0.48
2:B:865:LYS:HE3	2:B:961:LEU:HD22	1.94	0.48
10:J:54:VAL:HG12	10:J:56:LEU:HG	1.95	0.48
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.48	0.48
5:E:78:LEU:HD13	5:E:107:THR:HG22	1.95	0.48
8:H:6:PHE:CD1	8:H:130:ARG:HG3	2.48	0.48
13:T:12:DT:C2	14:N:6:DG:N2	2.82	0.48
1:A:648:ASN:O	1:A:652:VAL:HG23	2.13	0.48
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.95	0.48
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.96	0.48
12:L:31:CYS:SG	12:L:48:CYS:CB	2.94	0.48
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.54	0.48
1:A:709:THR:HG22	1:A:711:ARG:H	1.78	0.48
2:B:503:GLY:O	2:B:506:GLY:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:LEU:HD12	2:B:693:ILE:HG13	1.96	0.48
3:C:92:CYS:SG	3:C:94:LYS:HG3	2.53	0.48
2:B:91:SER:HB3	2:B:133:LYS:HB2	1.96	0.48
2:B:745:PRO:O	2:B:748:ILE:HG12	2.14	0.48
2:B:94:LYS:HD3	2:B:96:TYR:HE1	1.78	0.48
8:H:145:ARG:HG2	8:H:146:ARG:H	1.79	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.14	0.48
2:B:98:THR:HG23	2:B:126:SER:HB2	1.95	0.48
8:H:132:LEU:HD12	8:H:132:LEU:H	1.78	0.48
9:I:15:TYR:CD2	9:I:30:ARG:HD2	2.49	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.78	0.47
1:A:679:ILE:O	1:A:683:ILE:HG13	2.14	0.47
1:A:59:GLY:HA2	1:A:67:CYS:HA	1.96	0.47
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.48	0.47
1:A:61:ILE:HG22	1:A:257:ARG:HH22	1.79	0.47
2:B:616:ILE:HB	2:B:697:GLU:HA	1.96	0.47
2:B:884:ARG:HG2	2:B:935:ARG:HD2	1.96	0.47
4:D:130:LEU:O	4:D:134:THR:HG22	2.13	0.47
8:H:4:THR:HG22	8:H:6:PHE:H	1.79	0.47
2:B:308:TRP:CH2	9:I:45:ARG:HD3	2.49	0.47
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.95	0.47
1:A:49:LYS:NZ	1:A:61:ILE:H	2.11	0.47
1:A:666:ILE:O	1:A:669:THR:OG1	2.30	0.47
1:A:689:LYS:O	1:A:693:VAL:HG23	2.14	0.47
2:B:232:SER:H	2:B:261:ARG:NH2	2.06	0.47
2:B:272:THR:HG22	2:B:279:ASP:OD1	2.14	0.47
2:B:711:GLU:N	2:B:711:GLU:OE1	2.41	0.47
2:B:872:GLU:OE1	2:B:914:LYS:NZ	2.29	0.47
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.44	0.47
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.96	0.47
1:A:512:VAL:HA	1:A:519:PRO:HA	1.95	0.47
1:A:335:ARG:NH2	2:B:1206:GLU:OE2	2.40	0.47
2:B:211:VAL:O	2:B:480:SER:HA	2.13	0.47
2:B:542:MET:HG3	2:B:747:MET:HB3	1.97	0.47
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.95	0.47
7:G:153:GLN:N	7:G:153:GLN:OE1	2.48	0.47
8:H:26:ILE:HG12	8:H:42:ILE:HD12	1.95	0.47
11:K:21:ILE:HG12	11:K:33:ILE:HG23	1.96	0.47
13:T:21:DC:H2'	13:T:22:BRU:H6	1.95	0.47
13:T:27:DA:H61	15:P:2:C:H42	1.62	0.47
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1163:ILE:HG23	1:A:1166:ASP:HB2	1.96	0.47
1:A:33:ALA:HB2	1:A:56:PRO:O	2.14	0.47
1:A:80:HIS:O	1:A:243:PRO:HB3	2.14	0.47
1:A:711:ARG:NE	9:I:95:THR:O	2.47	0.47
2:B:1056:SER:OG	2:B:1066:SER:O	2.26	0.47
1:A:115:LEU:HB2	1:A:142:CYS:SG	2.55	0.47
1:A:591:PHE:HB3	1:A:595:THR:OG1	2.15	0.47
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.44	0.47
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.96	0.47
2:B:361:LEU:N	2:B:362:PRO:HD3	2.30	0.47
5:E:17:ARG:O	5:E:21:GLU:HG3	2.14	0.47
1:A:567:LYS:HD3	8:H:96:VAL:N	2.29	0.47
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.79	0.47
2:B:276:ILE:HD11	2:B:336:ARG:O	2.15	0.47
2:B:617:ARG:HG3	2:B:624:LEU:HD13	1.97	0.47
1:A:672:ASP:OD1	3:C:195:GLN:NE2	2.47	0.47
2:B:642:ASP:OD2	2:B:650:GLU:N	2.48	0.47
2:B:52:ASN:OD1	2:B:177:LYS:HB3	2.15	0.47
2:B:46:GLN:HG3	2:B:545:ILE:HD12	1.96	0.47
1:A:1206:ASP:O	1:A:1208:THR:HG23	2.14	0.46
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.97	0.46
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.51	0.46
2:B:879:ARG:HD3	2:B:880:THR:H	1.80	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.97	0.46
7:G:56:ILE:O	7:G:56:ILE:HG13	2.15	0.46
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.97	0.46
1:A:1276:VAL:HB	1:A:1279:ILE:HG13	1.97	0.46
1:A:885:THR:O	1:A:940:ARG:HG3	2.15	0.46
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.97	0.46
1:A:42:ASP:O	1:A:43:GLU:HG2	2.14	0.46
1:A:527:THR:HG23	1:A:653:VAL:HB	1.96	0.46
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.98	0.46
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.98	0.46
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.97	0.46
1:A:857:ARG:HD3	1:A:861:GLY:O	2.15	0.46
2:B:382:ILE:O	2:B:386:LEU:HG	2.16	0.46
4:D:197:SER:O	4:D:201:LYS:HD2	2.13	0.46
5:E:98:ILE:O	5:E:102:GLU:HB2	2.15	0.46
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.97	0.46
1:A:549:MET:CE	1:A:656:TRP:HD1	2.28	0.46
2:B:232:SER:N	2:B:261:ARG:HH22	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:63:VAL:HG23	11:K:63:VAL:O	2.15	0.46
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.97	0.46
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.36	0.46
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.34	0.46
12:L:33:GLU:HB2	12:L:53:HIS:ND1	2.30	0.46
1:A:901:LEU:O	1:A:920:LEU:HD12	2.16	0.46
2:B:580:VAL:O	2:B:586:TRP:HD1	1.99	0.46
7:G:106:MET:HG3	7:G:157:ILE:O	2.16	0.46
2:B:766:ARG:NH2	2:B:1020:ARG:HE	2.13	0.46
4:D:38:ILE:HD13	4:D:44:GLU:HA	1.98	0.46
1:A:1115:SER:H	1:A:1330:ASN:HD21	1.63	0.46
1:A:1422:ARG:HD3	2:B:1224:PHE:CE2	2.51	0.46
1:A:595:THR:CG2	1:A:603:ASN:HB3	2.46	0.46
2:B:878:GLN:HA	2:B:885:MET:HE1	1.98	0.46
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.98	0.46
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.97	0.46
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.81	0.46
1:A:1325:THR:O	5:E:148:GLU:HG3	2.16	0.46
1:A:34:LYS:HA	1:A:83:HIS:CE1	2.51	0.45
1:A:35:ILE:HA	1:A:52:GLY:O	2.15	0.45
1:A:856:THR:HB	1:A:865:GLN:HB2	1.98	0.45
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.19	0.45
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.51	0.45
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.16	0.45
1:A:130:ASP:OD1	1:A:131:SER:N	2.50	0.45
1:A:960:ILE:O	1:A:963:ILE:HG22	2.16	0.45
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.80	0.45
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.97	0.45
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.47	0.45
2:B:91:SER:H	2:B:133:LYS:HB3	1.80	0.45
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.97	0.45
2:B:916:THR:HA	2:B:917:PRO:HD3	1.83	0.45
12:L:49:LYS:HD2	12:L:50:ASP:N	2.31	0.45
1:A:976:THR:OG1	1:A:977:LYS:N	2.49	0.45
5:E:96:PHE:O	5:E:100:ILE:HG12	2.16	0.45
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.31	0.45
2:B:766:ARG:CZ	2:B:1020:ARG:HE	2.30	0.45
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.98	0.45
2:B:429:PHE:HA	2:B:432:MET:HE2	1.99	0.45
2:B:962:LYS:HB2	2:B:962:LYS:HE3	1.79	0.45
5:E:4:GLU:CG	5:E:5:ASN:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:O	1:A:221:SER:OG	2.23	0.45
5:E:55:ARG:HB2	5:E:84:ASP:OD1	2.17	0.45
13:T:23:DC:H2'	13:T:24:DC:C6	2.52	0.45
1:A:153:PRO:HA	1:A:161:LEU:HB3	1.99	0.45
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.99	0.45
2:B:1004:GLU:O	2:B:1006:ILE:N	2.49	0.45
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.98	0.45
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.97	0.45
2:B:94:LYS:HD3	2:B:96:TYR:CE1	2.52	0.45
5:E:128:PRO:HA	5:E:130:ALA:N	2.29	0.45
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.17	0.45
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.97	0.45
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.37	0.45
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.56	0.45
5:E:4:GLU:HA	5:E:7:ARG:HE	1.82	0.45
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.64	0.45
1:A:447:GLN:OE1	13:T:20:DC:H4'	2.17	0.45
3:C:148:ARG:HG2	3:C:149:LYS:H	1.81	0.45
8:H:13:SER:HB3	8:H:27:GLU:HB2	1.99	0.45
8:H:77:ARG:HA	8:H:77:ARG:HD3	1.64	0.45
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.16	0.45
1:A:50:ILE:C	1:A:52:GLY:H	2.20	0.44
1:A:650:GLN:O	1:A:654:ASN:HB2	2.16	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.48	0.44
1:A:50:ILE:HG23	1:A:52:GLY:N	2.32	0.44
1:A:534:LEU:O	1:A:574:GLY:HA3	2.16	0.44
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.81	0.44
2:B:640:VAL:HG23	2:B:640:VAL:O	2.17	0.44
5:E:65:THR:O	5:E:69:ILE:HG13	2.18	0.44
1:A:1205:LYS:HE3	1:A:1205:LYS:HB3	1.51	0.44
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.64	0.44
1:A:913:LEU:HD12	1:A:915:SER:N	2.32	0.44
2:B:46:GLN:N	2:B:46:GLN:OE1	2.42	0.44
5:E:39:LEU:HD12	5:E:40:GLU:HG2	2.00	0.44
5:E:39:LEU:HD12	5:E:40:GLU:N	2.31	0.44
8:H:15:VAL:HG12	8:H:26:ILE:CG2	2.46	0.44
11:K:12:LEU:HA	11:K:12:LEU:HD23	1.77	0.44
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.50	0.44
1:A:1140:HIS:O	1:A:1141:THR:HG23	2.17	0.44
1:A:629:LEU:O	1:A:633:VAL:HG23	2.18	0.44
6:F:132:LEU:O	6:F:148:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:127:PRO:HG2	7:G:139:ILE:HG21	1.99	0.44
10:J:37:SER:OG	10:J:47:ARG:NH2	2.50	0.44
1:A:121:LEU:HA	1:A:124:GLN:HG2	2.00	0.44
1:A:55:ASP:HB2	1:A:59:GLY:O	2.17	0.44
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.44
2:B:580:VAL:HG22	2:B:624:LEU:HD23	1.99	0.44
1:A:1081:LEU:CB	1:A:1082:ASN:HA	2.35	0.44
1:A:1207:LEU:CD1	1:A:1208:THR:H	2.31	0.44
1:A:224:PHE:HE2	1:A:231:PRO:HB3	1.81	0.44
1:A:64:ASN:OD1	1:A:64:ASN:N	2.49	0.44
1:A:984:LYS:O	1:A:988:LEU:HB2	2.18	0.44
2:B:242:SER:OG	2:B:252:SER:O	2.34	0.44
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.99	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HB2	2.00	0.44
4:D:118:THR:N	4:D:121:LYS:HB2	2.33	0.44
5:E:46:TYR:O	5:E:53:PRO:HA	2.18	0.44
1:A:1164:PRO:HA	1:A:1167:GLU:HG2	2.00	0.44
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.48	0.44
1:A:464:PRO:HG2	1:A:465:TYR:CD2	2.53	0.44
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.99	0.44
1:A:54:ASN:C	1:A:56:PRO:HD3	2.38	0.44
1:A:62:ASP:HB3	1:A:64:ASN:OD1	2.18	0.44
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.81	0.44
4:D:185:CYS:O	4:D:211:LEU:HD22	2.18	0.44
1:A:1339:LEU:HD13	5:E:147:HIS:HD2	1.81	0.44
11:K:60:ALA:O	11:K:73:LEU:HD12	2.17	0.44
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.38	0.44
2:B:634:TYR:CD2	2:B:692:TYR:HB3	2.53	0.44
2:B:68:THR:HA	2:B:90:ILE:O	2.18	0.44
3:C:20:PHE:HE1	3:C:232:VAL:HG23	1.82	0.44
4:D:72:ARG:HD3	4:D:72:ARG:HA	1.79	0.44
13:T:16:DT:H2"	13:T:17:DG:N7	2.32	0.44
1:A:34:LYS:HG2	1:A:36:ARG:NE	2.32	0.43
2:B:1106:ARG:HG2	2:B:1107:ALA:O	2.18	0.43
6:F:83:PRO:HA	6:F:146:TRP:CZ3	2.53	0.43
2:B:1076:HIS:ND1	11:K:40:HIS:CE1	2.86	0.43
2:B:295:GLY:O	2:B:299:GLU:HB2	2.18	0.43
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.53	0.43
2:B:582:VAL:HA	2:B:626:ILE:HG13	1.99	0.43
13:T:18:4DU:H8	13:T:19:DC:C6	2.52	0.43
1:A:219:PHE:HA	1:A:222:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LYS:HB2	2:B:422:LYS:HE3	1.76	0.43
2:B:510:LYS:HA	2:B:513:GLN:OE1	2.18	0.43
3:C:220:ASP:OD1	3:C:222:LYS:HE2	2.18	0.43
5:E:85:GLU:H	5:E:85:GLU:HG2	1.58	0.43
11:K:61:TYR:HA	11:K:72:LYS:O	2.18	0.43
12:L:65:VAL:HG23	12:L:67:PHE:CE1	2.53	0.43
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.69	0.43
5:E:31:THR:OG1	5:E:32:GLN:N	2.51	0.43
2:B:620:ARG:NE	9:I:89:GLN:OE1	2.46	0.43
2:B:640:VAL:HG12	2:B:651:LEU:HG	2.01	0.43
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.00	0.43
3:C:136:ASP:HB2	3:C:139:GLY:H	1.82	0.43
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.38	0.43
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.48	0.43
5:E:26:ARG:HH12	5:E:133:GLU:CD	2.22	0.43
3:C:165:LYS:O	11:K:6:ARG:NH1	2.52	0.43
1:A:25:GLU:N	1:A:25:GLU:OE1	2.44	0.43
1:A:924:LYS:HB2	1:A:924:LYS:HE2	1.78	0.43
2:B:216:GLU:OE1	2:B:537:LYS:HE3	2.18	0.43
8:H:96:VAL:HA	8:H:142:LEU:O	2.18	0.43
1:A:1220:PHE:CD2	1:A:1224:LEU:HD23	2.53	0.43
2:B:890:TYR:CE1	2:B:910:VAL:HG21	2.54	0.43
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.53	0.43
1:A:1074:GLU:O	1:A:1077:THR:HB	2.18	0.43
1:A:567:LYS:HD3	8:H:95:TYR:CA	2.47	0.43
1:A:745:GLN:HA	1:A:748:MET:HE2	2.00	0.43
8:H:62:SER:C	8:H:63:LEU:HD12	2.39	0.43
9:I:75:CYS:O	9:I:79:HIS:HA	2.19	0.43
2:B:218:SER:HA	2:B:404:LYS:HD3	2.01	0.43
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.01	0.43
2:B:299:GLU:OE2	2:B:572:HIS:HB3	2.19	0.42
2:B:766:ARG:HG3	2:B:1022:THR:HG22	2.00	0.42
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.01	0.42
10:J:7:CYS:HA	10:J:49:MET:HE3	2.00	0.42
12:L:40:LEU:HD12	12:L:40:LEU:HA	1.86	0.42
14:N:2:DA:C6	14:N:3:DG:C6	3.07	0.42
1:A:1215:ARG:NE	1:A:1272:THR:O	2.43	0.42
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.18	0.42
1:A:873:MET:C	1:A:1058:VAL:HG13	2.40	0.42
2:B:133:LYS:O	2:B:134:LYS:HG2	2.18	0.42
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.02	0.42
3:C:6:PRO:HB3	3:C:25:VAL:HB	2.02	0.42
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.49	0.42
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.54	0.42
3:C:40:GLU:HA	3:C:163:ILE:CG2	2.49	0.42
6:F:70:LYS:HA	6:F:70:LYS:HD3	1.83	0.42
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.42
14:N:1:DA:HO5'	14:N:1:DA:H8	1.66	0.42
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.01	0.42
1:A:726:ARG:HD3	1:A:766:GLY:HA3	2.01	0.42
2:B:244:LEU:HD12	2:B:244:LEU:H	1.83	0.42
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.49	0.42
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.85	0.42
1:A:567:LYS:HD3	8:H:96:VAL:H	1.84	0.42
2:B:986:GLN:NE2	2:B:1016:ALA:O	2.46	0.42
2:B:170:LEU:HD12	2:B:171:PRO:HD2	2.00	0.42
4:D:194:LEU:HB3	7:G:86:VAL:HG21	2.00	0.42
8:H:113:ALA:HA	8:H:125:LEU:O	2.19	0.42
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.20	0.42
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.45	0.42
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.19	0.42
2:B:457:LEU:HA	2:B:457:LEU:HD23	1.88	0.42
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.01	0.42
2:B:832:GLY:O	2:B:835:GLN:NE2	2.42	0.42
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.42
5:E:79:TRP:HB2	5:E:105:PHE:CE2	2.54	0.42
6:F:70:LYS:H	6:F:72:LYS:HG3	1.84	0.42
13:T:14:DC:H2'	13:T:15:DT:C6	2.54	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.59	0.42
13:T:27:DA:H61	15:P:2:C:N4	2.17	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.02	0.42
1:A:545:GLN:HG2	1:A:549:MET:HE3	2.02	0.42
1:A:618:GLU:OE2	1:A:620:LYS:HB2	2.19	0.42
2:B:418:LYS:HE3	2:B:422:LYS:HZ1	1.84	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.83	0.42
1:A:306:ASN:O	1:A:313:GLN:HG2	2.20	0.42
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.02	0.42
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.35	0.42
5:E:180:ARG:HB2	5:E:215:MET:HG3	2.01	0.42
8:H:98:TYR:CD1	8:H:141:TYR:CE1	3.08	0.42
1:A:677:ARG:NH1	1:A:681:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:HG3	2:B:1021:MET:HG2	2.00	0.42
1:A:998:LEU:HD23	1:A:1001:ARG:HG2	2.01	0.42
2:B:654:ARG:O	2:B:657:HIS:HB2	2.20	0.42
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.83	0.42
2:B:848:ARG:NH1	10:J:8:PHE:O	2.53	0.42
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.35	0.41
1:A:365:GLY:O	1:A:468:PHE:HA	2.20	0.41
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.54	0.41
1:A:956:LEU:HA	1:A:956:LEU:HD23	1.89	0.41
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.34	0.41
2:B:880:THR:HB	2:B:933:SER:HA	2.02	0.41
2:B:884:ARG:O	2:B:884:ARG:HG3	2.20	0.41
2:B:955:THR:HG23	12:L:54:ARG:O	2.20	0.41
4:D:7:THR:OG1	4:D:8:PHE:N	2.42	0.41
7:G:5:LYS:HA	7:G:5:LYS:HD2	1.81	0.41
1:A:800:VAL:HG13	1:A:812:GLU:HB3	2.02	0.41
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.02	0.41
2:B:1162:ILE:HD13	2:B:1194:ILE:HD13	2.02	0.41
2:B:955:THR:HG22	2:B:956:THR:N	2.35	0.41
3:C:88:CYS:CB	3:C:92:CYS:HB2	2.15	0.41
1:A:535:THR:HG21	1:A:617:VAL:N	2.35	0.41
1:A:710:LEU:HD12	1:A:710:LEU:HA	1.92	0.41
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	2.02	0.41
1:A:928:LEU:HA	1:A:928:LEU:HD23	1.96	0.41
2:B:383:ASN:O	2:B:387:LEU:HD13	2.20	0.41
8:H:63:LEU:HD11	8:H:141:TYR:CE2	2.55	0.41
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.20	0.41
1:A:399:HIS:O	1:A:401:GLY:N	2.54	0.41
2:B:121:ASN:HA	2:B:207:GLY:CA	2.50	0.41
2:B:273:LEU:HA	2:B:274:PRO:HD3	1.97	0.41
2:B:356:LEU:HA	2:B:356:LEU:HD23	1.74	0.41
2:B:521:LEU:HA	2:B:543:SER:OG	2.20	0.41
9:I:52:ILE:HG13	9:I:52:ILE:O	2.20	0.41
10:J:22:LEU:HD12	10:J:22:LEU:HA	1.56	0.41
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.21	0.41
1:A:1354:ASN:O	1:A:1358:SER:HB3	2.20	0.41
1:A:913:LEU:HD12	1:A:915:SER:H	1.85	0.41
2:B:534:GLY:O	2:B:537:LYS:NZ	2.36	0.41
2:B:685:LEU:HD12	2:B:685:LEU:HA	1.84	0.41
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.20	0.41
12:L:48:CYS:SG	12:L:48:CYS:O	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:ALA:O	2:B:513:GLN:NE2	2.53	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.56	0.41
9:I:72:ASP:N	9:I:72:ASP:OD1	2.54	0.41
11:K:21:ILE:HG22	11:K:31:VAL:HG21	2.03	0.41
8:H:93:TYR:HB3	8:H:144:ILE:O	2.21	0.41
9:I:27:PHE:O	9:I:35:VAL:HA	2.20	0.41
2:B:805:THR:HG21	2:B:1041:GLU:OE1	2.20	0.41
2:B:512:ARG:HH11	2:B:512:ARG:HD3	1.76	0.41
1:A:709:THR:HG23	9:I:94:ASP:HA	2.02	0.41
2:B:1077:THR:HG22	11:K:44:ASN:OD1	2.20	0.41
1:A:455:MET:HE3	1:A:455:MET:HB3	1.93	0.41
1:A:670:ILE:HA	1:A:670:ILE:HD13	1.91	0.41
2:B:845:SER:OG	2:B:1009:ASP:OD1	2.31	0.41
2:B:424:LEU:HA	2:B:427:ASP:HB2	2.03	0.41
2:B:651:LEU:HD23	2:B:652:LYS:H	1.86	0.41
2:B:706:GLN:O	2:B:710:LEU:HD22	2.20	0.41
6:F:70:LYS:C	6:F:72:LYS:H	2.24	0.41
11:K:107:THR:O	11:K:111:LEU:HD13	2.20	0.41
1:A:1155:ASP:HB3	1:A:1241:ARG:NH2	2.36	0.41
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.54	0.41
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.89	0.41
1:A:1168:GLU:C	1:A:1169:ILE:HG13	2.40	0.41
1:A:1313:LEU:HG	1:A:1317:MET:HE3	2.03	0.41
1:A:601:LYS:HA	1:A:601:LYS:HD3	1.88	0.41
6:F:140:ASP:OD1	6:F:140:ASP:N	2.53	0.41
6:F:154:ASP:O	6:F:155:LEU:HD12	2.20	0.41
8:H:37:LYS:HG3	8:H:38:LEU:N	2.35	0.41
8:H:56:THR:HG21	8:H:145:ARG:NH1	2.36	0.41
3:C:114:TYR:OH	10:J:19:GLU:OE2	2.35	0.41
1:A:1168:GLU:O	1:A:1169:ILE:HG13	2.21	0.40
1:A:147:VAL:HG13	1:A:149:GLU:HG2	2.02	0.40
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.56	0.40
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.56	0.40
2:B:95:ILE:HG13	2:B:129:PHE:O	2.21	0.40
2:B:203:PHE:O	2:B:209:GLU:HA	2.21	0.40
2:B:43:LEU:HD23	2:B:43:LEU:HA	1.86	0.40
5:E:10:SER:O	5:E:14:ARG:HG3	2.21	0.40
7:G:112:LYS:HA	7:G:115:MET:HE3	2.03	0.40
8:H:97:MET:HE3	8:H:118:PHE:CG	2.56	0.40
9:I:68:LEU:HD23	9:I:68:LEU:HA	1.87	0.40
2:B:1150:ARG:HA	2:B:1150:ARG:HD3	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:601:ARG:O	2:B:605:ARG:HG3	2.21	0.40
3:C:259:LEU:HD23	3:C:259:LEU:HA	1.90	0.40
13:T:15:DT:C6	13:T:16:DT:H72	2.56	0.40
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.21	0.40
4:D:20:GLU:CD	4:D:20:GLU:H	2.24	0.40
1:A:896:ARG:O	1:A:1029:ARG:HD2	2.21	0.40
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.21	0.40
1:A:332:LYS:HB3	1:A:332:LYS:HE2	1.90	0.40
1:A:990:VAL:O	1:A:994:GLN:HG3	2.22	0.40
2:B:210:LYS:HE2	2:B:462:ALA:HA	2.02	0.40
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.56	0.40
3:C:17:ASN:HA	3:C:232:VAL:O	2.21	0.40
3:C:34:ARG:HA	3:C:37:MET:HE3	2.03	0.40
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.03	0.40
8:H:11:GLN:HG2	8:H:52:GLN:HA	2.03	0.40
8:H:38:LEU:HD12	8:H:124:ARG:O	2.22	0.40
1:A:628:GLY:O	1:A:632:VAL:HG23	2.20	0.40
2:B:454:THR:HG22	2:B:458:LYS:HE3	2.02	0.40
2:B:638:PHE:HB2	2:B:741:CYS:HB3	2.02	0.40
2:B:794:ASN:C	2:B:795:ILE:HD12	2.42	0.40
2:B:893:LEU:HA	2:B:893:LEU:HD23	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:NZ	3:C:83:SER:O[4_555]	2.14	0.06

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1402/1733 (81%)	1302 (93%)	89 (6%)	11 (1%)	19 58
2	B	1084/1224 (89%)	990 (91%)	80 (7%)	14 (1%)	12 47
3	C	263/318 (83%)	244 (93%)	19 (7%)	0	100 100
4	D	171/221 (77%)	156 (91%)	13 (8%)	2 (1%)	13 49
5	E	210/215 (98%)	199 (95%)	11 (5%)	0	100 100
6	F	85/155 (55%)	77 (91%)	6 (7%)	2 (2%)	6 34
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	25 64
8	H	130/146 (89%)	113 (87%)	15 (12%)	2 (2%)	10 44
9	I	112/122 (92%)	99 (88%)	12 (11%)	1 (1%)	17 56
10	J	63/70 (90%)	57 (90%)	6 (10%)	0	100 100
11	K	112/120 (93%)	109 (97%)	3 (3%)	0	100 100
12	L	42/70 (60%)	36 (86%)	6 (14%)	0	100 100
All	All	3843/4565 (84%)	3538 (92%)	272 (7%)	33 (1%)	17 56

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	567	LYS
2	B	502	ILE
2	B	507	LYS
1	A	68	GLN
2	B	501	PRO
2	B	503	GLY
2	B	648	HIS
2	B	262	GLU
2	B	465	ASN
2	B	705	MET
2	B	1005	GLY
4	D	17	LYS
4	D	199	ASN
1	A	465	TYR
1	A	593	GLU
2	B	63	ILE
2	B	508	LEU
2	B	1017	ILE
6	F	139	PRO
6	F	154	ASP
7	G	63	PRO

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Mol	Chain	Res	Type
1	A	35	ILE
2	B	917	PRO
8	H	79	TRP
1	A	56	PRO
2	B	510	LYS
1	A	147	VAL
1	A	566	ILE
1	A	1097	GLY
1	A	1107	VAL
9	I	62	ILE
8	H	17	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1234/1520 (81%)	1214 (98%)	20 (2%)	62 84
2	B	956/1061 (90%)	943 (99%)	13 (1%)	67 86
3	C	233/274 (85%)	229 (98%)	4 (2%)	60 83
4	D	155/200 (78%)	153 (99%)	2 (1%)	69 87
5	E	194/197 (98%)	193 (100%)	1 (0%)	88 95
6	F	77/137 (56%)	77 (100%)	0	100 100
7	G	152/152 (100%)	151 (99%)	1 (1%)	84 94
8	H	118/128 (92%)	114 (97%)	4 (3%)	37 70
9	I	108/116 (93%)	104 (96%)	4 (4%)	34 68
10	J	60/65 (92%)	58 (97%)	2 (3%)	38 71
11	K	99/102 (97%)	96 (97%)	3 (3%)	41 73
12	L	39/57 (68%)	34 (87%)	5 (13%)	4 20
All	All	3425/4009 (85%)	3366 (98%)	59 (2%)	60 83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	67	CYS
1	A	98	LYS
1	A	107	CYS
1	A	116	ASP
1	A	143	LYS
1	A	161	LEU
1	A	517	ASN
1	A	542	GLU
1	A	567	LYS
1	A	676	MET
1	A	738	LYS
1	A	764	CYS
1	A	821	ARG
1	A	906	HIS
1	A	1120	LEU
1	A	1171	GLN
1	A	1215	ARG
1	A	1285	MET
1	A	1393	ASN
2	B	228	LYS
2	B	306	ASN
2	B	354	ASP
2	B	476	ARG
2	B	507	LYS
2	B	510	LYS
2	B	537	LYS
2	B	615	MET
2	B	904	ARG
2	B	1087	PHE
2	B	1092	TYR
2	B	1096	ARG
2	B	1177	HIS
3	C	12	GLU
3	C	26	ASP
3	C	34	ARG
3	C	136	ASP
4	D	72	ARG
4	D	74	GLN
5	E	83	CYS
7	G	94	CYS
8	H	52	GLN
8	H	106	GLU

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Mol	Chain	Res	Type
8	H	110	ASP
8	H	131	ASN
9	I	8	ARG
9	I	29	CYS
9	I	44	TYR
9	I	94	ASP
10	J	28	ASP
10	J	46	CYS
11	K	1	MET
11	K	44	ASN
11	K	70	ARG
12	L	27	LEU
12	L	33	GLU
12	L	38	LEU
12	L	49	LYS
12	L	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	253	ASN
1	A	736	ASN
2	B	843	GLN
7	G	97	HIS
9	I	83	ASN
11	K	96	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/11 (81%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	3	G

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
13	BRU	T	22	13,15	15,21,22	5.03	10 (66%)	17,30,33	2.00	3 (17%)
13	4DU	T	18	18,13	18,23,24	1.77	7 (38%)	21,33,36	2.46	4 (19%)

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	BRU	T	22	13,15	-	0/4/21/22	0/2/2/2
13	4DU	T	18	18,13	-	2/3/21/22	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	22	BRU	C4-N3	8.27	1.47	1.33
13	T	22	BRU	C4-C5	7.38	1.47	1.38
13	T	22	BRU	O4'-C1'	7.32	1.58	1.42
13	T	22	BRU	C2'-C3'	-7.15	1.34	1.52
13	T	22	BRU	O4'-C4'	-6.87	1.29	1.45
13	T	22	BRU	C2-N3	5.54	1.49	1.38
13	T	22	BRU	C1'-N1	-5.02	1.34	1.49
13	T	22	BRU	C6-C5	4.67	1.48	1.39
13	T	22	BRU	C3'-C4'	3.40	1.62	1.53
13	T	22	BRU	O4-C4	-3.28	1.16	1.24
13	T	18	4DU	C3-C2	3.25	1.41	1.36
13	T	18	4DU	C4-C5	2.98	1.46	1.40
13	T	18	4DU	C6-N6	2.70	1.43	1.34
13	T	18	4DU	C8-N7	2.59	1.39	1.34
13	T	18	4DU	C2-N1	2.43	1.39	1.34
13	T	18	4DU	O5'-C5'	-2.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	18	4DU	C5-N7	2.22	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	T	18	4DU	C2-C3-C4	-9.05	111.58	119.31
13	T	22	BRU	C4-N3-C2	6.33	120.48	115.14
13	T	18	4DU	C5-C6-N6	3.73	126.01	120.35
13	T	18	4DU	C3-C2-N1	3.25	127.01	123.81
13	T	22	BRU	C5-C4-N3	-2.71	120.39	123.64
13	T	18	4DU	C2-N1-C6	2.49	121.26	117.61
13	T	22	BRU	BR-C5-C6	2.34	122.63	117.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	18	4DU	C3'-C4'-C5'-O5'
13	T	18	4DU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	22	BRU	1	0
13	T	18	4DU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
18	AHW	T	101	13	15,15,15	1.86	6 (40%)	20,20,20	0.75	1 (5%)

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
18	AHW	T	101	13	-	2/4/4/4	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	101	AHW	C14-C13	2.74	1.48	1.42
18	T	101	AHW	C20-C17	2.48	1.41	1.36
18	T	101	AHW	C13-C12	-2.31	1.37	1.42
18	T	101	AHW	C15-C13	2.27	1.47	1.42
18	T	101	AHW	C11-C10	2.26	1.41	1.36
18	T	101	AHW	C17-C16	2.11	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	101	AHW	C17-C16-C15	-2.00	118.11	120.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	T	101	AHW	C17-C16-O21-C22
18	T	101	AHW	C15-C16-O21-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	101	AHW	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1412/1733 (81%)	-0.10	7 (0%) 91 86	79, 121, 194, 258	0
2	B	1104/1224 (90%)	0.03	21 (1%) 66 53	81, 134, 209, 272	0
3	C	265/318 (83%)	-0.22	0 100 100	91, 124, 162, 219	0
4	D	175/221 (79%)	-0.15	1 (0%) 89 83	101, 135, 197, 249	0
5	E	212/215 (98%)	-0.02	3 (1%) 75 63	100, 156, 215, 235	0
6	F	87/155 (56%)	-0.31	1 (1%) 80 69	81, 100, 142, 173	0
7	G	171/171 (100%)	-0.11	0 100 100	99, 120, 162, 184	0
8	H	134/146 (91%)	0.35	7 (5%) 27 15	130, 174, 226, 245	0
9	I	114/122 (93%)	-0.14	0 100 100	123, 164, 220, 276	0
10	J	65/70 (92%)	-0.21	0 100 100	102, 127, 175, 199	0
11	K	114/120 (95%)	-0.22	1 (0%) 84 75	87, 125, 168, 190	0
12	L	44/70 (62%)	-0.06	1 (2%) 60 47	106, 156, 213, 311	0
13	T	17/26 (65%)	-0.16	0 100 100	119, 170, 287, 305	0
14	N	7/14 (50%)	0.94	1 (14%) 2 1	254, 258, 314, 338	0
15	P	10/11 (90%)	-0.39	0 100 100	112, 136, 200, 205	0
All	All	3931/4616 (85%)	-0.06	43 (1%) 80 69	79, 129, 204, 338	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	139	ASN	5.1
2	B	715	ALA	4.9
2	B	712	PRO	4.0
2	B	918	ILE	3.7
2	B	868	MET	3.3
1	A	255	SER	3.3
2	B	643	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	865	LYS	3.2
4	D	18	VAL	3.1
2	B	714	GLU	3.0
2	B	709	ASP	3.0
14	N	7	DT	3.0
2	B	864	LYS	3.0
8	H	140	ALA	3.0
5	E	110	PHE	2.9
1	A	165	GLY	2.6
5	E	83	CYS	2.5
2	B	866	TYR	2.5
2	B	870	ILE	2.4
2	B	831	SER	2.4
2	B	132	VAL	2.4
2	B	869	SER	2.4
1	A	155	GLU	2.4
2	B	475	SER	2.3
12	L	27	LEU	2.3
2	B	92	PHE	2.3
8	H	134	ASN	2.3
2	B	130	VAL	2.3
2	B	708	GLU	2.2
11	K	114	LEU	2.2
8	H	123	MET	2.2
1	A	660	ASN	2.2
8	H	113	ALA	2.2
1	A	163	SER	2.2
2	B	473	MET	2.1
1	A	156	ASP	2.1
6	F	108	PHE	2.1
2	B	722	ASP	2.1
2	B	504	ARG	2.0
5	E	93	MET	2.0
8	H	54	SER	2.0
8	H	83	GLN	2.0
1	A	199	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	4DU	T	18	21/22	0.94	0.17	124,132,154,195	0
13	BRU	T	22	20/21	0.97	0.15	112,119,157,249	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	AHW	T	101	14/14	0.84	0.43	124,149,195,201	0
16	ZN	A	1801	1/1	0.95	0.07	204,204,204,204	0
16	ZN	A	1802	1/1	0.97	0.17	255,255,255,255	0
16	ZN	L	101	1/1	0.97	0.19	553,553,553,553	0
16	ZN	J	101	1/1	0.97	0.22	138,138,138,138	0
16	ZN	B	1301	1/1	0.98	0.18	111,111,111,111	0
16	ZN	C	401	1/1	0.98	0.10	106,106,106,106	0
17	MG	A	1803	1/1	0.98	0.14	97,97,97,97	0
16	ZN	I	201	1/1	0.99	0.10	147,147,147,147	0
16	ZN	I	202	1/1	0.99	0.07	284,284,284,284	0

6.5 Other polymers (i)

There are no such residues in this entry.