



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:51 PM UTC

PDB ID : 8WB0 / pdb_00008wb0
EMDB ID : EMD-37411
Title : De novo transcribing complex 17 (TC17), the early elongation complex with Pol II positioned 17nt downstream of TSS
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-08
Resolution : 2.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

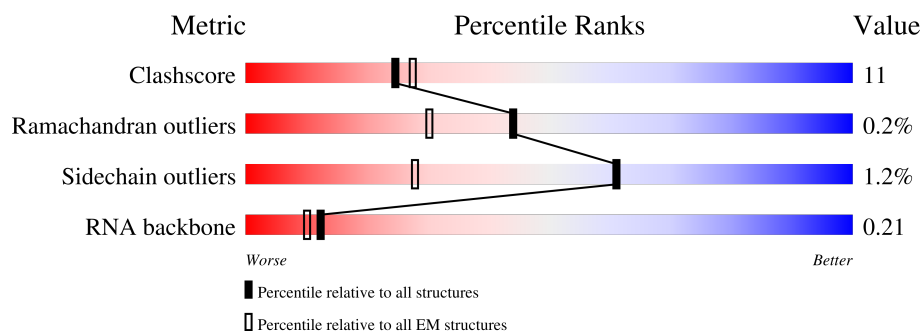
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	N	8	38% 38% 25%
2	S	517	22% 5% 73%
3	T	249	35% 6% 59%
4	X	99	15% 28% 57%
5	Y	99	30% 24% 45%
6	Z	13	31% 46% 15% 8%
7	o	1970	55% 18% . 26%

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Mol	Chain	Length	Quality of chain
8	p	1174	
9	q	275	
10	r	142	
11	s	210	
12	t	127	
13	u	172	
14	v	150	
15	w	125	
16	x	67	
17	y	117	
18	z	58	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 35758 atoms, of which 30 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 Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	8	Total	C	H	N	O	S	
			94	39	30	10	14	1	
								0	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	138	Total	C	N	O	S		
			1138	719	208	208	3		
								0	0

- Molecule 3 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	103	Total	C	N	O	S		
			789	492	142	154	1		
								0	0

- Molecule 4 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	43	Total	C	N	O	P		
			876	416	160	257	43		
								0	0

- Molecule 5 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	54	Total	C	N	O	P		
			1115	528	210	323	54		
								0	0

- Molecule 6 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	13	Total	C	N	O	P		
			270	122	42	93	13		
								0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	p	1146	Total	C	N	O	S	0	0
			9149	5782	1610	1693	64		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	y	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 18 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

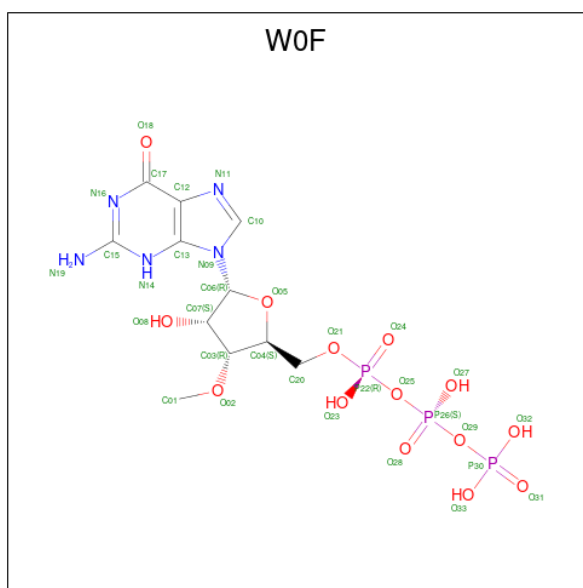
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	o	2	Total	Zn	0
			2	2	
19	p	1	Total	Zn	0
			1	1	
19	q	1	Total	Zn	0
			1	1	
19	w	2	Total	Zn	0
			2	2	
19	x	1	Total	Zn	0
			1	1	
19	z	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	o	1	Total	Mg	0
			1	1	

- Molecule 21 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	p	1	Total	C	N	O	P	0
			33	11	5	14	3	

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. 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. 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.

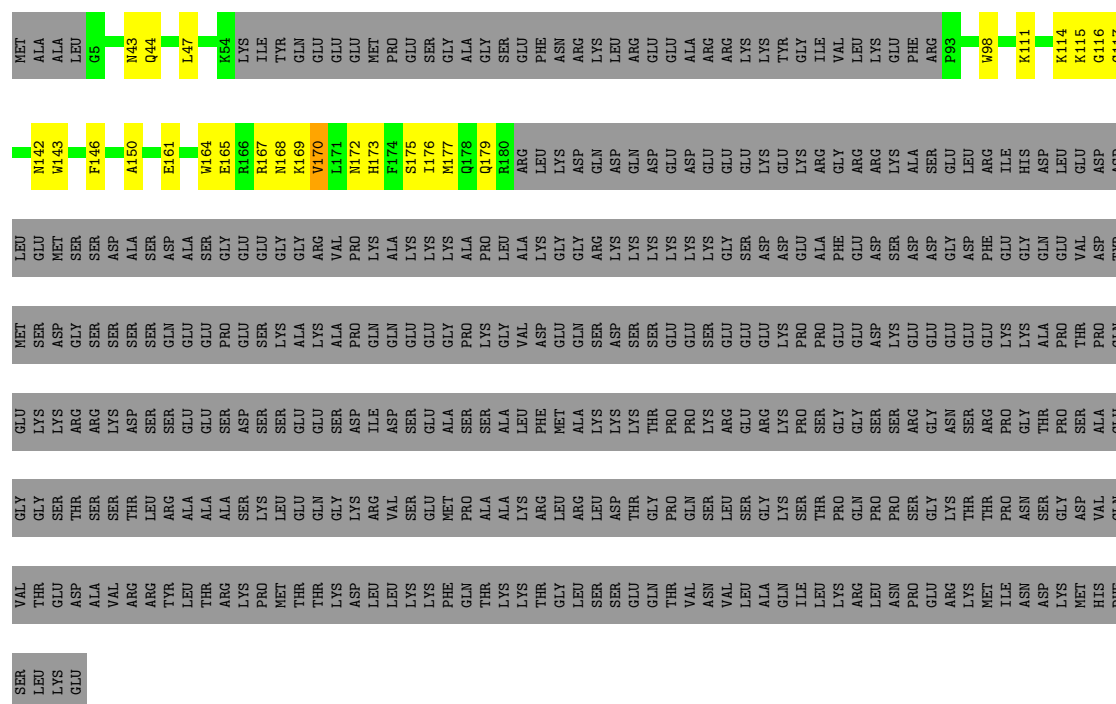
- Molecule 1: Alpha-amanitin

Chain N: 



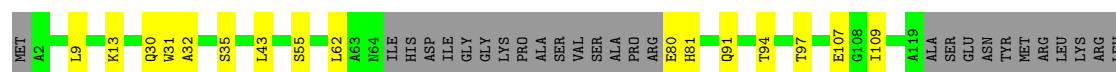
- Molecule 2: General transcription factor IIF subunit 1

Chain S: 



- Molecule 3: General transcription factor IIF subunit 2

Chain T: 



PHE	GLU	HIS	GLN	TYR	ASN	LEU	ASP	VAL	VAL	TYR	LYS	GLN	PRO	VAL	VAL	LYS	GLU	ILE	LEU	GLY	VAL	GLN	ASN	VAL	LYS	GLY	ILE	ILE	LYS	ASN	THR	TRP	GLU	LEU	LYS	PRO	GLU	TYR	ARG	HIS	THR	GLN	GLY	GLU	LYS	SER	ASP
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Chain X: 15% 28% 57%

C26		A29	C30	G31	T32		C35	T36	A37	C38		C42	C43	A44	T45	G46	DT	DC	DC	DC	DG	DG	DA	DA	DA	DA	DC	DC	DT	DG	DA	DA	DC
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Chain Y: 30% 24% 45%

DA DC DC DC DC DC DT DT DT DT DT DA DT DA DG DG DC DG DC DC DC DT DT

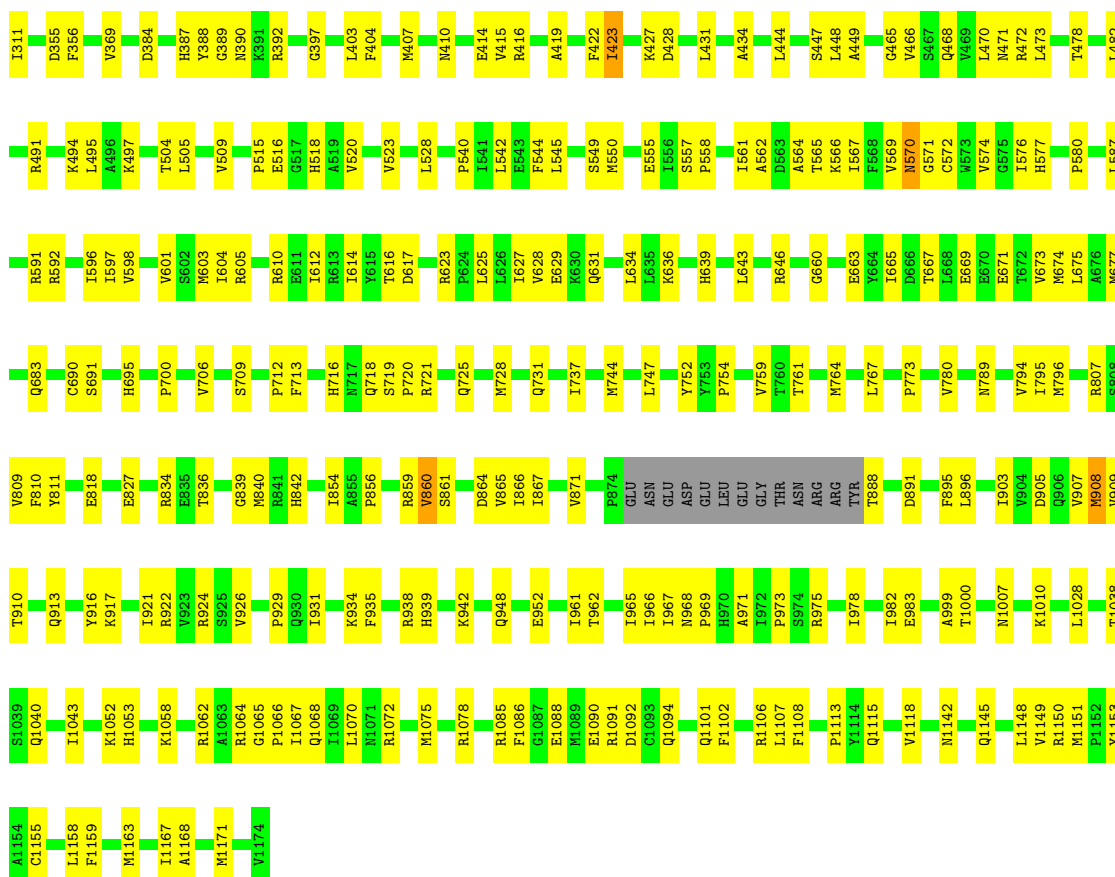
Chain Z: 31% 46% 15% 8%

A5	U8	C9	A10	U11	C12	U13		G17
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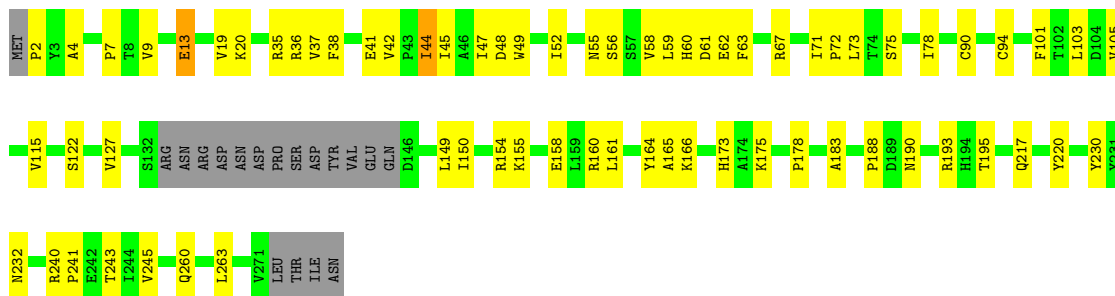
Chain o: 55% 18% 26%

M501	N502	L503	L508	L509	T510	T511	E514	E515	E516	Q516	E517	M520	M521	M522	M523	M524	I525	V526	T527	S530	N531	R532	P533	P534	M535	A544	V545	F548	T549	D552	V553	F554	L555	V560	M565	T569	Q576	P577	L580	K581	P582	L585	K589	Q590	T594
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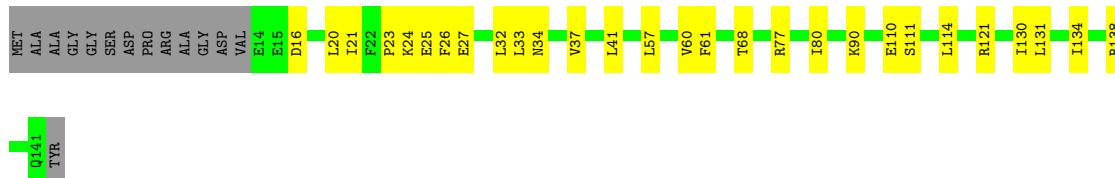
M601	M618	D625	T626	K627	V630	E631	I636	M637	L640	L645	F668	Y669	S670	N671	I672	Q673	T674	V675	I676	L680	H685	I686	I687	I689	I693	I706	A709	V713	I717	H721	P727	L733	T736	L745	A748	R749							
A756	L760	N765	M769	I779	N780	I781	V784	I785	A786	V787	G789	Q790	Q791	N792	F802	I811	P817	E824	L828	L847	V852	K853	L864	I865	K866	S867	Q865	D884	V901	L909	K910	P911	S912	F916	F920	K921	F922	Y924					
R931	E936	L938	V939	N945	I948	L952	E953	N959	R960	E961	D962	P971	T972	V978	L983	N988	N989	K992	T996	D1003	H1005	P1006	I1007	L1016	L1020	V1021	I1022	L1040	I1043	H1044	R1052	L1060	K1075	H1082	Q1230	K1234							
L1104	N1105	T1106	F1107	H1108	K1115	T1118	N1128	H1129	I1130	K1135	L1143	S1147	A1148	R1153	I1157	L1158	G1159	L1160	L1161	E1162	H1163	T1173	A1174	I1175	P1181	T1184	D1189	Q1190	E1191	W1192	R1206	I1207	S1208	P1209	W1210	L1211	R1213	V1214	E1215	Q1230	K1234		
V1256	L1257	I1258	R1259	I1261	M1262	S1264	D1265	E1266	N1267	K1268	E1271	V1275	M1279	D1280	D1282	E1289	L1283	T1297	L1298	Q1299	G1300	V1307	K1318	K1319	I1320	I1321	E1327	A1330	L1331	Q1332	E1333	E1337	V1346	L1347	V1374	V1385	I1386	L1398					
D1403	C1407	R1408	L1411	I1414	T1415	R1416	R1421	L1427	E1433	E1434	T1435	M1440	A1443	A1444	H1445	E1456	M1457	L1458	Q1462	F1471	D1472	L1473	A1477	E1478	K1479	K1481	E1485	I1486	P1487	THR	ASN	ILE	PRO	GLY	LEU	ALA	GLY	PRO	THR	GLY	MET	PHE	
PHE	GLY	ALA	TRP	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
PRO	ALA	TRP	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
PRO	SER	THR	PRO	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
PRO	THR	SER	PRO	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
PRO	THR	SER	PRO	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
PRO	THR	SER	PRO	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR	
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY	MET	GLY	ILE	ASN	GLN	GLY	ALA	TYR	GLY	ALA	TRP	THR	PRO	VAL	GLY	SER	GLY	ALA	ALA	GLY	PHE	PRO	THR	PRO	GLN	ALA	ASP	PRO	THR	GLY	PRO	TYR	THR	TYR
THR	SER	PRO	THR	SER	ALA	PRO	THR	PRO	GLY																																		



• Molecule 9: DNA-directed RNA polymerase II subunit RPB3

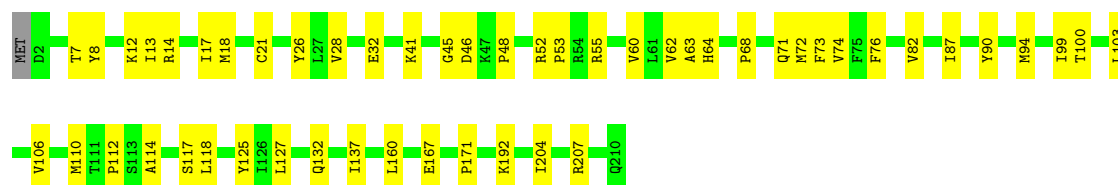


• Molecule 10: DNA-directed RNA polymerase II subunit RPB4



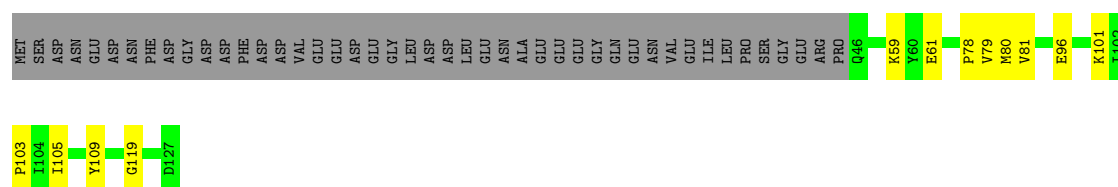
• Molecule 11: DNA-directed RNA polymerase II subunit E

Chain s:  75% 24%



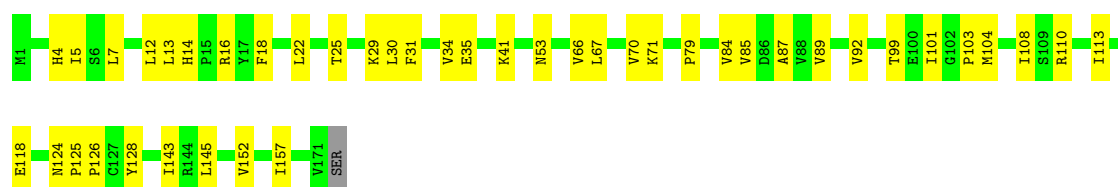
- Molecule 12: DNA-directed RNA polymerase II subunit F

Chain t:  55% 9% 35%



- Molecule 13: DNA-directed RNA polymerase II subunit RPB7

Chain u:  74% 25%



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain v:  77% 20% 3%



- Molecule 15: DNA-directed RNA polymerase II subunit RPB9

Chain w:  71% 19% 9%

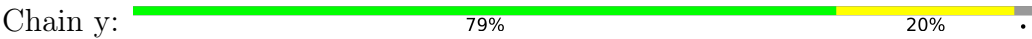


- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain x:  78% 21%



- Molecule 17: DNA-directed RNA polymerase II subunit RPB11-a



- Molecule 18: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: CSX, ILX, HYP, TRX, G2L, W0F, 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
1	N	0.42	0/22	0.98	0/26
2	S	0.09	0/1167	0.23	0/1576
3	T	0.09	0/799	0.25	0/1077
4	X	0.27	0/980	0.59	0/1506
5	Y	0.32	0/1252	0.55	0/1932
6	Z	0.26	0/272	0.45	0/419
7	o	0.24	0/11723	0.37	0/15830
8	p	0.26	0/9332	0.40	1/12598 (0.0%)
9	q	0.25	0/2102	0.37	0/2857
10	r	0.11	0/1064	0.22	0/1428
11	s	0.23	0/1751	0.35	1/2366 (0.0%)
12	t	0.23	0/667	0.28	0/901
13	u	0.15	0/1382	0.31	0/1874
14	v	0.23	0/1207	0.35	0/1628
15	w	0.19	0/948	0.34	0/1284
16	x	0.25	0/542	0.34	0/730
17	y	0.24	0/939	0.32	0/1271
18	z	0.20	0/377	0.36	0/500
All	All	0.24	0/36526	0.38	2/49803 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	46	ASP	CB-CA-C	-5.55	109.68	117.23
8	p	355	ASP	CB-CA-C	-5.12	110.27	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	64	30	51	11	0
2	S	1138	0	1103	19	0
3	T	789	0	795	10	0
4	X	876	0	484	24	0
5	Y	1115	0	607	25	0
6	Z	270	0	138	8	0
7	o	11510	0	11616	267	0
8	p	9149	0	9178	251	0
9	q	2059	0	2007	61	0
10	r	1050	0	1033	17	0
11	s	1720	0	1737	39	0
12	t	657	0	684	11	0
13	u	1351	0	1358	27	0
14	v	1186	0	1147	24	0
15	w	927	0	859	20	0
16	x	533	0	553	12	0
17	y	920	0	942	16	0
18	z	372	0	378	10	0
19	o	2	0	0	0	0
19	p	1	0	0	0	0
19	q	1	0	0	0	0
19	w	2	0	0	0	0
19	x	1	0	0	0	0
19	z	1	0	0	0	0
20	o	1	0	0	0	0
21	p	33	0	0	6	0
All	All	35728	30	34670	741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (741) 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)
5:Y:-16:DC:O2	6:Z:17:G2L:N2	1.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:91:GLN:HB2	8:p:555:GLU:HG3	1.57	0.85
4:X:18:DG:N2	5:Y:-18:DC:O2	2.11	0.84
8:p:597:ILE:HG23	8:p:601:VAL:HB	1.61	0.82
8:p:866:ILE:HG22	8:p:867:ILE:HG13	1.61	0.80
8:p:926:VAL:HG21	9:q:62:GLU:HG3	1.64	0.79
8:p:118:LEU:HD22	8:p:913:GLN:HG3	1.65	0.79
7:o:948:ILE:HG12	7:o:1007:ILE:HD11	1.64	0.78
8:p:975:ARG:NH2	21:p:1201:W0F:O32	2.17	0.78
8:p:1142:ASN:HD21	8:p:1145:GLN:HB2	1.50	0.76
7:o:497:ASP:OD2	21:p:1201:W0F:O33	2.04	0.75
7:o:922:PHE:H	7:o:1052:ARG:HD2	1.52	0.75
9:q:42:VAL:HB	9:q:178:PRO:HG3	1.69	0.74
5:Y:-7:DA:H5''	5:Y:-7:DA:H8	1.53	0.74
9:q:20:LYS:HG3	9:q:232:ASN:HD22	1.52	0.74
8:p:567:ILE:HA	8:p:612:ILE:HG22	1.70	0.73
8:p:665:ILE:HG23	8:p:669:GLU:HB3	1.71	0.72
8:p:718:GLN:HG2	8:p:720:PRO:HD2	1.69	0.72
7:o:1458:ILE:HD12	8:p:1091:ARG:HH21	1.52	0.72
4:X:20:DG:H4'	4:X:21:DC:H5'	1.72	0.72
9:q:60:HIS:HD2	9:q:62:GLU:HG2	1.56	0.71
10:r:25:GLU:HG3	13:u:41:LYS:HE2	1.70	0.71
14:v:26:SER:HB3	14:v:45:ILE:HD11	1.72	0.71
8:p:761:THR:H	8:p:764:MET:HE3	1.55	0.71
7:o:204:HIS:HA	7:o:211:GLU:HB3	1.73	0.71
9:q:193:ARG:HH12	9:q:217:GLN:HB3	1.56	0.70
8:p:924:ARG:HH11	9:q:60:HIS:HB2	1.56	0.70
10:r:16:ASP:H	10:r:21:ILE:HB	1.56	0.70
8:p:274:ARG:NH1	8:p:311:ILE:O	2.24	0.70
5:Y:-17:DC:O2	21:p:1201:W0F:N19	2.24	0.70
7:o:358:ARG:NH2	8:p:1068:GLN:OE1	2.24	0.70
7:o:1148:ALA:HB1	7:o:1333:GLU:HB2	1.73	0.70
1:N:1:ILX:HG23	7:o:791:GLN:NE2	2.07	0.70
17:y:45:ILE:HG22	17:y:94:LEU:HD13	1.75	0.69
9:q:48:ASP:HB3	9:q:166:LYS:HE2	1.75	0.69
8:p:544:PHE:HB2	8:p:596:ILE:HD13	1.73	0.69
9:q:67:ARG:NH2	16:x:3:ILE:O	2.26	0.69
17:y:7:PHE:HB2	17:y:11:LEU:HD12	1.74	0.68
7:o:784:VAL:HG22	8:p:978:ILE:HD11	1.75	0.68
2:S:115:LYS:NZ	2:S:117:GLY:O	2.27	0.68
7:o:141:LEU:HD13	7:o:1445:HIS:HE1	1.56	0.68
8:p:910:THR:HG22	18:z:43:ILE:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:744:MET:HE3	8:p:922:ARG:HB2	1.74	0.68
5:Y:-30:DG:H1'	5:Y:-29:DT:H5'	1.76	0.67
10:r:33:LEU:HD12	10:r:80:ILE:HG23	1.76	0.67
8:p:572:CYS:O	8:p:574:VAL:HG23	1.95	0.67
4:X:5:DC:H2''	4:X:6:DT:C5	2.29	0.67
7:o:358:ARG:HA	8:p:1085:ARG:HA	1.77	0.67
8:p:566:LYS:HA	8:p:576:ILE:HG22	1.77	0.67
8:p:80:GLU:O	8:p:82:PRO:HD3	1.95	0.67
4:X:5:DC:O2	5:Y:-5:DG:N2	2.26	0.66
7:o:508:SER:HB3	7:o:511:THR:HG22	1.76	0.66
7:o:527:THR:HB	7:o:534:VAL:HG22	1.76	0.66
8:p:827:GLU:HG2	8:p:871:VAL:HG22	1.77	0.66
9:q:90:CYS:SG	9:q:94:CYS:HB3	2.35	0.66
1:N:1:ILX:HG23	7:o:791:GLN:HE22	1.60	0.66
4:X:37:DA:H2''	4:X:38:DC:C5	2.30	0.66
9:q:190:ASN:ND2	9:q:195:THR:O	2.28	0.66
11:s:8:TYR:CZ	11:s:12:LYS:HD2	2.31	0.66
5:Y:-38:DG:H2''	5:Y:-37:DT:H72	1.78	0.66
11:s:17:ILE:HD13	11:s:74:VAL:HG11	1.78	0.66
7:o:26:LEU:HG	8:p:1168:ALA:HB2	1.79	0.65
8:p:505:LEU:HD22	8:p:509:VAL:HB	1.78	0.65
8:p:108:MET:HE2	8:p:118:LEU:HD12	1.78	0.65
7:o:1213:ARG:NH1	7:o:1215:GLU:OE2	2.29	0.64
7:o:733:LEU:HB3	15:w:106:ASP:HB2	1.80	0.64
8:p:1115:GLN:HB3	8:p:1148:LEU:HD11	1.79	0.64
7:o:1262:MET:HB3	7:o:1265:ASP:HB3	1.78	0.64
7:o:478:PRO:O	7:o:483:ARG:NH2	2.31	0.64
7:o:375:ILE:HD11	7:o:669:TYR:HB2	1.80	0.64
7:o:121:SER:HA	7:o:126:ILE:HG21	1.80	0.64
8:p:407:MET:HE1	8:p:444:LEU:HG	1.79	0.64
11:s:171:PRO:HB2	11:s:207:ARG:HD3	1.78	0.64
7:o:549:THR:HG21	7:o:640:LEU:HD12	1.79	0.63
2:S:170:VAL:HG23	7:o:1279:MET:HG3	1.80	0.63
8:p:403:LEU:HD23	8:p:444:LEU:HD23	1.80	0.63
5:Y:4:DG:H2''	5:Y:5:DA:C8	2.32	0.63
7:o:636:ILE:HG22	7:o:637:MET:HG2	1.80	0.63
7:o:924:TYR:OH	7:o:953:GLU:OE2	2.17	0.63
7:o:576:GLN:O	7:o:590:GLN:NE2	2.32	0.63
11:s:82:VAL:HG23	11:s:106:VAL:HG13	1.81	0.63
8:p:859:ARG:HG2	8:p:903:ILE:HG12	1.81	0.62
17:y:49:GLN:HB2	17:y:94:LEU:HD21	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:42:DC:H2''	4:X:43:DC:C5	2.35	0.62
8:p:193:VAL:HG21	8:p:470:LEU:HD13	1.82	0.62
5:Y:-13:DT:H2'	5:Y:-12:DA:C8	2.35	0.62
8:p:545:LEU:HB3	8:p:550:MET:HG3	1.81	0.62
7:o:1485:GLU:HB3	12:t:78:PRO:HB3	1.82	0.62
8:p:565:THR:H	8:p:610:ARG:HB3	1.65	0.62
9:q:19:VAL:HG23	9:q:241:PRO:HB2	1.82	0.62
7:o:760:LEU:HD11	7:o:781:ILE:HG21	1.82	0.61
8:p:905:ASP:HB2	8:p:924:ARG:HG3	1.82	0.61
7:o:1474:LEU:HB2	12:t:105:ILE:HG13	1.83	0.61
12:t:81:VAL:HG22	12:t:101:LYS:HD3	1.83	0.61
3:T:94:THR:HG22	3:T:109:ILE:HG22	1.81	0.61
5:Y:-17:DC:H2'	5:Y:-16:DC:C6	2.35	0.61
7:o:201:GLU:HG2	7:o:203:LYS:H	1.66	0.61
2:S:167:ARG:O	8:p:248:LYS:NZ	2.33	0.61
7:o:322:LEU:HB3	7:o:325:LEU:HD12	1.82	0.61
7:o:98:GLY:HA3	7:o:1440:MET:HE2	1.82	0.60
8:p:298:MET:HE3	15:w:14:ILE:HB	1.83	0.60
14:v:96:VAL:HG22	14:v:116:VAL:HG22	1.83	0.60
18:z:16:ILE:HG12	18:z:27:GLU:HG2	1.83	0.60
7:o:560:VAL:HG22	7:o:591:ILE:HD11	1.83	0.60
8:p:37:LYS:HB3	8:p:41:ARG:HG3	1.83	0.60
8:p:157:ARG:NH2	8:p:177:CYS:O	2.34	0.60
7:o:1268:LYS:HD3	7:o:1275:VAL:HG13	1.83	0.60
7:o:367:ILE:HG21	7:o:501:MET:HG3	1.84	0.60
8:p:285:LEU:HD11	8:p:305:LEU:HD11	1.83	0.60
13:u:99:THR:HG21	13:u:143:ILE:HD11	1.84	0.60
7:o:792:ASN:HD21	7:o:1108:HIS:CE1	2.20	0.60
7:o:1128:ILE:HG23	7:o:1414:ILE:HB	1.83	0.60
8:p:387:HIS:HD2	8:p:504:THR:HG21	1.67	0.60
8:p:625:LEU:HD13	8:p:675:LEU:HD21	1.84	0.60
13:u:89:VAL:HA	13:u:99:THR:HG22	1.82	0.60
4:X:19:DA:H2''	4:X:20:DG:H2'	1.84	0.59
8:p:591:ARG:HH22	8:p:592:ARG:HE	1.49	0.59
8:p:860:VAL:HG12	8:p:864:ASP:HB2	1.84	0.59
11:s:82:VAL:HB	11:s:110:MET:HG2	1.85	0.59
18:z:17:TYR:HB3	18:z:44:MET:HB3	1.85	0.59
14:v:58:LEU:HD11	14:v:143:LEU:HD11	1.85	0.59
9:q:9:VAL:HG11	17:y:105:PHE:HD1	1.67	0.59
8:p:627:ILE:HD11	8:p:663:GLU:HB2	1.85	0.58
7:o:671:ASN:O	7:o:675:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:917:LYS:HG3	18:z:34:ILE:HD11	1.84	0.58
10:r:60:VAL:HG13	13:u:103:PRO:HB3	1.85	0.58
8:p:387:HIS:CD2	8:p:504:THR:HG21	2.39	0.58
8:p:747:LEU:HD23	8:p:810:PHE:CE1	2.38	0.58
4:X:23:DG:H2"	4:X:24:DA:C8	2.38	0.58
7:o:555:LEU:HD12	7:o:591:ILE:HD12	1.86	0.58
8:p:392:ARG:NE	8:p:617:ASP:OD2	2.33	0.58
9:q:105:VAL:HG11	9:q:115:VAL:HG22	1.86	0.58
2:S:168:ASN:HA	8:p:248:LYS:HD3	1.84	0.57
8:p:403:LEU:HD21	8:p:447:SER:OG	2.03	0.57
7:o:370:ASP:HB2	7:o:483:ARG:HB3	1.86	0.57
7:o:1386:ILE:HD12	7:o:1398:LEU:HD21	1.87	0.57
9:q:4:ALA:HB2	17:y:93:ASP:HB3	1.85	0.57
12:t:105:ILE:HG22	12:t:119:GLY:HA2	1.86	0.57
15:w:69:ILE:HG22	15:w:71:ASP:H	1.68	0.57
7:o:1258:ARG:HH22	7:o:1260:ARG:HH21	1.52	0.57
7:o:1471:PHE:CZ	12:t:61:GLU:HA	2.40	0.57
8:p:550:MET:SD	8:p:577:HIS:HB2	2.44	0.57
9:q:37:VAL:HG13	9:q:41:GLU:HB2	1.87	0.57
5:Y:-28:DC:H5"	11:s:112:PRO:HB3	1.85	0.57
7:o:864:LEU:HD23	7:o:1414:ILE:HG21	1.86	0.57
7:o:461:GLN:NE2	8:p:1090:GLU:OE2	2.38	0.57
7:o:867:SER:HB3	7:o:1414:ILE:HG23	1.87	0.57
8:p:516:GLU:HA	8:p:520:VAL:HG22	1.86	0.57
7:o:901:VAL:HB	7:o:978:VAL:HG12	1.86	0.57
8:p:834:ARG:HD2	8:p:840:MET:HE2	1.87	0.57
7:o:996:ILE:HD13	7:o:1060:LEU:HA	1.87	0.56
7:o:545:VAL:HG22	7:o:676:ILE:HG12	1.85	0.56
7:o:601:ASN:ND2	7:o:989:ASN:OD1	2.38	0.56
8:p:540:PRO:HB2	8:p:596:ILE:HG23	1.87	0.56
11:s:45:GLY:HA3	11:s:52:ARG:HB2	1.87	0.56
7:o:1189:ASP:HA	7:o:1192:TRP:CE2	2.40	0.56
7:o:721:HIS:HE1	15:w:98:GLN:HE21	1.51	0.56
8:p:50:PHE:HB2	8:p:397:GLY:HA2	1.87	0.56
8:p:924:ARG:NH1	9:q:60:HIS:HB2	2.21	0.56
7:o:1472:ASP:HB2	12:t:109:TYR:HE2	1.69	0.56
7:o:631:GLU:HG2	7:o:988:TRP:HZ2	1.70	0.55
7:o:1403:ASP:O	7:o:1407:CYS:HB2	2.06	0.55
7:o:581:LYS:HG2	7:o:582:PRO:HA	1.88	0.55
12:t:80:MET:HE3	12:t:103:PRO:HG3	1.88	0.55
7:o:626:THR:OG1	7:o:627:LYS:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:91:ILE:HD12	8:p:126:VAL:HG22	1.87	0.55
8:p:570:ASN:OD1	8:p:616:THR:N	2.39	0.55
8:p:709:SER:HB2	8:p:767:LEU:HD11	1.89	0.55
7:o:62:GLN:HG3	7:o:84:HIS:O	2.07	0.55
9:q:260:GLN:HB2	17:y:91:ILE:HG21	1.89	0.55
13:u:30:LEU:HD22	13:u:70:VAL:HG11	1.89	0.55
8:p:952:GLU:HB2	9:q:36:ARG:HG3	1.89	0.54
5:Y:-7:DA:H5''	5:Y:-7:DA:C8	2.39	0.54
7:o:938:LEU:HD22	7:o:1005:HIS:HD1	1.71	0.54
8:p:557:SER:N	8:p:558:PRO:HD2	2.23	0.54
8:p:636:LYS:H	8:p:639:HIS:HD2	1.55	0.54
8:p:65:ILE:HB	8:p:86:LEU:HB2	1.89	0.54
11:s:18:MET:HE2	11:s:32:GLU:HB3	1.89	0.54
7:o:554:PHE:HZ	14:v:121:LEU:HD11	1.72	0.54
11:s:26:TYR:HB3	11:s:62:VAL:HG12	1.90	0.54
16:x:3:ILE:HD12	16:x:4:PRO:HD2	1.88	0.54
8:p:495:LEU:HG	8:p:497:LYS:H	1.73	0.54
7:o:1381:GLU:O	7:o:1385:VAL:HG13	2.07	0.53
7:o:413:TYR:O	7:o:449:HIS:HD2	1.91	0.53
8:p:569:VAL:O	8:p:571:GLY:N	2.42	0.53
8:p:570:ASN:ND2	8:p:616:THR:O	2.41	0.53
7:o:693:ILE:HD13	7:o:828:LEU:HD21	1.90	0.53
7:o:894:ASP:O	7:o:1022:ILE:HD13	2.09	0.53
8:p:761:THR:HG23	8:p:1000:THR:HA	1.91	0.53
9:q:183:ALA:HB3	9:q:232:ASN:HB3	1.89	0.53
7:o:1161:LEU:HD22	7:o:1346:VAL:HG22	1.91	0.53
15:w:115:THR:HG22	15:w:116:ALA:H	1.74	0.53
13:u:14:HIS:HD2	13:u:16:ARG:H	1.56	0.53
7:o:93:PRO:HD2	7:o:219:GLU:HG2	1.90	0.53
7:o:756:ALA:HB2	7:o:786:ALA:HB2	1.90	0.53
7:o:1147:SER:HA	7:o:1153:ARG:HB2	1.91	0.53
17:y:64:PRO:HG3	17:y:70:LYS:HE2	1.91	0.53
7:o:1347:LEU:HB3	11:s:137:ILE:HD12	1.90	0.53
13:u:53:ASN:HD22	13:u:71:LYS:HE3	1.73	0.53
6:Z:5:A:H2'	8:p:842:HIS:CE1	2.44	0.53
7:o:769:MET:HE1	8:p:969:PRO:HB2	1.91	0.53
8:p:1007:ASN:HB2	8:p:1010:LYS:HG3	1.91	0.53
21:p:1201:W0F:C01	21:p:1201:W0F:C20	2.85	0.53
7:o:689:ILE:HD11	8:p:982:ILE:HA	1.91	0.52
8:p:472:ARG:NH1	8:p:737:ILE:HD11	2.24	0.52
13:u:108:ILE:HD11	13:u:145:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:50:PHE:O	8:p:51:ILE:C	2.51	0.52
11:s:73:PHE:HE1	11:s:99:ILE:HD13	1.74	0.52
1:N:2:TRX:CE3	7:o:749:ARG:HD2	2.39	0.52
8:p:388:TYR:CZ	8:p:505:LEU:HD21	2.45	0.52
7:o:1206:ARG:HB2	7:o:1267:ASN:HB2	1.91	0.52
4:X:31:DG:H2"	4:X:32:DT:C6	2.45	0.52
7:o:1262:MET:HB3	7:o:1265:ASP:CB	2.40	0.52
8:p:1062:ARG:NE	8:p:1065:GLY:H	2.07	0.52
13:u:92:VAL:HB	13:u:126:PRO:HB2	1.91	0.52
8:p:545:LEU:O	8:p:550:MET:HG2	2.09	0.52
11:s:55:ARG:HE	11:s:76:PHE:HB3	1.74	0.52
7:o:1130:ILE:HD13	7:o:1411:LEU:HB3	1.90	0.52
8:p:587:LEU:HB3	8:p:603:MET:SD	2.49	0.52
7:o:1005:HIS:HD2	7:o:1007:ILE:HB	1.75	0.52
9:q:78:ILE:HD11	9:q:127:VAL:HG23	1.91	0.52
9:q:56:SER:HG	9:q:158:GLU:H	1.58	0.52
7:o:112:PHE:HD1	7:o:113:PHE:HD2	1.58	0.51
8:p:192:LYS:NZ	8:p:449:ALA:O	2.43	0.51
8:p:561:ILE:HG21	8:p:610:ARG:HB2	1.92	0.51
8:p:1088:GLU:O	8:p:1091:ARG:HG2	2.09	0.51
7:o:544:ALA:HB2	7:o:680:LEU:HD13	1.92	0.51
9:q:44:ILE:HG12	9:q:45:ILE:H	1.75	0.51
7:o:344:LYS:O	7:o:1435:THR:HG21	2.10	0.51
9:q:101:PHE:CE2	9:q:122:SER:HB3	2.45	0.51
7:o:111:CYS:SG	7:o:114:CYS:HB3	2.50	0.51
10:r:32:LEU:HD11	13:u:4:HIS:HB2	1.92	0.51
3:T:97:THR:OG1	3:T:107:GLU:OE2	2.25	0.51
10:r:20:LEU:HD12	10:r:121:ARG:HH22	1.74	0.51
2:S:114:LYS:HB3	8:p:356:PHE:CZ	2.45	0.51
7:o:675:VAL:HG22	7:o:676:ILE:HD12	1.92	0.51
7:o:1082:HIS:CD2	12:t:59:LYS:HE3	2.46	0.51
7:o:1347:LEU:HB3	11:s:137:ILE:CD1	2.40	0.51
8:p:754:PRO:HB2	8:p:773:PRO:HG2	1.91	0.51
18:z:36:CYS:HB2	18:z:44:MET:HE1	1.92	0.51
7:o:916:PHE:HE2	7:o:960:ARG:HG2	1.76	0.51
7:o:1163:HIS:CE1	7:o:1297:THR:HG23	2.46	0.51
7:o:1181:PRO:HG3	7:o:1207:ILE:HG21	1.93	0.51
11:s:87:ILE:HD12	11:s:114:ALA:HB1	1.92	0.51
13:u:30:LEU:O	13:u:34:VAL:HG22	2.11	0.51
14:v:79:ASP:O	14:v:82:PRO:HD2	2.11	0.51
7:o:618:TYR:HE1	14:v:40:ILE:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:u:14:HIS:CD2	13:u:16:ARG:H	2.29	0.51
7:o:516:GLN:O	7:o:520:MET:HB2	2.10	0.50
8:p:515:PRO:HG3	8:p:523:VAL:HB	1.93	0.50
8:p:574:VAL:HG12	8:p:574:VAL:O	2.11	0.50
8:p:604:ILE:O	8:p:612:ILE:HA	2.11	0.50
8:p:789:ASN:O	8:p:968:ASN:HB2	2.11	0.50
7:o:46:THR:HG22	7:o:47:THR:HG23	1.93	0.50
8:p:86:LEU:HD22	8:p:431:LEU:HD21	1.93	0.50
8:p:1062:ARG:HE	8:p:1065:GLY:H	1.60	0.50
4:X:20:DG:H1'	4:X:21:DC:C6	2.46	0.50
8:p:1028:LEU:HD11	8:p:1043:ILE:HD11	1.93	0.50
11:s:118:LEU:HD22	11:s:127:LEU:HB2	1.94	0.50
2:S:116:GLY:HA2	8:p:356:PHE:HD2	1.76	0.50
7:o:909:LEU:C	7:o:911:PRO:HD2	2.37	0.50
7:o:577:PRO:HG2	7:o:580:LEU:HD23	1.93	0.50
7:o:865:ILE:HG21	8:p:1092:ASP:CG	2.37	0.50
7:o:1208:SER:HB3	7:o:1260:ARG:HB3	1.94	0.50
7:o:1427:LEU:HB2	7:o:1456:GLU:HG2	1.94	0.50
6:Z:17:G2L:H2'	21:p:1201:W0F:C10	2.41	0.50
7:o:1230:GLN:HG2	7:o:1234:LYS:HE3	1.93	0.50
7:o:1443:ALA:HB2	8:p:1167:ILE:HG23	1.92	0.50
8:p:49:GLU:O	8:p:50:PHE:C	2.54	0.50
8:p:567:ILE:O	8:p:567:ILE:HG13	2.12	0.50
2:S:164:TRP:CZ2	2:S:167:ARG:HD3	2.47	0.50
8:p:465:GLY:O	8:p:468:GLN:NE2	2.39	0.50
8:p:796:MET:HE3	8:p:948:GLN:HE21	1.77	0.49
7:o:631:GLU:HG2	7:o:988:TRP:CZ2	2.47	0.49
6:Z:17:G2L:OP1	8:p:934:LYS:NZ	2.43	0.49
7:o:350:VAL:O	7:o:355:MET:HG2	2.11	0.49
8:p:759:VAL:HG12	8:p:999:ALA:HB2	1.93	0.49
9:q:49:TRP:HB3	9:q:164:TYR:HB2	1.94	0.49
9:q:52:ILE:HG21	9:q:55:ASN:HB2	1.94	0.49
11:s:192:LYS:HE3	11:s:204:ILE:HD13	1.93	0.49
7:o:548:PHE:HE1	7:o:555:LEU:HD11	1.78	0.49
8:p:591:ARG:NH2	8:p:592:ARG:HG3	2.27	0.49
2:S:169:LYS:HD2	2:S:173:HIS:CD2	2.47	0.49
8:p:77:GLU:HA	8:p:80:GLU:HB2	1.94	0.49
8:p:752:TYR:CE2	8:p:807:ARG:HD2	2.48	0.49
8:p:961:ILE:HG23	16:x:9:THR:HG21	1.94	0.49
9:q:7:PRO:HB2	17:y:101:LEU:HD13	1.94	0.49
10:r:34:ASN:O	10:r:68:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:t:81:VAL:HG23	12:t:96:GLU:HG2	1.93	0.49
2:S:142:ASN:OD1	2:S:143:TRP:N	2.45	0.49
7:o:1321:ILE:HD12	7:o:1331:LEU:HD12	1.95	0.49
9:q:101:PHE:HZ	9:q:127:VAL:HG12	1.77	0.49
11:s:7:THR:OG1	11:s:48:PRO:HD3	2.13	0.49
16:x:27:ALA:O	16:x:28:GLU:HB2	2.13	0.49
7:o:471:GLY:O	7:o:521:VAL:HG23	2.12	0.49
7:o:769:MET:SD	8:p:973:PRO:HG3	2.53	0.49
7:o:909:LEU:O	7:o:910:LYS:HB2	2.12	0.49
7:o:936:GLU:HA	7:o:939:VAL:HG12	1.95	0.49
8:p:794:VAL:HG22	8:p:967:ILE:HG22	1.95	0.49
14:v:58:LEU:HD12	14:v:145:MET:HG2	1.95	0.49
7:o:18:ILE:HD11	8:p:1149:VAL:HG11	1.94	0.49
7:o:885:GLN:HE22	7:o:1408:ARG:HH12	1.61	0.49
7:o:527:THR:HG22	7:o:532:ARG:O	2.13	0.49
8:p:69:ALA:H	8:p:82:PRO:HD2	1.76	0.49
8:p:565:THR:HA	8:p:610:ARG:O	2.13	0.49
4:X:-7:DC:H2"	4:X:-6:DT:C5	2.48	0.48
5:Y:-8:DG:H2"	5:Y:-7:DA:H5"	1.95	0.48
7:o:112:PHE:HD1	7:o:113:PHE:CD2	2.31	0.48
8:p:187:ILE:HD13	8:p:448:LEU:HB3	1.94	0.48
8:p:706:VAL:HG13	8:p:767:LEU:HD22	1.94	0.48
11:s:13:ILE:HD11	11:s:132:GLN:HG3	1.95	0.48
8:p:561:ILE:HB	8:p:610:ARG:HH11	1.78	0.48
7:o:469:MET:HE1	8:p:1086:PHE:CZ	2.49	0.48
7:o:525:ILE:HG12	7:o:535:MET:HE3	1.96	0.48
8:p:564:ALA:HA	8:p:610:ARG:HD2	1.94	0.48
9:q:103:LEU:HB3	9:q:161:LEU:HG	1.94	0.48
14:v:40:ILE:O	14:v:123:MET:HA	2.14	0.48
18:z:36:CYS:HB3	18:z:39:CYS:SG	2.54	0.48
7:o:709:ALA:HB2	7:o:748:ALA:HB2	1.96	0.48
7:o:912:SER:HB2	7:o:1327:GLU:HG2	1.94	0.48
8:p:811:TYR:CE2	8:p:924:ARG:HG2	2.49	0.48
3:T:31:TRP:HD1	3:T:62:LEU:HD21	1.78	0.48
7:o:931:ARG:HG2	7:o:939:VAL:HG11	1.95	0.48
8:p:860:VAL:HB	8:p:896:LEU:HD11	1.95	0.48
9:q:58:VAL:HG11	16:x:59:LEU:HB3	1.95	0.48
11:s:21:CYS:SG	11:s:62:VAL:HG11	2.53	0.48
7:o:457:ILE:HG12	7:o:515:ILE:HD13	1.96	0.48
7:o:847:LEU:HD11	8:p:720:PRO:HB3	1.96	0.48
8:p:85:LEU:HB2	8:p:131:THR:OG1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:s:72:MET:HE3	11:s:72:MET:HB2	1.78	0.48
2:S:161:GLU:O	2:S:165:GLU:HG2	2.14	0.48
7:o:343:LEU:HD22	8:p:1158:LEU:HD12	1.95	0.48
8:p:260:LEU:HB2	8:p:263:ILE:HD12	1.96	0.48
8:p:674:MET:HG2	15:w:77:THR:HA	1.95	0.48
11:s:21:CYS:SG	11:s:26:TYR:HB2	2.53	0.48
7:o:362:SER:HA	7:o:503:LEU:O	2.13	0.48
8:p:473:LEU:HD22	8:p:1052:LYS:HD3	1.95	0.48
8:p:747:LEU:HD23	8:p:810:PHE:HE1	1.76	0.48
9:q:72:PRO:HG3	16:x:13:ILE:HD11	1.94	0.48
7:o:1211:LEU:HD11	7:o:1258:ARG:HB3	1.95	0.48
8:p:470:LEU:HD11	8:p:478:THR:HG23	1.95	0.48
8:p:569:VAL:HG12	8:p:572:CYS:HB2	1.94	0.48
8:p:712:PRO:HD3	8:p:938:ARG:HD2	1.96	0.48
15:w:64:GLU:O	15:w:68:ILE:HG12	2.13	0.48
7:o:360:ASP:O	8:p:1106:ARG:NH2	2.46	0.47
8:p:404:PHE:HA	8:p:407:MET:HE2	1.96	0.47
9:q:67:ARG:NH1	9:q:149:LEU:O	2.47	0.47
13:u:13:LEU:HB3	13:u:66:VAL:HG12	1.96	0.47
7:o:1212:LEU:HD23	7:o:1259:ILE:HD12	1.96	0.47
8:p:88:PHE:HD2	8:p:126:VAL:HG11	1.79	0.47
8:p:938:ARG:NH2	8:p:983:GLU:OE2	2.47	0.47
15:w:73:SER:HA	15:w:95:VAL:HG11	1.96	0.47
7:o:375:ILE:HD11	7:o:669:TYR:CB	2.45	0.47
7:o:972:THR:HA	7:o:1320:ILE:HG13	1.96	0.47
11:s:60:VAL:HG12	11:s:62:VAL:HG23	1.95	0.47
15:w:12:VAL:HG23	15:w:50:ASN:HD21	1.79	0.47
7:o:1479:LYS:HD2	12:t:103:PRO:HA	1.96	0.47
8:p:861:SER:O	8:p:896:LEU:HD12	2.15	0.47
8:p:971:ALA:O	8:p:975:ARG:HD2	2.14	0.47
7:o:87:HIS:HD2	7:o:89:GLU:HG3	1.79	0.47
7:o:545:VAL:HG11	7:o:645:LEU:HD12	1.95	0.47
7:o:802:PHE:HD2	8:p:671:GLU:HG2	1.79	0.47
8:p:117:ASN:HA	8:p:189:GLY:HA3	1.97	0.47
10:r:57:LEU:HD13	10:r:61:PHE:CE1	2.49	0.47
5:Y:-16:DC:N3	6:Z:17:G2L:N1	2.55	0.47
8:p:491:ARG:HB3	8:p:518:HIS:HB3	1.97	0.47
8:p:744:MET:SD	8:p:908:MET:HG2	2.54	0.47
14:v:65:TYR:CD1	14:v:84:ARG:HG2	2.50	0.47
7:o:565:MET:HE1	17:y:74:ARG:HB2	1.96	0.47
7:o:1105:ASN:HB3	7:o:1107:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:1347:LEU:C	11:s:137:ILE:HD11	2.40	0.47
8:p:185:PHE:HB2	8:p:187:ILE:HD11	1.97	0.47
9:q:59:LEU:HD13	9:q:63:PHE:CE1	2.49	0.47
3:T:80:GLU:OE1	3:T:81:HIS:N	2.47	0.47
5:Y:-11:DG:H2''	5:Y:-10:DA:H8	1.80	0.47
7:o:76:GLY:HA2	7:o:81:CYS:HB2	1.97	0.47
8:p:564:ALA:HB3	8:p:580:PRO:HD3	1.97	0.47
8:p:854:ILE:O	8:p:907:VAL:HG21	2.15	0.47
4:X:45:DT:H2''	4:X:46:DG:C8	2.50	0.47
7:o:421:ARG:CZ	7:o:427:ILE:HD11	2.45	0.47
7:o:585:LEU:HD12	14:v:47:ILE:HD11	1.96	0.47
8:p:565:THR:HA	8:p:610:ARG:C	2.40	0.47
8:p:1072:ARG:HD2	8:p:1153:TYR:CE1	2.49	0.47
11:s:63:ALA:HB1	11:s:68:PRO:HA	1.97	0.47
5:Y:1:DG:H2''	5:Y:2:DA:C8	2.50	0.47
8:p:297:MET:O	8:p:301:VAL:HG23	2.14	0.47
7:o:460:ARG:HD3	7:o:492:TYR:O	2.15	0.46
7:o:1263:ASN:OD1	7:o:1263:ASN:N	2.46	0.46
13:u:18:PHE:HA	13:u:22:LEU:HD13	1.97	0.46
8:p:427:LYS:HG3	8:p:428:ASP:H	1.79	0.46
8:p:561:ILE:HG21	8:p:610:ARG:CB	2.44	0.46
13:u:124:ASN:HB2	13:u:125:PRO:HD3	1.98	0.46
7:o:1261:ILE:HG22	7:o:1262:MET:H	1.81	0.46
8:p:747:LEU:HA	8:p:810:PHE:HE1	1.79	0.46
4:X:22:DC:H2''	4:X:23:DG:C8	2.51	0.46
6:Z:13:U:H5''	8:p:465:GLY:HA2	1.98	0.46
7:o:41:ILE:HG21	7:o:57:LEU:HD23	1.97	0.46
8:p:384:ASP:O	8:p:390:ASN:ND2	2.44	0.46
8:p:565:THR:HG21	8:p:612:ILE:HB	1.97	0.46
5:Y:-13:DT:H2'	5:Y:-12:DA:H8	1.78	0.46
7:o:201:GLU:HB2	7:o:213:LYS:HG2	1.98	0.46
8:p:550:MET:HE1	8:p:577:HIS:ND1	2.31	0.46
8:p:1151:MET:HE2	8:p:1155:CYS:HB3	1.97	0.46
15:w:36:LEU:HD23	15:w:47:GLU:HA	1.97	0.46
18:z:46:LYS:O	18:z:47:LYS:HB3	2.15	0.46
7:o:515:ILE:HD11	8:p:1102:PHE:CE1	2.51	0.46
7:o:952:LEU:HD21	7:o:1006:PRO:HB2	1.98	0.46
8:p:50:PHE:O	8:p:54:SER:N	2.39	0.46
8:p:665:ILE:HD13	8:p:673:VAL:HG21	1.96	0.46
9:q:154:ARG:HB2	16:x:60:LEU:HD22	1.97	0.46
17:y:84:GLN:O	17:y:88:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:929:PRO:HB3	8:p:935:PHE:HZ	1.81	0.46
9:q:263:LEU:HD22	17:y:87:PHE:HD2	1.80	0.46
7:o:282:ASP:O	7:o:286:ILE:HG12	2.16	0.46
7:o:460:ARG:HB2	7:o:501:MET:SD	2.56	0.46
8:p:713:PHE:HB3	8:p:716:HIS:CD2	2.50	0.46
8:p:859:ARG:HG3	18:z:53:VAL:HG11	1.96	0.46
2:S:172:ASN:HB2	7:o:1280:ASP:OD1	2.15	0.46
3:T:32:ALA:HA	3:T:35:SER:HB2	1.97	0.46
7:o:421:ARG:NE	7:o:427:ILE:HD11	2.30	0.46
7:o:733:LEU:HA	7:o:736:THR:HG22	1.98	0.46
7:o:811:ILE:HD11	8:p:690:CYS:HB2	1.98	0.46
8:p:43:GLN:HE21	8:p:43:GLN:HB3	1.64	0.46
10:r:37:VAL:O	10:r:41:LEU:HG	2.15	0.46
10:r:90:LYS:HE2	10:r:130:ILE:HD11	1.98	0.46
14:v:60:ILE:HG21	14:v:135:PHE:CZ	2.51	0.46
7:o:26:LEU:HD13	7:o:31:LEU:HD21	1.97	0.46
7:o:113:PHE:CE1	7:o:186:ARG:HD2	2.51	0.46
7:o:226:LYS:HG2	7:o:246:GLU:OE1	2.16	0.46
7:o:515:ILE:HD11	8:p:1102:PHE:CD1	2.51	0.46
7:o:673:GLN:HE21	7:o:673:GLN:HB3	1.56	0.46
8:p:158:SER:O	8:p:164:ASN:HB2	2.17	0.45
7:o:15:LEU:HD11	8:p:1150:ARG:HG3	1.98	0.45
7:o:1477:ALA:O	7:o:1481:LYS:HG2	2.16	0.45
8:p:40:VAL:HG11	8:p:482:LEU:HD13	1.98	0.45
8:p:422:PHE:HB3	8:p:428:ASP:O	2.16	0.45
11:s:8:TYR:CE2	11:s:12:LYS:HD2	2.51	0.45
13:u:79:PRO:HG3	13:u:104:MET:SD	2.56	0.45
8:p:236:TRP:HB2	8:p:259:THR:HB	1.98	0.45
7:o:353:ASN:O	7:o:357:LYS:HE2	2.16	0.45
7:o:852:VAL:HG13	8:p:494:LYS:HB3	1.98	0.45
8:p:818:GLU:HG2	8:p:917:LYS:HB3	1.99	0.45
9:q:9:VAL:HG11	17:y:105:PHE:CD1	2.48	0.45
11:s:7:THR:HG21	11:s:41:LYS:HG2	1.97	0.45
4:X:-6:DT:H2"	4:X:-5:DT:H72	1.98	0.45
7:o:357:LYS:HD2	8:p:1107:LEU:O	2.16	0.45
7:o:517:GLU:O	7:o:523:ARG:HD2	2.17	0.45
7:o:1016:LEU:O	7:o:1020:LEU:HG	2.17	0.45
8:p:237:VAL:HG11	8:p:369:VAL:HG22	1.98	0.45
17:y:47:LYS:HD3	17:y:61:TYR:HD1	1.82	0.45
8:p:298:MET:HB3	15:w:14:ILE:HD12	1.99	0.45
8:p:1038:THR:HA	9:q:195:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:910:LYS:N	7:o:911:PRO:HD2	2.31	0.45
7:o:1318:LYS:HE2	7:o:1330:ALA:HB1	1.98	0.45
8:p:387:HIS:CD2	8:p:389:GLY:H	2.35	0.45
8:p:631:GLN:NE2	8:p:691:SER:O	2.47	0.45
10:r:77:ARG:HA	10:r:80:ILE:HD12	1.98	0.45
7:o:155:GLU:H	7:o:181:HIS:CD2	2.35	0.45
7:o:470:MET:HB3	7:o:521:VAL:HG22	1.99	0.45
7:o:526:VAL:HA	7:o:533:PRO:HA	1.98	0.45
8:p:725:GLN:HA	8:p:728:MET:HE2	1.99	0.45
8:p:780:VAL:HG22	8:p:965:ILE:HB	1.98	0.45
13:u:25:THR:O	13:u:29:LYS:HG2	2.17	0.45
2:S:175:SER:O	2:S:179:GLN:HG2	2.17	0.45
5:Y:-24:DT:H2''	5:Y:-23:DC:H5'	1.98	0.45
7:o:706:ILE:HD13	7:o:824:GLU:HB2	1.98	0.45
9:q:2:PRO:HB3	17:y:54:PRO:HD2	1.99	0.45
9:q:154:ARG:HD3	16:x:64:PRO:HD3	1.99	0.45
11:s:18:MET:HE3	11:s:28:VAL:HG13	1.99	0.45
5:Y:-17:DC:H2'	5:Y:-16:DC:H6	1.80	0.45
7:o:971:PRO:O	7:o:972:THR:OG1	2.28	0.45
13:u:87:ALA:HB2	13:u:101:ILE:HG12	1.98	0.45
8:p:415:VAL:HA	8:p:434:ALA:HB1	1.98	0.44
8:p:472:ARG:CZ	8:p:737:ILE:HD11	2.47	0.44
8:p:561:ILE:O	8:p:610:ARG:NH1	2.50	0.44
11:s:160:LEU:HD11	11:s:167:GLU:HG2	1.99	0.44
15:w:69:ILE:HG22	15:w:71:ASP:N	2.32	0.44
1:N:2:TRX:CZ3	7:o:749:ARG:HD2	2.47	0.44
2:S:177:MET:HG2	15:w:40:ARG:O	2.17	0.44
8:p:42:GLN:HG3	8:p:43:GLN:H	1.81	0.44
8:p:51:ILE:O	8:p:52:GLN:C	2.58	0.44
1:N:2:TRX:O	7:o:790:GLN:N	2.50	0.44
4:X:35:DC:H2''	4:X:36:DT:H72	1.98	0.44
7:o:253:LEU:HD11	7:o:317:MET:HE1	1.98	0.44
9:q:13:GLU:HB2	9:q:20:LYS:HB2	1.99	0.44
11:s:106:VAL:HG21	11:s:110:MET:HG3	2.00	0.44
17:y:58:PHE:HB3	17:y:76:GLN:HB3	1.99	0.44
4:X:18:DG:H2'	4:X:18:DG:OP2	2.18	0.44
7:o:721:HIS:CE1	15:w:98:GLN:HE21	2.32	0.44
7:o:1118:THR:HG21	7:o:1135:LYS:HB2	2.00	0.44
7:o:1268:LYS:HG3	7:o:1271:GLU:OE2	2.18	0.44
11:s:14:ARG:O	11:s:18:MET:HG2	2.16	0.44
11:s:26:TYR:HA	11:s:64:HIS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:s:90:TYR:O	11:s:94:MET:HG2	2.17	0.44
15:w:14:ILE:HG21	15:w:23:MET:HE2	1.98	0.44
7:o:1158:LEU:HG	7:o:1307:VAL:HB	2.00	0.44
8:p:818:GLU:O	8:p:916:TYR:HB3	2.18	0.44
8:p:1142:ASN:ND2	8:p:1145:GLN:HB2	2.27	0.44
9:q:52:ILE:HD12	9:q:61:ASP:HB3	1.99	0.44
10:r:23:PRO:HG2	10:r:26:PHE:HB2	1.99	0.44
7:o:1209:PRO:HG2	7:o:1210:TRP:CD1	2.52	0.44
8:p:558:PRO:O	8:p:562:ALA:N	2.50	0.44
8:p:1072:ARG:HB2	8:p:1153:TYR:CD2	2.53	0.44
9:q:71:ILE:HD11	9:q:150:ILE:HG12	1.98	0.44
9:q:103:LEU:O	9:q:160:ARG:HA	2.18	0.44
10:r:24:LYS:HA	10:r:27:GLU:CD	2.43	0.44
14:v:47:ILE:H	14:v:47:ILE:HG13	1.63	0.44
15:w:22:ASN:ND2	15:w:41:ASN:HD22	2.16	0.44
7:o:1440:MET:SD	8:p:1167:ILE:HD11	2.56	0.44
8:p:795:ILE:HB	8:p:966:ILE:HB	2.00	0.44
8:p:1159:PHE:O	8:p:1163:MET:HG3	2.17	0.44
9:q:44:ILE:HG12	9:q:45:ILE:N	2.33	0.44
9:q:63:PHE:CE1	9:q:67:ARG:HD2	2.52	0.44
16:x:17:LYS:HB3	16:x:38:LEU:HD13	2.00	0.44
1:N:1:ILX:HA	7:o:791:GLN:NE2	2.32	0.44
1:N:2:TRX:HE3	7:o:788:VAL:O	2.18	0.44
7:o:53:LYS:HE3	7:o:53:LYS:HB2	1.75	0.44
7:o:1282:ASP:N	7:o:1282:ASP:OD1	2.51	0.44
8:p:252:ILE:HD12	8:p:255:ARG:HD3	2.00	0.44
14:v:52:LEU:HD23	14:v:52:LEU:HA	1.77	0.44
15:w:106:ASP:OD1	15:w:106:ASP:N	2.51	0.44
1:N:1:ILX:CG2	7:o:791:GLN:HE22	2.27	0.44
8:p:591:ARG:HH12	8:p:592:ARG:HE	1.66	0.44
8:p:1053:HIS:HB3	8:p:1058:LYS:HE3	1.99	0.44
8:p:1115:GLN:HG2	8:p:1150:ARG:HG2	2.00	0.44
9:q:35:ARG:O	9:q:38:PHE:HB2	2.17	0.44
11:s:114:ALA:O	11:s:117:SER:HB2	2.18	0.44
8:p:163:LEU:HA	8:p:166:LEU:HD12	2.00	0.43
8:p:561:ILE:HB	8:p:610:ARG:NH1	2.33	0.43
8:p:643:LEU:O	8:p:646:ARG:HB2	2.18	0.43
13:u:84:VAL:HA	13:u:145:LEU:O	2.18	0.43
7:o:194:SER:HB3	7:o:199:TYR:HE2	1.82	0.43
7:o:368:THR:HG21	8:p:931:ILE:O	2.18	0.43
7:o:530:SER:O	7:o:532:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:o:601:ASN:HA	7:o:630:VAL:O	2.18	0.43
7:o:853:LYS:HA	7:o:1104:LEU:HD21	1.99	0.43
7:o:1075:LYS:HE3	7:o:1075:LYS:HB2	1.86	0.43
7:o:1434:GLU:C	7:o:1435:THR:HG1	2.24	0.43
8:p:419:ALA:O	8:p:423:ILE:HG12	2.18	0.43
10:r:110:GLU:O	10:r:114:LEU:HG	2.17	0.43
7:o:569:THR:HG23	7:o:671:ASN:HD21	1.82	0.43
7:o:1416:ARG:HB3	7:o:1433:GLU:OE1	2.17	0.43
8:p:193:VAL:HG23	8:p:470:LEU:HB2	2.00	0.43
8:p:628:VAL:HG21	8:p:683:GLN:NE2	2.34	0.43
10:r:121:ARG:HD3	10:r:121:ARG:HA	1.79	0.43
5:Y:-13:DT:OP1	8:p:1078:ARG:N	2.51	0.43
7:o:916:PHE:CE2	7:o:960:ARG:HG2	2.52	0.43
8:p:926:VAL:CG2	9:q:62:GLU:HG3	2.42	0.43
14:v:76:ASN:HB3	14:v:79:ASP:HB2	2.00	0.43
7:o:379:GLY:O	7:o:482:PHE:HA	2.18	0.43
4:X:25:DG:H4'	4:X:26:DC:OP1	2.19	0.43
5:Y:-8:DG:H2''	5:Y:-7:DA:C5'	2.49	0.43
5:Y:-3:DT:H2''	5:Y:-2:DG:C8	2.54	0.43
7:o:1208:SER:O	7:o:1260:ARG:NH1	2.52	0.43
8:p:177:CYS:HB3	8:p:180:ASP:HB2	2.00	0.43
8:p:713:PHE:HB3	8:p:716:HIS:HD2	1.83	0.43
14:v:37:MET:HE2	14:v:37:MET:HB3	1.79	0.43
8:p:1118:VAL:HG21	8:p:1171:MET:HE3	2.01	0.43
9:q:49:TRP:CE3	9:q:164:TYR:HD2	2.36	0.43
7:o:58:MET:HE3	7:o:65:ILE:HD13	2.00	0.43
7:o:668:PHE:CZ	7:o:672:ILE:HD11	2.54	0.43
7:o:983:LEU:HD12	7:o:1044:HIS:CD2	2.54	0.43
7:o:1206:ARG:HA	7:o:1206:ARG:HD3	1.74	0.43
8:p:942:LYS:HE2	21:p:1201:W0F:O31	2.19	0.43
10:r:134:ILE:O	10:r:138:ARG:HG3	2.18	0.43
1:N:3:GLY:HA3	7:o:749:ARG:NH1	2.33	0.43
7:o:212:LYS:H	7:o:212:LYS:HD3	1.83	0.43
7:o:381:PRO:HB3	7:o:480:SER:HA	2.00	0.43
7:o:1153:ARG:O	7:o:1157:ILE:HG12	2.19	0.43
7:o:1160:ARG:O	7:o:1300:GLY:HA2	2.18	0.43
7:o:1215:GLU:HG2	7:o:1256:VAL:HG22	2.00	0.43
9:q:154:ARG:HG2	9:q:155:LYS:N	2.34	0.43
15:w:97:PHE:HB2	15:w:100:HIS:HE2	1.83	0.43
7:o:123:ASN:HD21	7:o:125:LYS:HB2	1.83	0.43
7:o:309:LEU:HD12	7:o:309:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:627:ILE:HD12	8:p:660:GLY:O	2.19	0.43
8:p:764:MET:HE1	8:p:938:ARG:NH1	2.34	0.43
2:S:43:ASN:OD1	2:S:44:GLN:N	2.52	0.42
7:o:87:HIS:CD2	7:o:89:GLU:HG3	2.53	0.42
7:o:920:PHE:CD1	7:o:959:MET:HE1	2.54	0.42
7:o:1175:ILE:HG12	7:o:1212:LEU:HD12	2.01	0.42
8:p:528:LEU:HA	8:p:528:LEU:HD23	1.74	0.42
8:p:1028:LEU:HD23	8:p:1028:LEU:HA	1.76	0.42
9:q:47:ILE:HA	9:q:165:ALA:HA	2.01	0.42
9:q:173:HIS:ND1	9:q:175:LYS:HB3	2.33	0.42
13:u:152:VAL:HG22	13:u:157:ILE:HG12	2.00	0.42
7:o:34:MET:HE2	7:o:34:MET:HB3	1.91	0.42
7:o:510:GLU:O	7:o:514:GLU:HG3	2.19	0.42
7:o:1234:LYS:HZ3	7:o:1298:LEU:C	2.25	0.42
7:o:1458:ILE:HD12	8:p:1091:ARG:NH2	2.27	0.42
8:p:296:GLU:O	8:p:300:MET:HG2	2.19	0.42
8:p:719:SER:OG	8:p:720:PRO:HD3	2.19	0.42
7:o:1130:ILE:HD13	7:o:1411:LEU:HD22	2.01	0.42
8:p:65:ILE:HG23	8:p:416:ARG:HD3	2.01	0.42
9:q:72:PRO:HG3	16:x:13:ILE:CD1	2.49	0.42
9:q:193:ARG:HG2	9:q:220:TYR:CD1	2.54	0.42
9:q:240:ARG:O	9:q:243:THR:HG22	2.18	0.42
11:s:62:VAL:O	11:s:71:GLN:HA	2.19	0.42
7:o:685:HIS:NE2	7:o:769:MET:HE3	2.34	0.42
7:o:745:LEU:HD21	7:o:817:PRO:HB3	2.00	0.42
7:o:1486:ILE:HB	7:o:1487:PRO:HD3	2.00	0.42
8:p:623:ARG:CZ	8:p:625:LEU:HD21	2.49	0.42
9:q:35:ARG:HA	9:q:38:PHE:CD2	2.54	0.42
14:v:36:LYS:HA	14:v:36:LYS:HD2	1.82	0.42
6:Z:9:C:H2'	6:Z:10:A:C8	2.55	0.42
7:o:96:HIS:HB3	7:o:99:PHE:HB2	2.01	0.42
7:o:375:ILE:HD13	7:o:375:ILE:HG21	1.70	0.42
8:p:504:THR:HB	8:p:667:THR:HG21	2.02	0.42
8:p:794:VAL:HG13	8:p:965:ILE:HG23	2.01	0.42
7:o:18:ILE:HB	7:o:1462:GLN:HE22	1.84	0.42
7:o:727:PRO:HA	7:o:736:THR:HG21	2.01	0.42
7:o:1173:THR:HG23	7:o:1214:VAL:HG22	2.02	0.42
7:o:1421:ARG:HA	7:o:1421:ARG:HD3	1.86	0.42
9:q:38:PHE:CE1	9:q:245:VAL:HA	2.54	0.42
10:r:111:SER:HB2	10:r:131:LEU:HD21	2.01	0.42
13:u:12:LEU:HD11	13:u:67:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:v:37:MET:HE3	14:v:127:GLY:HA3	2.02	0.42
2:S:111:LYS:O	2:S:146:PHE:HA	2.20	0.42
5:Y:-15:DA:H5"	8:p:1085:ARG:HG3	2.01	0.42
8:p:169:ARG:H	8:p:169:ARG:HG3	1.69	0.42
8:p:629:GLU:HG3	8:p:634:LEU:HD21	2.01	0.42
7:o:210:GLN:HB2	7:o:214:ILE:HD11	2.00	0.42
7:o:938:LEU:HD11	7:o:1003:ASP:C	2.45	0.42
8:p:19:PRO:C	8:p:21:LEU:H	2.27	0.42
8:p:780:VAL:HA	8:p:965:ILE:O	2.19	0.42
8:p:1066:PRO:HB2	8:p:1075:MET:SD	2.60	0.42
9:q:188:PRO:HD3	9:q:230:TYR:HE2	1.85	0.42
11:s:74:VAL:HG22	11:s:103:LEU:HD12	2.01	0.42
13:u:5:ILE:HD12	13:u:7:LEU:HD21	2.02	0.42
14:v:90:TYR:HB3	14:v:145:MET:HB2	2.02	0.42
7:o:93:PRO:HB2	7:o:218:PRO:HB2	2.00	0.42
7:o:1184:THR:HG21	7:o:1190:GLN:HA	2.01	0.42
14:v:57:ARG:HB2	14:v:148:LEU:HD11	2.02	0.42
16:x:22:LEU:O	16:x:26:GLN:HG2	2.20	0.42
2:S:47:LEU:HD11	2:S:98:TRP:HB3	2.01	0.41
8:p:473:LEU:HD23	8:p:731:GLN:HA	2.02	0.41
8:p:542:LEU:HD22	8:p:574:VAL:HG11	2.01	0.41
11:s:100:THR:HA	11:s:125:TYR:HD1	1.84	0.41
7:o:62:GLN:HE22	7:o:255:VAL:HG12	1.85	0.41
7:o:552:ASP:CG	14:v:22:PHE:HB3	2.44	0.41
7:o:1234:LYS:NZ	7:o:1298:LEU:O	2.46	0.41
8:p:569:VAL:HG22	8:p:570:ASN:H	1.85	0.41
8:p:865:VAL:HG22	8:p:895:PHE:CE1	2.54	0.41
2:S:150:ALA:HB2	15:w:20:CYS:HB3	2.01	0.41
3:T:9:LEU:O	3:T:13:LYS:HG2	2.20	0.41
4:X:19:DA:H2"	4:X:20:DG:C8	2.55	0.41
4:X:30:DC:N3	5:Y:-30:DG:O6	2.53	0.41
7:o:1143:LEU:HB2	7:o:1148:ALA:HB2	2.03	0.41
7:o:1487:PRO:HD2	12:t:79:VAL:H	1.85	0.41
14:v:60:ILE:HG23	14:v:141:VAL:HG13	2.02	0.41
5:Y:-15:DA:H5"	8:p:1085:ARG:CG	2.51	0.41
7:o:106:VAL:O	7:o:110:VAL:HG23	2.19	0.41
7:o:349:ARG:NH2	8:p:1070:LEU:HD21	2.36	0.41
7:o:447:GLU:CD	8:p:1064:ARG:HH12	2.27	0.41
7:o:685:HIS:HE2	7:o:769:MET:HE3	1.85	0.41
7:o:1207:ILE:O	7:o:1266:GLU:HG2	2.20	0.41
8:p:836:THR:O	8:p:888:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:839:GLY:O	8:p:891:ASP:HB2	2.20	0.41
8:p:856:PRO:HG2	18:z:48:ARG:HA	2.03	0.41
8:p:1108:PHE:CE1	8:p:1113:PRO:HA	2.55	0.41
2:S:172:ASN:O	2:S:176:ILE:HG12	2.20	0.41
7:o:316:THR:HG21	7:o:328:ALA:HB3	2.01	0.41
7:o:377:GLN:HA	7:o:473:ARG:O	2.21	0.41
7:o:1115:LYS:HD3	7:o:1337:GLU:HB3	2.01	0.41
8:p:569:VAL:HG13	8:p:570:ASN:N	2.35	0.41
13:u:31:PHE:O	13:u:35:GLU:HB2	2.20	0.41
4:X:24:DA:N1	4:X:25:DG:C6	2.88	0.41
4:X:29:DA:H4'	4:X:30:DC:H5'	2.03	0.41
7:o:154:CYS:O	7:o:185:GLY:HA2	2.20	0.41
7:o:202:TRP:NE1	7:o:209:SER:OG	2.54	0.41
7:o:365:THR:HG22	7:o:482:PHE:CD2	2.55	0.41
7:o:514:GLU:CD	8:p:1101:GLN:HB3	2.46	0.41
7:o:713:VAL:O	7:o:717:ILE:HG13	2.20	0.41
7:o:1374:VAL:HG11	7:o:1411:LEU:HD21	2.02	0.41
8:p:230:ARG:O	8:p:231:PRO:C	2.63	0.41
8:p:605:ARG:O	8:p:605:ARG:HG3	2.20	0.41
8:p:809:VAL:HG21	9:q:60:HIS:CE1	2.56	0.41
13:u:101:ILE:HD11	13:u:145:LEU:HD11	2.02	0.41
13:u:118:GLU:O	13:u:128:TYR:HA	2.21	0.41
14:v:64:LEU:HD23	14:v:64:LEU:HA	1.91	0.41
4:X:42:DC:H2''	4:X:43:DC:C6	2.55	0.41
6:Z:8:U:H2'	6:Z:9:C:H6	1.85	0.41
7:o:102:LYS:HB3	7:o:102:LYS:HE3	1.81	0.41
7:o:548:PHE:CE1	7:o:555:LEU:HD11	2.56	0.41
8:p:52:GLN:O	8:p:53:MET:C	2.64	0.41
11:s:94:MET:HE3	11:s:99:ILE:O	2.20	0.41
3:T:31:TRP:CD1	3:T:62:LEU:HD21	2.56	0.41
3:T:43:LEU:HD12	3:T:55:SER:O	2.21	0.41
7:o:992:LYS:HD3	7:o:992:LYS:HA	1.85	0.41
8:p:675:LEU:HD23	8:p:695:HIS:HB2	2.03	0.41
8:p:721:ARG:HD3	8:p:721:ARG:HA	1.85	0.41
11:s:73:PHE:CE1	11:s:99:ILE:HD13	2.55	0.41
1:N:2:TRX:CE2	7:o:779:ILE:HG23	2.51	0.41
7:o:187:TYR:H	7:o:207:GLU:HG2	1.85	0.41
7:o:340:LYS:O	7:o:344:LYS:HB2	2.21	0.41
7:o:456:VAL:HG21	7:o:503:LEU:HD11	2.03	0.41
7:o:589:LYS:HZ3	7:o:625:ASP:CG	2.29	0.41
7:o:1128:ILE:CG2	7:o:1414:ILE:HB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:497:LYS:HA	8:p:497:LYS:HD2	1.74	0.41
9:q:60:HIS:CD2	9:q:62:GLU:HG2	2.45	0.41
9:q:193:ARG:HG2	9:q:220:TYR:HD1	1.84	0.41
14:v:6:PHE:HB3	14:v:60:ILE:HB	2.03	0.41
14:v:48:TYR:OH	14:v:147:LYS:HG3	2.20	0.41
1:n:1:ILX:CB	7:o:791:GLN:HE22	2.34	0.41
7:o:346:LYS:HE2	7:o:346:LYS:HB3	1.92	0.41
7:o:1289:GLU:O	7:o:1293:LEU:HG	2.21	0.41
8:p:1086:PHE:HE2	8:p:1094:GLN:HG3	1.86	0.41
9:q:73:LEU:HB3	9:q:127:VAL:HG13	2.02	0.41
8:p:410:ASN:O	8:p:414:GLU:HG2	2.21	0.40
8:p:591:ARG:NH2	8:p:592:ARG:HE	2.17	0.40
8:p:677:MET:CE	8:p:700:PRO:HB3	2.51	0.40
8:p:962:THR:O	16:x:9:THR:HG23	2.21	0.40
4:X:3:DA:H2"	4:X:4:DA:C8	2.55	0.40
7:o:111:CYS:HB3	7:o:114:CYS:HB3	2.02	0.40
7:o:255:VAL:HG13	7:o:280:LEU:HD13	2.03	0.40
7:o:267:GLN:C	7:o:269:SER:H	2.29	0.40
8:p:603:MET:HE3	8:p:603:MET:HB2	1.92	0.40
18:z:15:MET:HG3	18:z:46:LYS:HE2	2.02	0.40
2:S:164:TRP:CH2	2:S:167:ARG:HD3	2.57	0.40
3:T:30:GLN:O	3:T:62:LEU:HD11	2.22	0.40
7:o:330:GLN:HB3	7:o:336:LEU:HG	2.04	0.40
7:o:687:ILE:HD13	7:o:765:ASN:HB2	2.02	0.40
7:o:784:VAL:HG13	8:p:978:ILE:HD11	2.02	0.40
7:o:1040:LEU:HA	7:o:1040:LEU:HD12	1.87	0.40
17:y:20:THR:OG1	17:y:34:THR:HB	2.21	0.40
4:X:35:DC:H2"	4:X:36:DT:C7	2.51	0.40
7:o:102:LYS:HZ1	7:o:141:LEU:HD13	1.86	0.40
7:o:123:ASN:ND2	7:o:125:LYS:HB2	2.37	0.40
7:o:226:LYS:HB3	7:o:226:LYS:HE2	1.91	0.40
7:o:962:ASP:HB3	7:o:1043:ILE:HG23	2.02	0.40
8:p:712:PRO:O	8:p:939:HIS:HE1	2.04	0.40
8:p:747:LEU:HA	8:p:810:PHE:CE1	2.55	0.40
9:q:20:LYS:HG3	9:q:232:ASN:ND2	2.30	0.40
11:s:48:PRO:HA	11:s:53:PRO:HG2	2.02	0.40
13:u:104:MET:HE2	13:u:104:MET:HB3	1.94	0.40
13:u:110:ARG:HA	13:u:113:ILE:HD12	2.04	0.40
7:o:99:PHE:HB3	7:o:248:MET:HB3	2.04	0.40
7:o:945:ASN:HB2	7:o:948:ILE:HG13	2.02	0.40
8:p:796:MET:HG2	8:p:965:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:1040:GLN:CD	8:p:1040:GLN:H	2.29	0.40
15:w:117:PRO:HB2	15:w:118:HIS:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
2	S	134/517 (26%)	134 (100%)	0	0	100	100
3	T	99/249 (40%)	95 (96%)	4 (4%)	0	100	100
7	o	1448/1970 (74%)	1394 (96%)	52 (4%)	2 (0%)	48	71
8	p	1142/1174 (97%)	1074 (94%)	65 (6%)	3 (0%)	36	59
9	q	253/275 (92%)	245 (97%)	8 (3%)	0	100	100
10	r	126/142 (89%)	126 (100%)	0	0	100	100
11	s	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
12	t	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
13	u	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
14	v	146/150 (97%)	139 (95%)	6 (4%)	1 (1%)	18	40
15	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
16	x	65/67 (97%)	63 (97%)	0	2 (3%)	3	8
17	y	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
18	z	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
All	All	4140/5361 (77%)	3966 (96%)	166 (4%)	8 (0%)	44	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	o	910	LYS
16	x	28	GLU
8	p	549	SER
14	v	34	SER
16	x	6	ARG
8	p	570	ASN
7	o	184	CYS
8	p	614	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	2/2 (100%)	2 (100%)	0	100	100
2	S	121/448 (27%)	120 (99%)	1 (1%)	73	84
3	T	85/218 (39%)	85 (100%)	0	100	100
7	o	1280/1749 (73%)	1262 (99%)	18 (1%)	59	76
8	p	1001/1027 (98%)	986 (98%)	15 (2%)	57	75
9	q	234/252 (93%)	231 (99%)	3 (1%)	61	77
10	r	118/126 (94%)	118 (100%)	0	100	100
11	s	191/192 (100%)	191 (100%)	0	100	100
12	t	71/111 (64%)	71 (100%)	0	100	100
13	u	152/153 (99%)	151 (99%)	1 (1%)	76	86
14	v	129/131 (98%)	127 (98%)	2 (2%)	55	74
15	w	103/112 (92%)	102 (99%)	1 (1%)	68	81
16	x	56/56 (100%)	55 (98%)	1 (2%)	51	72
17	y	104/106 (98%)	103 (99%)	1 (1%)	68	81
18	z	41/55 (74%)	41 (100%)	0	100	100
All	All	3688/4738 (78%)	3645 (99%)	43 (1%)	61	78

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

Mol	Chain	Res	Type
2	S	170	VAL
7	o	46	THR
7	o	48	GLU
7	o	184	CYS
7	o	302	VAL
7	o	484	LEU
7	o	488	VAL
7	o	490	THR
7	o	495	ASP
7	o	534	VAL
7	o	626	THR
7	o	636	ILE
7	o	675	VAL
7	o	676	ILE
7	o	1087	VAL
7	o	1207	ILE
7	o	1279	MET
7	o	1385	VAL
7	o	1458	ILE
8	p	18	THR
8	p	42	GLN
8	p	51	ILE
8	p	59	VAL
8	p	235	ILE
8	p	279	VAL
8	p	423	ILE
8	p	466	VAL
8	p	471	ASN
8	p	598	VAL
8	p	860	VAL
8	p	908	MET
8	p	909	VAL
8	p	921	ILE
8	p	1067	ILE
9	q	13	GLU
9	q	44	ILE
9	q	75	SER
13	u	85	VAL
14	v	47	ILE
14	v	58	LEU
15	w	95	VAL
16	x	14	VAL
17	y	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	44	GLN
2	S	178	GLN
3	T	59	ASN
3	T	64	ASN
7	o	62	GLN
7	o	181	HIS
7	o	449	HIS
7	o	531	ASN
7	o	539	GLN
7	o	599	HIS
7	o	671	ASN
7	o	721	HIS
7	o	731	ASN
7	o	780	ASN
7	o	791	GLN
7	o	792	ASN
7	o	804	HIS
7	o	888	GLN
7	o	904	GLN
7	o	1032	GLN
7	o	1044	HIS
7	o	1082	HIS
7	o	1093	GLN
7	o	1163	HIS
7	o	1190	GLN
7	o	1194	ASN
7	o	1230	GLN
7	o	1410	HIS
7	o	1417	HIS
7	o	1422	GLN
7	o	1445	HIS
7	o	1462	GLN
8	p	43	GLN
8	p	68	GLN
8	p	117	ASN
8	p	144	HIS
8	p	164	ASN
8	p	245	GLN
8	p	312	GLN
8	p	387	HIS
8	p	430	ASN

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Mol	Chain	Res	Type
8	p	481	HIS
8	p	486	ASN
8	p	500	GLN
8	p	518	HIS
8	p	525	ASN
8	p	639	HIS
8	p	699	HIS
8	p	725	GLN
8	p	755	GLN
8	p	797	ASN
8	p	838	GLN
8	p	941	GLN
8	p	948	GLN
8	p	1071	ASN
8	p	1094	GLN
8	p	1142	ASN
9	q	18	ASN
9	q	190	ASN
9	q	232	ASN
9	q	262	GLN
10	r	66	ASN
10	r	129	GLN
11	s	35	GLN
11	s	64	HIS
12	t	46	GLN
13	u	14	HIS
13	u	53	ASN
14	v	131	ASN
15	w	41	ASN
15	w	118	HIS
17	y	49	GLN
17	y	69	HIS
18	z	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Z	12/13 (92%)	6 (50%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	Z	6	C
6	Z	7	U
6	Z	8	U
6	Z	12	C
6	Z	13	U
6	Z	17	G2L

There are no RNA pucker outliers to report.

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

5 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
6	G2L	Z	17	6,5,20	23,26,30	1.20	3 (13%)	31,38,44	2.12	7 (22%)
1	HYP	N	8	1	7,8,9	0.83	0	5,10,12	2.34	2 (40%)
1	CSX	N	6	1	3,6,7	1.08	0	1,6,8	2.14	1 (100%)
1	ILX	N	1	1	8,9,10	0.63	0	8,11,13	1.40	1 (12%)
1	TRX	N	2	1	15,16,17	1.11	1 (6%)	17,22,24	0.96	0

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
6	G2L	Z	17	6,5,20	-	2/9/27/31	0/3/3/3
1	HYP	N	8	1	-	0/0/11/13	0/1/1/1
1	CSX	N	6	1	-	2/2/5/7	-
1	ILX	N	1	1	-	7/11/12/14	-
1	TRX	N	2	1	-	2/5/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	17	G2L	C5-C4	3.18	1.47	1.38
6	Z	17	G2L	C6-N1	-2.41	1.34	1.38
1	N	2	TRX	CD2-CE2	2.40	1.44	1.41
6	Z	17	G2L	C5-N7	-2.01	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	17	G2L	C5-C4-N3	-6.22	118.49	128.39
6	Z	17	G2L	C2-N3-C4	5.04	120.98	112.30
6	Z	17	G2L	N9-C4-N3	4.57	135.09	125.95
1	N	8	HYP	CB-CG-CD	3.43	106.97	103.16
1	N	8	HYP	O-C-CA	-3.31	116.25	124.77
6	Z	17	G2L	C6-C5-N7	3.21	136.14	130.29
1	N	1	ILX	OD1-CD1-CG1	-3.05	104.75	111.16
6	Z	17	G2L	C3'-C2'-C1'	2.72	105.86	99.89
6	Z	17	G2L	C4-C5-N7	-2.62	106.52	110.67
1	N	6	CSX	CA-CB-SG	2.14	118.21	113.17
6	Z	17	G2L	O6-C6-C5	-2.08	121.06	126.53

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	ILX	C-CA-CB-CG2
1	N	1	ILX	OD1-CD1-CG1-CB
1	N	1	ILX	OD1-CD1-CG1-OG1
1	N	6	CSX	N-CA-CB-SG
1	N	6	CSX	C-CA-CB-SG
6	Z	17	G2L	C3'-C4'-C5'-O5'
1	N	2	TRX	CA-CB-CG-CD2
6	Z	17	G2L	O4'-C4'-C5'-O5'
1	N	2	TRX	CA-CB-CG-CD1
1	N	1	ILX	C-CA-CB-CG1
1	N	1	ILX	N-CA-CB-CG2
1	N	1	ILX	CG2-CB-CG1-CD1
1	N	1	ILX	CG2-CB-CG1-OG1

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	17	G2L	4	0
1	N	1	ILX	5	0
1	N	2	TRX	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
21	W0F	p	1201	-	34,35,35	4.05	14 (41%)	43,55,55	3.45	17 (39%)

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
21	W0F	p	1201	-	-	3/24/40/40	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	p	1201	W0F	P26-O29	13.80	1.74	1.59
21	p	1201	W0F	C03-C04	-9.74	1.27	1.52
21	p	1201	W0F	P22-O25	8.41	1.68	1.59
21	p	1201	W0F	O05-C04	6.90	1.60	1.45
21	p	1201	W0F	O05-C06	-5.97	1.28	1.42
21	p	1201	W0F	C12-C13	5.68	1.47	1.38
21	p	1201	W0F	P26-O25	5.30	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	p	1201	W0F	C13-N09	-3.20	1.34	1.37
21	p	1201	W0F	C07-C03	-2.96	1.46	1.53
21	p	1201	W0F	C20-C04	2.56	1.59	1.51
21	p	1201	W0F	C06-N09	2.34	1.54	1.47
21	p	1201	W0F	P22-O21	2.16	1.67	1.59
21	p	1201	W0F	C12-N11	-2.12	1.34	1.39
21	p	1201	W0F	C17-N16	-2.08	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	p	1201	W0F	O05-C06-N09	-14.57	75.35	108.36
21	p	1201	W0F	C07-C06-N09	8.28	136.31	113.25
21	p	1201	W0F	O05-C04-C03	-5.80	92.69	104.92
21	p	1201	W0F	O27-P26-O25	-5.28	92.99	107.27
21	p	1201	W0F	O05-C04-C20	4.94	125.15	109.33
21	p	1201	W0F	O05-C06-C07	-4.15	97.74	106.62
21	p	1201	W0F	O21-C20-C04	3.97	122.52	108.99
21	p	1201	W0F	O32-P30-O29	3.91	117.75	104.64
21	p	1201	W0F	O33-P30-O31	-3.37	97.70	110.83
21	p	1201	W0F	C06-N09-C10	-3.24	117.53	126.73
21	p	1201	W0F	O08-C07-C06	2.82	119.80	110.10
21	p	1201	W0F	O33-P30-O29	2.66	113.55	104.64
21	p	1201	W0F	O29-P26-O28	2.28	117.56	110.70
21	p	1201	W0F	O21-P22-O24	-2.28	99.91	108.94
21	p	1201	W0F	O27-P26-O29	2.15	113.09	107.27
21	p	1201	W0F	C13-C12-N11	-2.11	106.52	109.26
21	p	1201	W0F	C10-N09-C13	2.08	108.42	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

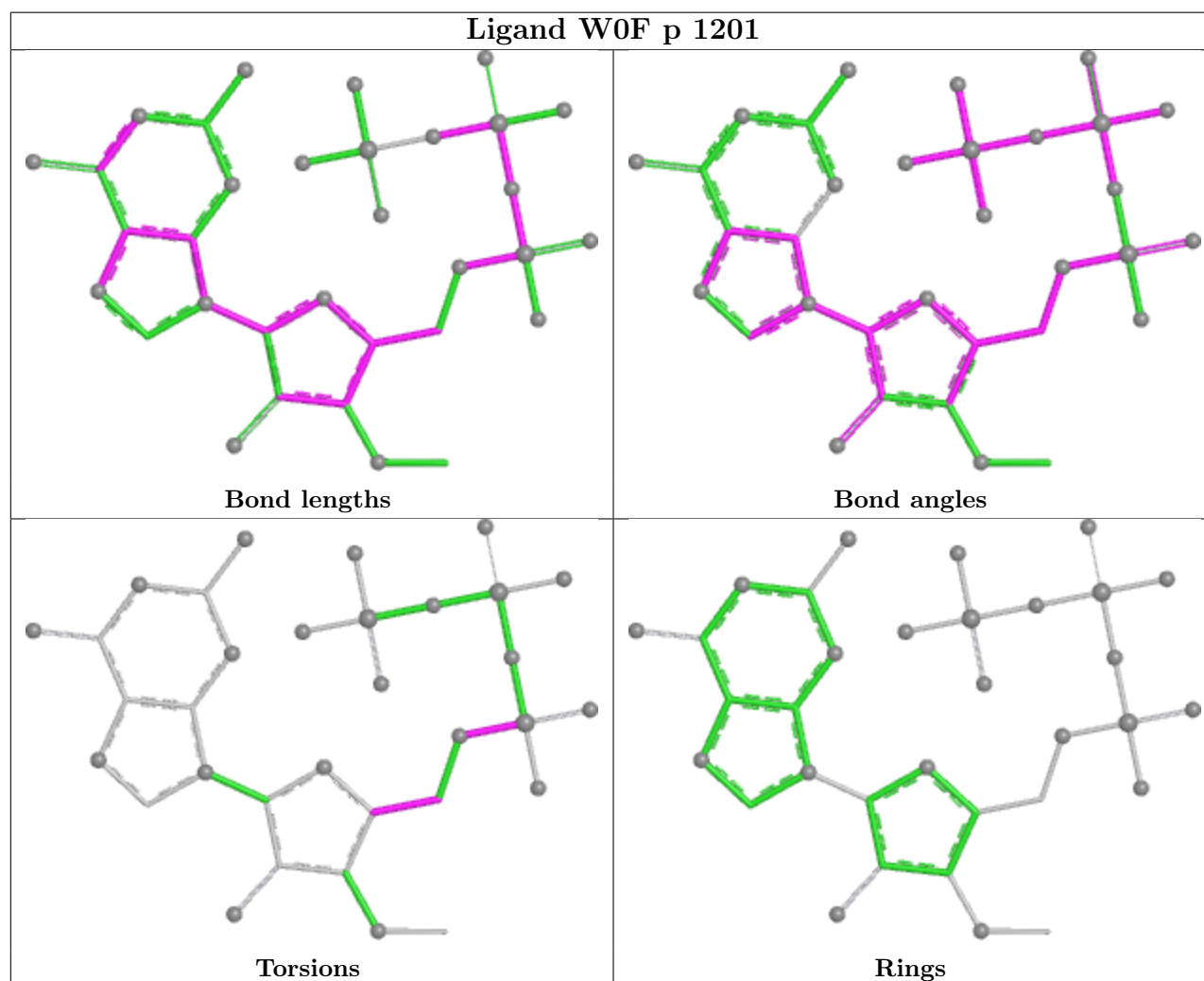
Mol	Chain	Res	Type	Atoms
21	p	1201	W0F	C20-O21-P22-O24
21	p	1201	W0F	C20-O21-P22-O25
21	p	1201	W0F	C03-C04-C20-O21

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	p	1201	W0F	6	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37411. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section was not generated.