



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 04:20 PM EST

PDB ID : 7RIY
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 2 soaked with UTP
Authors : Oh, J.; Dervan, P.B.; Wang, D.
Deposited on : 2021-07-20
Resolution : 3.70 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	:	2.25
buster-report	:	1.1.7 (2018)
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)	:	2.25

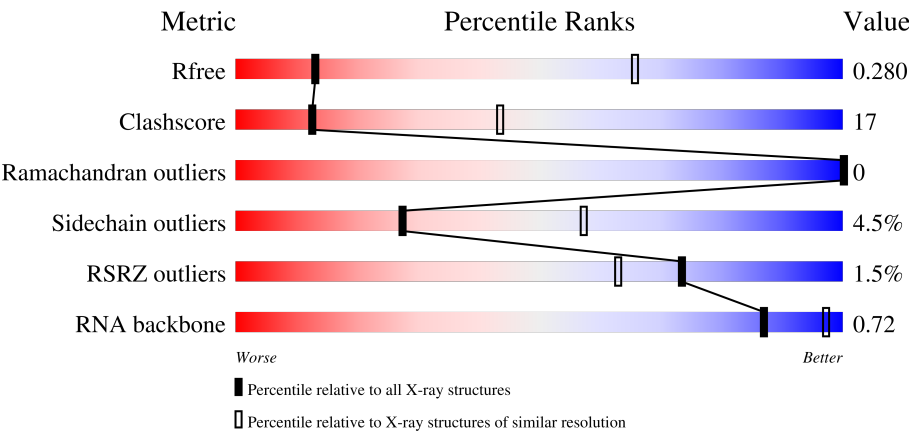
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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 of 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 $\leq 5\%$. 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	R	11	<div><div>18%</div><div>64%</div><div>18%</div></div>
2	T	30	<div><div>20%</div><div>63%</div><div>13%</div></div>
3	N	20	<div><div>40%</div><div>30%</div><div>30%</div></div>
4	A	1733	<div><div>2%</div><div>49%</div><div>29%</div><div>20%</div></div>

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29168 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			525	252	84	163	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			293	138	63	78	14			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

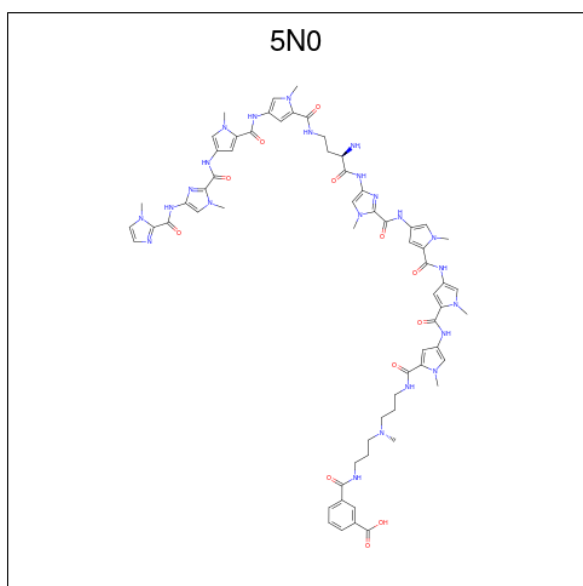
- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	R	1	Total	Mg	0	0
			1	1		

- Molecule 15 is 3-({3-[(3-[(4-[(4-[(2R)-2-amino-4-[(1-methyl-4-[(1-methyl-4-[(1-methyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methyl)amino]propyl}carbamoyl)benzoic acid (three-letter code: 5N0) (formula: C₆₄H₇₅N₂₃O₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	T	1	Total	C	N	O	0	0
			99	64	23	12		

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

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

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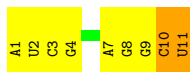
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: RNA

Chain R: 



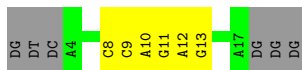
• Molecule 2: Template strand DNA

Chain T: 



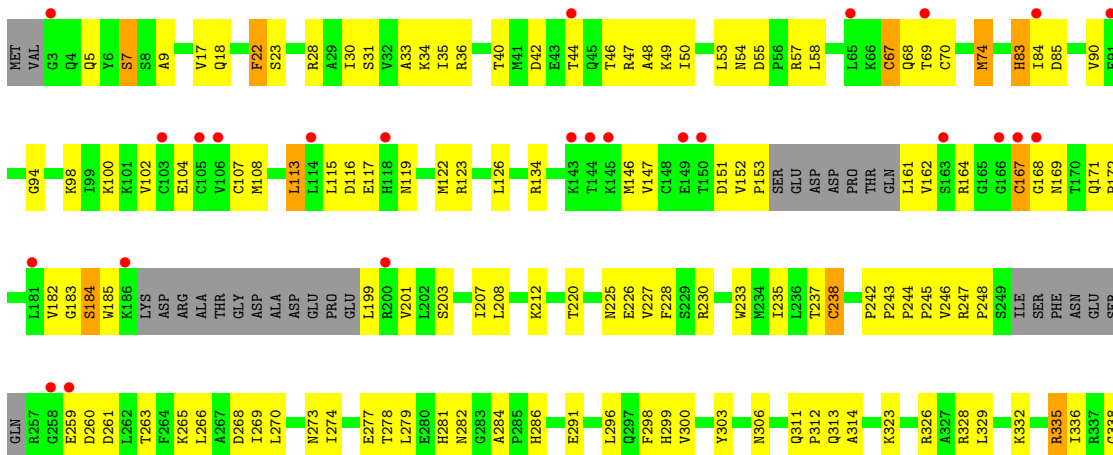
• Molecule 3: Non-template strand DNA

Chain N: 



• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

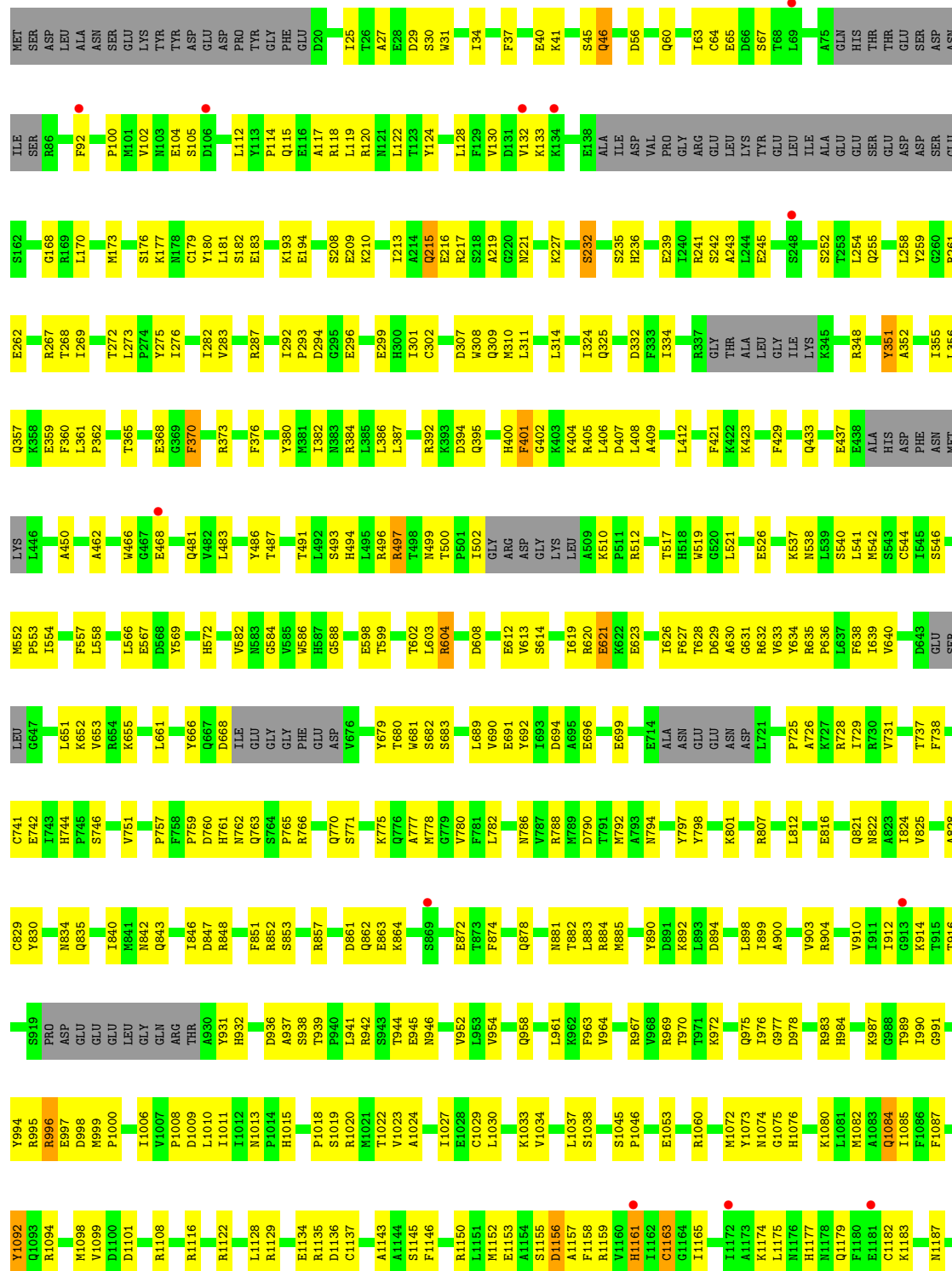
Chain A: 

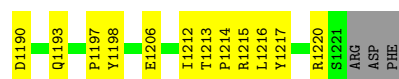


PRO	THR	PRO	THR	PRO	THR	GLY	VAL	GLY	GLU	C1400	V1308	S1229	R1135	V1044	W954	T848	N717	1607	K533	P481	K343
THR	SER	TYR	SER	PRO	ALA	GLY	SER	LEU	SER	S1401	M1312	E1230	I1138	V1045	P955	D853	V718	1608	L534	V442	K344
PRO	PRO	SER	SER	PRO	VAL	VAL	PRO	VAL	LEU	E1402	E1315	D1233	E1139	L1046	P957	N854	D609	6610	R537	F443	V345
TYR	SER	THR	GLY	ASN	ALA	ASN	PRO	GLY	ASN	V1406	V1316	K1235	H1140	A1051	N958	T855	F721	1612	D538	N445	D346
SER	PRO	SER	PHE	SER	ALA	ALA	THR	THR	ASP	V1410	V1319	I1237	L1143	R1055	I960	R857	K738	1613	I541	R446	F347
PRO	THR	SER	SER	PRO	ASP	ASP	PRO	PRO	ASP	E1411	V1322	I1239	T1147	P1060	R961	R859	N741	6614	E542	Q447	R350
THR	THR	TYR	THR	THR	VAL	VAL	THR	THR	THR	A1412	I1322	C1239	E1151	G1061	I964	N858	N742	6618	L543	T351	V352
PRO	PRO	PRO	THR	THR	VAL	VAL	PRO	PRO	PRO	E1417	P1324	R1241	I1152	E1062	N965	L860	Q745	6619	Q544	S449	
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PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO	G1423	Y1328	PRO	E1165	L1067	D974	E870	I759	6629	M456	A459	E360
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PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO	A1440	I1341	GLU	S1175	I1072	K984	L883	I775	6639	P562	S473	A371
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PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1357	GLU	GLU	GLY	L993	D890	E801	6654	K573	Y383	Y383
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1358	GLU	GLU	GLY	L993	D890	E801	6655	K574	M487	D386
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		D1359	GLU	GLU	GLY	L993	D890	E801	6656	K575	N488	R387
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PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6696	H603	D626	I436
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PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6700	H603	D626	I436
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6701	H603	D626	I436
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6702	H603	D626	I436
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6703	H603	D626	I436
PRO	PRO	PRO	PRO	PRO	VAL	VAL	PRO	PRO	PRO		Y1399	GLU	GLU	GLY	L993	D890	E801	6704	H603	D626	I436
PRO	PRO	PRO	PRO	PRO	VAL																

ALA
TYR
SER
PRO
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
ASN
ARG

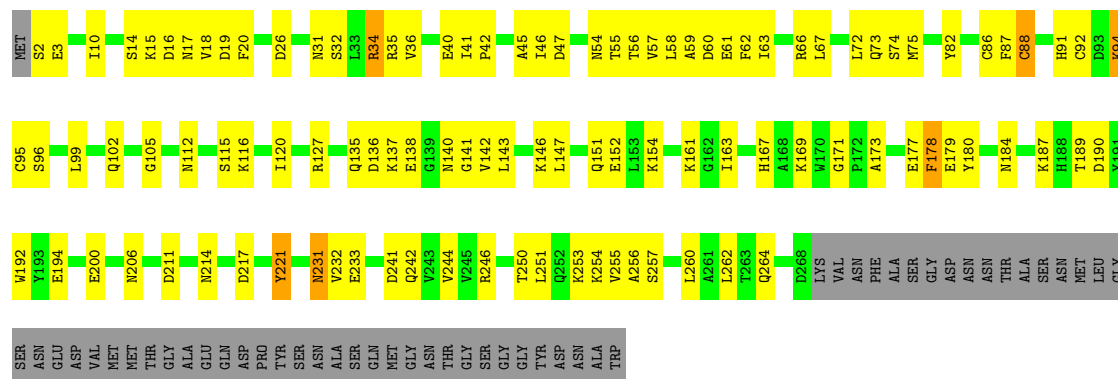
● Molecule 5: DNA-directed RNA polymerase II subunit RPB2





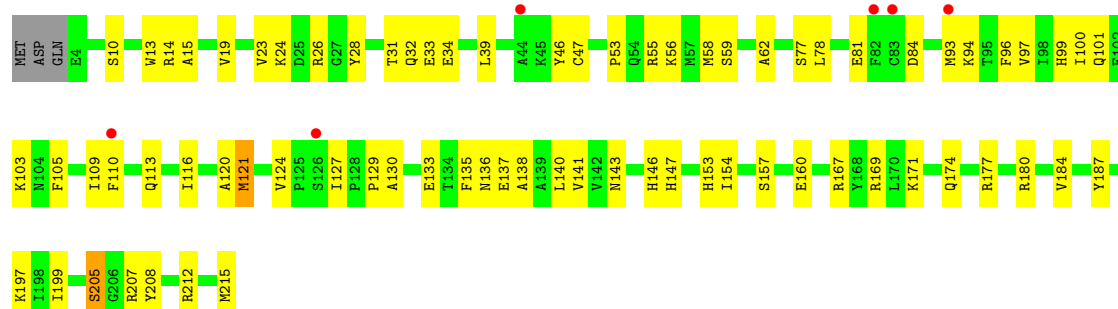
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C: 50% 32% 16%



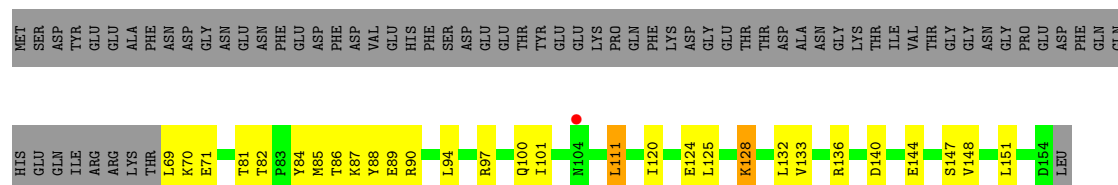
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 3% 64% 33% 2%



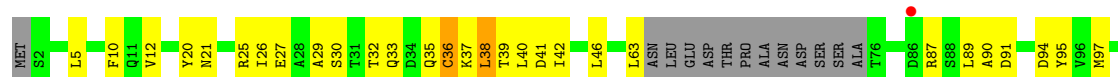
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 37% 17% 45%



• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 2% 56% 32% 9%

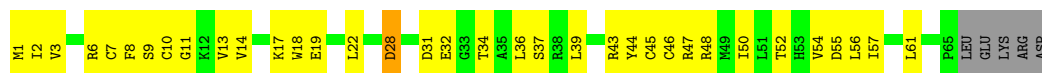




- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



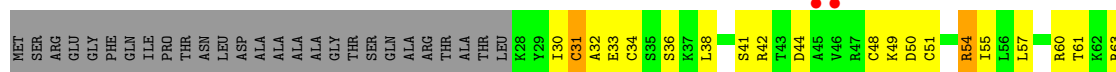
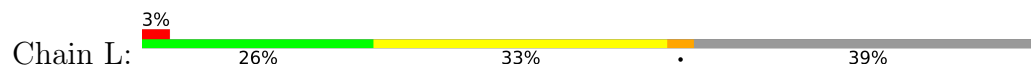
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.78Å 222.76Å 192.96Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	49.53 – 3.70 49.53 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.53-3.70) 99.9 (49.53-3.70)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.232 , 0.281 0.232 , 0.280	Depositor DCC
R_{free} test set	1888 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	106.3	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29168	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MG, ZN, 5N0

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	R	0.34	0/263	1.12	0/409
2	T	0.76	0/584	1.09	1/898 (0.1%)
3	N	0.57	0/331	0.79	0/509
4	A	0.29	0/11020	0.48	0/14907
5	B	0.29	0/9030	0.48	0/12186
6	C	0.30	0/2139	0.49	0/2899
7	E	0.28	0/1767	0.46	0/2378
8	F	0.29	0/696	0.48	0/943
9	H	0.28	0/1082	0.51	0/1466
10	I	0.31	0/970	0.50	0/1308
11	J	0.29	0/541	0.48	0/727
12	K	0.30	0/937	0.48	0/1265
13	L	0.28	0/339	0.56	0/450
All	All	0.31	0/29699	0.52	1/40345 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	T	14	DC	O4'-C1'-N1	5.48	111.84	108.00

There are no chirality outliers.

There are no planarity outliers.

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	R	235	0	121	7	0
2	T	525	0	297	32	0
3	N	293	0	156	9	0
4	A	10828	0	10876	386	0
5	B	8859	0	8816	329	0
6	C	2101	0	2056	87	0
7	E	1731	0	1758	50	0
8	F	684	0	692	28	0
9	H	1064	0	1029	38	0
10	I	952	0	897	42	0
11	J	532	0	542	33	0
12	K	919	0	929	30	0
13	L	337	0	352	16	0
14	R	1	0	0	0	0
15	T	99	0	0	5	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
All	All	29168	0	28521	963	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 17.

All (963) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:446:ARG:NH2	4:A:480:ALA:HA	1.53	1.23
4:A:446:ARG:HH21	4:A:480:ALA:CA	1.76	0.98
4:A:446:ARG:HH21	4:A:480:ALA:HA	0.79	0.94
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.46	0.89
4:A:1224:LEU:HD11	4:A:1240:CYS:HB3	1.57	0.84
5:B:118:ARG:NH1	5:B:209:GLU:OE1	2.12	0.82
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.62	0.80
5:B:400:HIS:NE2	5:B:699:GLU:OE1	2.13	0.80
4:A:54:ASN:HD22	4:A:244:PRO:HG3	1.46	0.80
4:A:7:SER:HA	5:B:1175:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.16	0.79
11:J:43:ARG:NH2	11:J:46:CYS:SG	2.56	0.79
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.16	0.79
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.16	0.78
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.16	0.78
4:A:446:ARG:HB2	4:A:487:MET:HE2	1.66	0.78
5:B:604:ARG:NH2	5:B:613:VAL:O	2.16	0.78
4:A:1385:THR:HG22	4:A:1386:ARG:H	1.47	0.78
6:C:17:ASN:HB3	6:C:233:GLU:HG2	1.68	0.76
7:E:14:ARG:HH11	7:E:141:VAL:HG12	1.51	0.76
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.66	0.76
4:A:738:LYS:HE3	6:C:194:GLU:HA	1.69	0.74
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.68	0.74
4:A:1437:GLY:HA3	8:F:88:TYR:HD2	1.53	0.74
10:I:111:THR:HG22	10:I:113:ASP:H	1.51	0.74
4:A:929:LEU:HD21	4:A:983:ILE:HG21	1.70	0.74
2:T:15:DA:H2'	2:T:16:DT:C6	2.23	0.74
4:A:55:ASP:O	4:A:57:ARG:N	2.21	0.73
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.70	0.73
2:T:21:DC:H5'	5:B:1129:ARG:HD3	1.70	0.73
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.21	0.73
5:B:1084:GLN:NE2	6:C:190:ASP:O	2.21	0.72
5:B:104:GLU:OE2	13:L:54:ARG:NH1	2.22	0.72
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.54	0.72
5:B:173:MET:O	5:B:176:SER:OG	2.05	0.72
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.68	0.72
4:A:608:ILE:HB	4:A:613:ILE:HD11	1.70	0.72
7:E:56:LYS:HE2	7:E:84:ASP:HB3	1.72	0.71
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.54	0.71
4:A:506:ALA:HB3	4:A:509:LEU:HG	1.71	0.71
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.24	0.71
5:B:996:ARG:NH2	6:C:173:ALA:O	2.24	0.71
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.54	0.71
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.73	0.70
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.70	0.70
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.72	0.70
4:A:562:THR:O	4:A:576:GLN:NE2	2.24	0.70
6:C:86:CYS:SG	6:C:87:PHE:N	2.64	0.70
5:B:213:ILE:O	5:B:215:GLN:NE2	2.24	0.70
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.26	0.69
2:T:7:DC:H2''	2:T:8:DT:H5''	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:660:ASN:ND2	5:B:1082:MET:HB3	2.07	0.69
4:A:636:GLU:OE2	4:A:966:ASN:ND2	2.25	0.69
5:B:287:ARG:NH1	5:B:324:ILE:O	2.24	0.69
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.38	0.69
5:B:882:THR:OG1	5:B:885:MET:SD	2.51	0.69
6:C:40:GLU:OE1	6:C:254:LYS:HE2	1.93	0.69
4:A:167:CYS:SG	4:A:168:GLY:N	2.66	0.68
4:A:579:SER:HB3	4:A:612:ILE:HG22	1.76	0.68
4:A:67:CYS:HB3	4:A:70:CYS:HB3	1.76	0.68
4:A:183:GLY:O	4:A:199:LEU:N	2.27	0.68
4:A:134:ARG:NH2	4:A:220:THR:O	2.26	0.68
4:A:362:ASP:OD1	4:A:459:ARG:NH1	2.27	0.68
4:A:500:GLU:OE2	5:B:1145:SER:OG	2.11	0.67
5:B:332:ASP:OD1	5:B:348:ARG:NH2	2.27	0.67
4:A:1385:THR:HG22	4:A:1386:ARG:N	2.08	0.67
5:B:629:ASP:O	5:B:632:ARG:NH1	2.27	0.67
4:A:329:LEU:HA	4:A:335:ARG:H	1.60	0.67
4:A:1390:ASN:O	4:A:1399:ARG:NH1	2.27	0.67
4:A:281:HIS:ND1	4:A:282:ASN:OD1	2.27	0.67
4:A:17:VAL:HG22	5:B:1216:LEU:HD22	1.76	0.67
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.28	0.67
5:B:613:VAL:HG23	5:B:628:THR:HG22	1.77	0.67
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.59	0.67
4:A:983:ILE:HG23	4:A:1028:THR:HG21	1.75	0.67
11:J:9:SER:OG	11:J:48:ARG:NH2	2.27	0.67
9:H:37:LYS:H	9:H:126:GLU:HG2	1.60	0.67
5:B:892:LYS:NZ	5:B:904:ARG:O	2.28	0.67
4:A:146:MET:HG3	4:A:147:VAL:HG23	1.76	0.67
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.75	0.67
2:T:13:DT:H2'	2:T:14:DC:C6	2.30	0.66
5:B:219:ALA:HB2	5:B:405:ARG:HD3	1.77	0.66
5:B:619:ILE:HD12	10:I:65:ASP:HB2	1.77	0.66
1:R:11:U:O2'	5:B:1019:SER:OG	2.11	0.66
4:A:1352:VAL:O	4:A:1356:ILE:HD13	1.94	0.66
12:K:100:ALA:O	12:K:104:ASN:ND2	2.28	0.66
5:B:744:HIS:ND1	5:B:746:SER:OG	2.25	0.66
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.78	0.66
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.76	0.66
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.21	0.65
6:C:40:GLU:OE1	6:C:254:LYS:CE	2.45	0.65
10:I:29:CYS:SG	10:I:30:ARG:N	2.68	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:2:SER:OG	6:C:3:GLU:N	2.29	0.65
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.77	0.65
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.25	0.65
5:B:56:ASP:OD2	5:B:177:LYS:NZ	2.29	0.65
4:A:660:ASN:HD21	5:B:1082:MET:HB3	1.61	0.65
6:C:16:ASP:OD2	6:C:135:GLN:NE2	2.29	0.65
1:R:3:C:H2'	1:R:4:G:C8	2.32	0.65
4:A:306:ASN:ND2	4:A:313:GLN:O	2.25	0.65
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.79	0.65
5:B:115:GLN:NE2	5:B:193:LYS:O	2.30	0.65
5:B:402:GLY:HA3	5:B:696:GLU:HG2	1.79	0.65
2:T:19:DG:H2'	2:T:20:DC:C6	2.31	0.64
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.31	0.64
5:B:232:SER:O	5:B:261:ARG:NH2	2.31	0.64
7:E:177:ARG:O	7:E:212:ARG:NH2	2.29	0.64
8:F:82:THR:HG22	8:F:84:TYR:H	1.62	0.64
5:B:640:VAL:HA	5:B:651:LEU:HA	1.80	0.64
4:A:247:ARG:NH1	4:A:263:THR:OG1	2.31	0.64
5:B:176:SER:O	5:B:182:SER:OG	2.12	0.64
5:B:208:SER:OG	5:B:210:LYS:NZ	2.27	0.64
4:A:795:GLU:HG3	5:B:731:VAL:HG11	1.80	0.64
4:A:1276:VAL:HG12	4:A:1277:GLU:H	1.62	0.63
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.79	0.63
4:A:537:ARG:NH1	4:A:602:ASP:OD1	2.31	0.63
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.79	0.63
5:B:566:LEU:HD13	5:B:588:GLY:HA2	1.80	0.63
5:B:63:ILE:HA	5:B:421:PHE:HE2	1.63	0.63
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.26	0.63
1:R:3:C:H2'	1:R:4:G:H8	1.61	0.63
5:B:496:ARG:NH1	5:B:540:SER:O	2.31	0.63
5:B:1006:ILE:HD11	11:J:43:ARG:HB3	1.80	0.63
4:A:541:ILE:HD12	4:A:577:ILE:HG21	1.81	0.63
4:A:663:SER:O	4:A:742:ASN:ND2	2.32	0.63
4:A:1062:GLU:OE2	8:F:88:TYR:OH	2.16	0.63
6:C:169:LYS:NZ	13:L:69:ALA:O	2.25	0.63
4:A:153:PRO:HA	4:A:161:LEU:HB2	1.80	0.62
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.80	0.62
4:A:888:GLY:O	4:A:940:ARG:NH2	2.32	0.62
2:T:11:DG:H2''	2:T:12:DG:C8	2.34	0.62
4:A:825:ILE:HD13	5:B:512:ARG:HB2	1.81	0.62
5:B:680:THR:O	5:B:683:SER:OG	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:182:VAL:HG12	4:A:201:VAL:HA	1.81	0.62
4:A:44:THR:OG1	4:A:46:THR:OG1	2.17	0.62
4:A:547:LEU:HB3	12:K:58:PHE:HE1	1.63	0.62
4:A:882:SER:H	4:A:961:ARG:HH12	1.48	0.62
4:A:1165:GLU:OE2	4:A:1235:LYS:NZ	2.33	0.62
5:B:848:ARG:NH1	11:J:8:PHE:O	2.32	0.62
4:A:807:GLY:HA2	5:B:761:HIS:CD2	2.35	0.62
4:A:1130:GLN:O	4:A:1134:ILE:HG12	1.99	0.62
5:B:612:GLU:O	5:B:632:ARG:NH2	2.32	0.62
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.32	0.62
4:A:31:SER:O	5:B:1183:LYS:NZ	2.27	0.62
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.32	0.62
2:T:19:DG:H2'	2:T:20:DC:H6	1.64	0.62
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.81	0.62
4:A:1212:VAL:O	4:A:1216:ILE:HG13	1.99	0.62
4:A:1312:ASN:ND2	4:A:1315:GLU:OE2	2.32	0.62
10:I:44:TYR:HE1	10:I:46:HIS:HB2	1.64	0.62
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.82	0.61
5:B:481:GLN:OE1	5:B:494:HIS:NE2	2.25	0.61
2:T:16:DT:H2'	2:T:17:DG:C8	2.35	0.61
2:T:17:DG:C2	2:T:18:DA:C8	2.89	0.61
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.31	0.61
6:C:242:GLN:OE1	6:C:246:ARG:NH2	2.33	0.61
7:E:47:CYS:HA	7:E:53:PRO:HA	1.80	0.61
5:B:255:GLN:H	5:B:272:THR:HG22	1.65	0.61
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.35	0.61
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.82	0.61
6:C:66:ARG:NH1	6:C:143:LEU:O	2.33	0.61
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.29	0.61
7:E:55:ARG:NH2	7:E:137:GLU:OE1	2.34	0.61
2:T:18:DA:H2'	2:T:18:DA:N3	2.16	0.61
4:A:407:ARG:NH2	4:A:409:SER:OG	2.33	0.61
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.81	0.61
6:C:184:ASN:ND2	6:C:189:THR:O	2.31	0.61
5:B:1082:MET:HA	6:C:189:THR:HA	1.82	0.60
8:F:128:LYS:NZ	8:F:151:LEU:O	2.33	0.60
4:A:1355:VAL:HG23	4:A:1356:ILE:HD12	1.82	0.60
5:B:309:GLN:OE1	5:B:392:ARG:NH2	2.34	0.60
8:F:97:ARG:NH2	8:F:124:GLU:OE2	2.29	0.60
5:B:822:ASN:O	11:J:48:ARG:NH1	2.32	0.60
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:713:SER:O	4:A:717:ASN:ND2	2.34	0.60
4:A:765:VAL:HG11	4:A:804:TYR:CD2	2.37	0.60
7:E:143:ASN:ND2	7:E:187:TYR:OH	2.35	0.60
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.83	0.60
5:B:227:LYS:N	5:B:395:GLN:OE1	2.28	0.60
5:B:798:TYR:O	5:B:821:GLN:NE2	2.33	0.60
2:T:12:DG:H2''	2:T:13:DT:H5''	1.84	0.60
6:C:56:THR:HG22	6:C:147:LEU:HD21	1.83	0.60
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.84	0.60
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.66	0.60
4:A:273:ASN:ND2	4:A:277:GLU:OE2	2.33	0.59
4:A:808:LEU:O	5:B:728:ARG:NH1	2.34	0.59
6:C:179:GLU:OE1	6:C:206:ASN:ND2	2.35	0.59
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.31	0.59
5:B:384:ARG:NH2	5:B:623:GLU:OE2	2.34	0.59
4:A:771:GLU:N	4:A:822:GLU:OE2	2.33	0.59
5:B:259:TYR:HB2	5:B:268:THR:HG23	1.83	0.59
5:B:1213:THR:OG1	5:B:1215:ARG:NH2	2.35	0.59
10:I:50:THR:HG22	10:I:52:ILE:H	1.66	0.59
4:A:167:CYS:SG	4:A:169:ASN:ND2	2.64	0.59
4:A:306:ASN:ND2	4:A:313:GLN:OE1	2.35	0.59
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.83	0.59
5:B:759:PRO:HD2	5:B:1046:PRO:HG3	1.85	0.59
5:B:995:ARG:HD3	12:K:6:ARG:HH12	1.67	0.59
6:C:47:ASP:OD1	13:L:70:ARG:NH1	2.33	0.59
5:B:996:ARG:NH1	6:C:173:ALA:HB1	2.17	0.59
4:A:533:LYS:HE2	4:A:745:GLN:OE1	2.02	0.59
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.85	0.59
6:C:17:ASN:HA	6:C:232:VAL:O	2.03	0.59
4:A:607:ILE:HG12	4:A:612:ILE:HA	1.84	0.59
4:A:979:SER:OG	4:A:980:ASP:N	2.34	0.59
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.38	0.59
5:B:60:GLN:NE2	5:B:64:CYS:SG	2.76	0.59
5:B:179:CYS:O	5:B:182:SER:OG	2.21	0.59
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.83	0.59
5:B:499:ASN:OD1	5:B:500:THR:N	2.36	0.59
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.35	0.59
4:A:74:MET:O	5:B:1116:ARG:NH2	2.36	0.59
4:A:351:THR:OG1	4:A:352:VAL:N	2.36	0.59
4:A:1165:GLU:OE1	4:A:1194:ARG:NH2	2.36	0.59
4:A:1276:VAL:HG11	4:A:1316:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:27:ALA:O	5:B:30:SER:OG	2.18	0.58
5:B:797:TYR:O	11:J:1:MET:N	2.36	0.58
4:A:274:ILE:O	4:A:278:THR:OG1	2.18	0.58
4:A:707:GLY:O	4:A:1281:ARG:NH1	2.36	0.58
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.36	0.58
4:A:1351:GLU:O	4:A:1355:VAL:HG13	2.03	0.58
5:B:620:ARG:NH2	10:I:89:GLN:OE1	2.35	0.58
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.36	0.58
5:B:1082:MET:HG3	6:C:189:THR:HA	1.85	0.58
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.67	0.58
7:E:113:GLN:HG3	7:E:137:GLU:HB2	1.85	0.58
5:B:299:GLU:OE1	5:B:572:HIS:ND1	2.37	0.58
5:B:653:VAL:HG12	5:B:689:LEU:HB3	1.84	0.58
4:A:841:LEU:HD21	4:A:1105:LEU:HD22	1.85	0.58
10:I:59:VAL:H	10:I:62:ILE:HD13	1.69	0.58
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.27	0.58
9:H:33:GLN:HB3	9:H:35:GLN:HE22	1.69	0.58
10:I:29:CYS:SG	10:I:31:THR:N	2.73	0.58
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.50	0.58
9:H:118:PHE:CZ	9:H:142:LEU:HD12	2.39	0.58
4:A:151:ASP:OD1	4:A:164:ARG:N	2.35	0.57
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.39	0.57
4:A:592:ASP:H	4:A:595:THR:HG21	1.67	0.57
5:B:41:LYS:NZ	5:B:692:TYR:OH	2.27	0.57
4:A:1118:VAL:HG22	4:A:1327:ILE:HD11	1.86	0.57
4:A:515:GLN:HB2	4:A:1071:SER:HB3	1.86	0.57
4:A:960:ILE:HG23	4:A:964:ILE:HD13	1.86	0.57
5:B:25:ILE:HG21	5:B:653:VAL:HG23	1.86	0.57
5:B:128:LEU:HD21	5:B:170:LEU:HB2	1.85	0.57
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.87	0.57
4:A:40:THR:HA	4:A:53:LEU:HD23	1.85	0.57
4:A:446:ARG:NH2	4:A:479:ASN:O	2.36	0.57
8:F:111:LEU:HD23	8:F:111:LEU:H	1.70	0.57
12:K:85:ASP:O	12:K:89:ASN:ND2	2.33	0.57
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.86	0.57
7:E:99:HIS:CD2	7:E:103:LYS:HG3	2.39	0.57
4:A:596:THR:HG22	4:A:598:LEU:H	1.68	0.57
4:A:884:ASP:OD2	4:A:1030:ARG:NH2	2.29	0.57
5:B:1023:VAL:HG12	5:B:1027:ILE:HD11	1.87	0.57
2:T:10:DT:O4	3:N:9:DC:N4	2.38	0.57
4:A:42:ASP:HA	4:A:50:ILE:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.34	0.57
7:E:136:ASN:OD1	7:E:138:ALA:N	2.34	0.57
4:A:663:SER:HB2	5:B:1085:ILE:HA	1.86	0.57
4:A:939:ASP:OD2	4:A:1023:ARG:NH1	2.37	0.57
10:I:92:ARG:O	10:I:95:THR:OG1	2.22	0.57
2:T:9:DC:H2''	2:T:10:DT:H71	1.85	0.56
3:N:11:DG:H2'	3:N:12:DA:C8	2.40	0.56
5:B:770:GLN:O	5:B:770:GLN:NE2	2.39	0.56
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.87	0.56
4:A:1303:GLU:OE2	4:A:1326:ARG:NH1	2.39	0.56
4:A:525:GLN:HB2	5:B:1015:HIS:CD2	2.41	0.56
5:B:1020:ARG:HB2	5:B:1022:THR:HG23	1.86	0.56
11:J:37:SER:OG	11:J:47:ARG:NH2	2.39	0.56
4:A:226:GLU:HG3	4:A:227:VAL:HG23	1.87	0.56
9:H:87:ARG:HA	9:H:87:ARG:HH21	1.69	0.56
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.87	0.56
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.06	0.56
5:B:235:SER:OG	5:B:236:HIS:ND1	2.38	0.56
4:A:563:PRO:HB3	4:A:572:TRP:CE2	2.41	0.56
10:I:19:ASP:O	10:I:23:ASN:HA	2.06	0.56
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.88	0.55
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.73	0.55
5:B:1163:CYS:SG	5:B:1187:ASN:ND2	2.73	0.55
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.88	0.55
4:A:1436:ILE:O	4:A:1440:ALA:N	2.38	0.55
13:L:34:CYS:SG	13:L:36:SER:OG	2.53	0.55
4:A:116:ASP:OD2	4:A:117:GLU:N	2.38	0.55
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.23	0.55
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.40	0.55
4:A:746:MET:SD	5:B:1015:HIS:ND1	2.74	0.55
5:B:221:ASN:OD1	5:B:243:ALA:N	2.32	0.55
5:B:307:ASP:OD1	5:B:392:ARG:NH1	2.30	0.55
5:B:788:ARG:NH1	5:B:790:ASP:OD2	2.36	0.55
5:B:1034:VAL:O	5:B:1038:SER:OG	2.21	0.55
6:C:167:HIS:ND1	6:C:169:LYS:HG2	2.22	0.55
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.72	0.55
5:B:40:GLU:OE1	5:B:682:SER:OG	2.24	0.55
4:A:645:LEU:HD12	4:A:645:LEU:O	2.07	0.55
4:A:1067:LEU:O	4:A:1071:SER:OG	2.20	0.55
5:B:213:ILE:HD12	5:B:497:ARG:HB3	1.89	0.55
4:A:360:GLU:N	4:A:363:GLN:OE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:124:TYR:HH	5:B:179:CYS:HG	1.55	0.55
5:B:546:SER:OG	5:B:631:GLY:N	2.40	0.55
5:B:969:ARG:NH1	6:C:61:GLU:OE2	2.37	0.55
5:B:519:TRP:NE1	5:B:742:GLU:OE1	2.34	0.54
9:H:63:LEU:HB3	9:H:90:ALA:HB2	1.87	0.54
4:A:961:ARG:NH1	4:A:1025:ARG:HH22	2.04	0.54
5:B:210:LYS:HE2	5:B:462:ALA:HA	1.88	0.54
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.22	0.54
6:C:256:ALA:O	6:C:260:LEU:HG	2.06	0.54
5:B:862:GLN:O	5:B:914:LYS:NZ	2.30	0.54
10:I:72:ASP:O	10:I:81:ARG:NH2	2.27	0.54
2:T:25:DC:OP1	5:B:942:ARG:NH2	2.40	0.54
4:A:631:HIS:CE1	4:A:879:GLU:HG2	2.41	0.54
5:B:63:ILE:HA	5:B:421:PHE:CE2	2.42	0.54
10:I:73:ARG:O	10:I:83:ASN:ND2	2.41	0.54
5:B:976:ILE:HA	5:B:990:ILE:HG22	1.90	0.54
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.41	0.54
9:H:5:LEU:HG	9:H:133:ASN:HB3	1.87	0.54
2:T:16:DT:C2	2:T:17:DG:C8	2.95	0.54
4:A:1329:THR:HG22	4:A:1331:SER:H	1.71	0.54
4:A:1385:THR:HG22	4:A:1386:ARG:HG2	1.90	0.54
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.89	0.54
6:C:116:LYS:HD3	6:C:140:ASN:HA	1.89	0.54
4:A:446:ARG:NH2	4:A:480:ALA:CA	2.48	0.54
7:E:180:ARG:N	7:E:215:MET:OXT	2.41	0.54
5:B:423:LYS:NZ	5:B:468:GLU:OE1	2.27	0.54
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.89	0.54
4:A:646:PHE:O	4:A:650:GLN:HG3	2.09	0.54
4:A:1215:ARG:NH1	4:A:1272:THR:O	2.41	0.54
4:A:119:ASN:OD1	4:A:122:MET:N	2.37	0.53
4:A:547:LEU:HB3	12:K:58:PHE:CE1	2.43	0.53
4:A:1095:THR:HG21	4:A:1112:LYS:HB2	1.90	0.53
5:B:1174:LYS:NZ	5:B:1179:GLN:OE1	2.33	0.53
10:I:85:PHE:CD1	10:I:99:LEU:HD13	2.43	0.53
4:A:758:ILE:O	4:A:762:SER:OG	2.26	0.53
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.90	0.53
5:B:487:THR:OG1	5:B:777:ALA:O	2.24	0.53
5:B:599:THR:O	5:B:603:LEU:HG	2.07	0.53
5:B:640:VAL:HG22	5:B:651:LEU:HB3	1.90	0.53
5:B:864:LYS:N	5:B:872:GLU:OE1	2.41	0.53
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:172:PRO:HB2	4:A:183:GLY:HA3	1.90	0.53
4:A:1140:HIS:CE1	4:A:1272:THR:HG22	2.43	0.53
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.90	0.53
9:H:27:GLU:OE2	9:H:38:LEU:O	2.26	0.53
4:A:46:THR:HG22	4:A:47:ARG:H	1.73	0.53
4:A:113:LEU:HD23	4:A:113:LEU:H	1.72	0.53
5:B:899:ILE:HD11	5:B:903:VAL:HG11	1.91	0.53
6:C:251:LEU:O	6:C:255:VAL:HG23	2.09	0.53
7:E:101:GLN:O	7:E:101:GLN:NE2	2.37	0.53
9:H:30:SER:OG	9:H:36:CYS:SG	2.61	0.53
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.44	0.53
6:C:92:CYS:SG	6:C:94:LYS:HG3	2.48	0.53
7:E:62:ALA:HB3	7:E:78:LEU:HD12	1.90	0.53
5:B:544:CYS:HB2	5:B:634:TYR:CE1	2.43	0.53
5:B:553:PRO:O	5:B:557:PHE:N	2.38	0.53
5:B:1116:ARG:HD2	5:B:1198:TYR:CG	2.43	0.53
4:A:152:VAL:O	4:A:162:VAL:N	2.42	0.53
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.41	0.53
4:A:369:SER:OG	12:K:2:ASN:OD1	2.19	0.53
5:B:373:ARG:HE	5:B:567:GLU:CD	2.12	0.53
5:B:944:THR:HG21	5:B:1122:ARG:NH1	2.23	0.53
5:B:1187:ASN:ND2	5:B:1190:ASP:O	2.36	0.53
10:I:92:ARG:HD2	10:I:93:LYS:H	1.74	0.52
4:A:350:ARG:HD2	5:B:1128:LEU:HD11	1.89	0.52
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.91	0.52
12:K:12:LEU:HD12	12:K:12:LEU:H	1.74	0.52
4:A:628:GLY:O	4:A:632:VAL:HG23	2.09	0.52
4:A:1297:GLU:OE2	4:A:1297:GLU:N	2.37	0.52
4:A:858:ASN:HD21	4:A:860:LEU:HB2	1.75	0.52
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.30	0.52
7:E:171:LYS:HB3	7:E:174:GLN:HG3	1.91	0.52
4:A:649:ILE:O	4:A:653:VAL:HG23	2.09	0.52
4:A:1140:HIS:HE1	4:A:1272:THR:HG22	1.72	0.52
6:C:112:ASN:ND2	11:J:19:GLU:OE2	2.43	0.52
4:A:545:GLN:O	4:A:549:MET:HG3	2.09	0.52
10:I:10:CYS:SG	10:I:31:THR:OG1	2.67	0.52
4:A:108:MET:SD	4:A:108:MET:N	2.82	0.52
4:A:336:ILE:HG21	4:A:1401:SER:HA	1.92	0.52
4:A:804:TYR:OH	4:A:816:HIS:NE2	2.31	0.52
4:A:931:GLU:OE2	4:A:991:LYS:NZ	2.37	0.52
4:A:1116:LEU:HD13	4:A:1329:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:384:ARG:HH22	5:B:621:GLU:HG2	1.74	0.52
6:C:34:ARG:HD2	6:C:178:PHE:CD1	2.45	0.52
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.43	0.51
4:A:866:PHE:N	7:E:208:TYR:OH	2.42	0.51
5:B:120:ARG:HB2	5:B:122:LEU:HG	1.91	0.51
5:B:861:ASP:OD1	5:B:862:GLN:N	2.37	0.51
9:H:25:ARG:HD2	9:H:39:THR:HG22	1.92	0.51
4:A:534:LEU:O	4:A:574:GLY:HA3	2.10	0.51
4:A:697:ALA:HA	4:A:702:LEU:HD23	1.93	0.51
5:B:429:PHE:O	5:B:433:GLN:HG3	2.10	0.51
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.36	0.51
5:B:780:VAL:HG21	11:J:56:LEU:HD11	1.93	0.51
1:R:1:A:H2'	1:R:2:U:C6	2.46	0.51
4:A:873:MET:HG3	4:A:957:PRO:HG3	1.93	0.51
5:B:130:VAL:HG23	5:B:132:VAL:HG23	1.93	0.51
8:F:94:LEU:HD21	8:F:125:LEU:HD22	1.93	0.51
4:A:35:ILE:O	4:A:84:ILE:HD13	2.11	0.51
4:A:311:GLN:N	4:A:312:PRO:HD3	2.26	0.51
5:B:497:ARG:HH21	5:B:538:ASN:HD21	1.57	0.51
10:I:72:ASP:N	10:I:72:ASP:OD1	2.43	0.51
4:A:900:ASP:O	4:A:907:THR:OG1	2.28	0.51
5:B:325:GLN:OE1	10:I:12:ASN:ND2	2.44	0.51
5:B:1033:LYS:NZ	5:B:1087:PHE:O	2.32	0.51
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.93	0.51
4:A:806:ARG:NH1	5:B:725:PRO:O	2.42	0.51
8:F:90:ARG:O	8:F:94:LEU:HG	2.11	0.51
4:A:469:ARG:NH2	5:B:991:GLY:O	2.32	0.50
5:B:807:ARG:HG2	5:B:1045:SER:HB3	1.93	0.50
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.39	0.50
4:A:323:LYS:HE2	4:A:328:ARG:HG3	1.93	0.50
4:A:483:ASP:HB2	5:B:987:LYS:HB2	1.92	0.50
4:A:585:GLY:N	4:A:609:ASP:OD1	2.43	0.50
10:I:19:ASP:HB3	10:I:24:ARG:HB2	1.93	0.50
2:T:17:DG:N3	2:T:18:DA:C8	2.79	0.50
4:A:9:ALA:O	5:B:1193:GLN:NE2	2.27	0.50
4:A:569:LYS:HD2	4:A:571:LEU:HD11	1.93	0.50
8:F:128:LYS:NZ	8:F:148:VAL:O	2.27	0.50
4:A:122:MET:O	4:A:126:LEU:HG	2.12	0.50
4:A:881:GLN:NE2	4:A:958:VAL:O	2.34	0.50
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.26	0.50
4:A:1235:LYS:HB3	4:A:1237:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.94	0.50
4:A:557:ASP:OD1	4:A:559:VAL:N	2.44	0.50
4:A:662:PHE:O	5:B:828:ALA:HA	2.11	0.50
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.46	0.50
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.92	0.50
6:C:32:SER:OG	12:K:41:THR:O	2.16	0.50
10:I:103:CYS:SG	10:I:104:LEU:N	2.84	0.50
3:N:10:DA:H2''	3:N:11:DG:C8	2.47	0.50
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.45	0.50
4:A:629:LEU:O	4:A:633:VAL:HG23	2.12	0.50
10:I:71:SER:HB3	10:I:85:PHE:CD2	2.47	0.50
2:T:18:DA:H5''	4:A:332:LYS:NZ	2.27	0.50
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.11	0.50
4:A:843:LYS:NZ	4:A:1401:SER:OG	2.34	0.50
4:A:1323:ASP:OD1	4:A:1325:THR:OG1	2.19	0.50
5:B:977:GLY:HA3	5:B:1099:VAL:HG21	1.93	0.50
7:E:77:SER:HB2	7:E:105:PHE:CD2	2.46	0.50
10:I:25:LEU:HB3	10:I:38:ALA:HB2	1.93	0.50
13:L:42:ARG:N	13:L:44:ASP:OD2	2.42	0.50
4:A:601:LYS:HB2	4:A:603:ASN:OD1	2.12	0.50
5:B:846:ILE:O	5:B:852:ARG:NH2	2.44	0.50
6:C:20:PHE:HE2	6:C:232:VAL:HG23	1.77	0.50
8:F:81:THR:OG1	8:F:144:GLU:OE1	2.23	0.50
4:A:266:LEU:HD11	4:A:303:TYR:CE1	2.47	0.49
4:A:881:GLN:HE21	4:A:956:LEU:HB2	1.77	0.49
6:C:40:GLU:OE1	6:C:254:LYS:HE3	2.12	0.49
9:H:32:THR:HG22	9:H:32:THR:O	2.11	0.49
10:I:44:TYR:CE1	10:I:46:HIS:HB2	2.46	0.49
6:C:34:ARG:HD2	6:C:178:PHE:HD1	1.76	0.49
9:H:29:ALA:HA	9:H:37:LYS:HA	1.93	0.49
9:H:113:ALA:HA	9:H:125:LEU:O	2.11	0.49
15:T:101:5N0:N23	3:N:11:DG:H1'	2.28	0.49
2:T:16:DT:H2'	2:T:17:DG:H8	1.75	0.49
4:A:237:THR:OG1	4:A:238:CYS:N	2.45	0.49
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	2.28	0.49
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.76	0.49
4:A:974:ASP:HA	9:H:136:LYS:HE3	1.94	0.49
6:C:214:ASN:HB2	6:C:217:ASP:CG	2.33	0.49
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.12	0.49
8:F:82:THR:O	8:F:136:ARG:NH1	2.25	0.49
4:A:1229:SER:OG	4:A:1230:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:102:VAL:HG13	5:B:112:LEU:HB2	1.95	0.49
7:E:94:LYS:HA	7:E:97:VAL:HG22	1.95	0.49
10:I:8:ARG:NE	10:I:9:ASP:OD1	2.37	0.49
11:J:2:ILE:HG12	11:J:3:VAL:H	1.77	0.49
11:J:10:CYS:SG	11:J:11:GLY:N	2.85	0.49
4:A:538:ASP:OD2	9:H:21:ASN:N	2.41	0.49
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.94	0.49
5:B:614:SER:OG	5:B:627:PHE:HB2	2.12	0.49
5:B:944:THR:HG21	5:B:1122:ARG:HH12	1.77	0.49
5:B:406:LEU:N	5:B:631:GLY:O	2.42	0.49
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.77	0.49
5:B:878:GLN:HB2	5:B:881:ASN:HB3	1.94	0.49
6:C:66:ARG:NH2	11:J:3:VAL:O	2.38	0.49
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.94	0.49
11:J:44:TYR:O	11:J:48:ARG:HG2	2.13	0.49
4:A:378:GLU:OE1	4:A:434:ARG:NE	2.45	0.49
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.48	0.49
4:A:998:LEU:HD12	4:A:1001:ARG:HH11	1.77	0.49
4:A:1412:ALA:HA	4:A:1417:GLU:HG3	1.94	0.49
5:B:41:LYS:HB3	5:B:45:SER:OG	2.12	0.49
4:A:901:LEU:HA	4:A:907:THR:HG23	1.95	0.48
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.13	0.48
5:B:168:GLY:HA2	5:B:450:ALA:HB1	1.95	0.48
5:B:384:ARG:NH2	5:B:621:GLU:HG2	2.28	0.48
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.35	0.48
6:C:105:GLY:N	6:C:151:GLN:O	2.41	0.48
4:A:100:LYS:O	4:A:104:GLU:N	2.46	0.48
4:A:107:CYS:SG	4:A:171:GLN:NE2	2.86	0.48
4:A:208:LEU:HD21	4:A:212:LYS:HE3	1.95	0.48
4:A:1206:ASP:OD1	4:A:1274:ARG:NH1	2.46	0.48
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.13	0.48
6:C:102:GLN:HB3	6:C:154:LYS:HG3	1.95	0.48
7:E:121:MET:HA	7:E:124:VAL:HG23	1.95	0.48
4:A:440:ASP:O	4:A:460:VAL:HG23	2.13	0.48
4:A:464:PRO:O	12:K:2:ASN:HB3	2.13	0.48
4:A:494:SER:HB3	4:A:496:GLU:OE1	2.14	0.48
4:A:1152:ILE:HB	10:I:44:TYR:HB3	1.94	0.48
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.60	0.48
5:B:437:GLU:N	5:B:437:GLU:OE1	2.47	0.48
5:B:883:LEU:HD12	5:B:884:ARG:H	1.78	0.48
10:I:82:GLU:OE1	10:I:82:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1066:VAL:O	4:A:1070:GLN:HG3	2.13	0.48
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.61	0.48
4:A:1444:MET:HG3	8:F:133:VAL:HG13	1.95	0.48
5:B:1084:GLN:NE2	5:B:1084:GLN:H	2.11	0.48
9:H:10:PHE:CD2	9:H:38:LEU:HD22	2.49	0.48
9:H:12:VAL:HG13	9:H:26:ILE:HD11	1.94	0.48
4:A:22:PHE:CD1	5:B:1213:THR:HG22	2.48	0.48
4:A:1224:LEU:HD12	4:A:1241:ARG:O	2.13	0.48
5:B:638:PHE:HB2	5:B:741:CYS:O	2.13	0.48
6:C:246:ARG:O	6:C:250:THR:OG1	2.30	0.48
9:H:104:PHE:HD2	9:H:114:VAL:HG22	1.78	0.48
10:I:82:GLU:HB3	10:I:104:LEU:HD12	1.96	0.48
11:J:14:VAL:HA	11:J:17:LYS:HD2	1.96	0.48
4:A:396:PRO:HB3	4:A:403:LYS:HA	1.96	0.48
5:B:402:GLY:O	5:B:405:ARG:NH1	2.47	0.48
5:B:936:ASP:OD1	5:B:937:ALA:N	2.46	0.48
11:J:32:GLU:O	11:J:36:LEU:HG	2.13	0.48
4:A:900:ASP:OD1	4:A:926:GLN:NE2	2.47	0.48
4:A:982:THR:N	4:A:985:ASP:OD2	2.47	0.48
5:B:242:SER:OG	5:B:252:SER:O	2.21	0.48
5:B:1080:LYS:HG3	6:C:180:TYR:OH	2.13	0.48
6:C:92:CYS:N	6:C:95:CYS:SG	2.86	0.48
4:A:259:GLU:OE1	4:A:260:ASP:N	2.46	0.48
4:A:544:ASP:N	4:A:544:ASP:OD1	2.45	0.48
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.79	0.48
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.96	0.48
4:A:809:THR:OG1	4:A:812:GLU:OE1	2.32	0.48
4:A:881:GLN:HE22	4:A:958:VAL:C	2.17	0.48
5:B:114:PRO:HG2	5:B:181:LEU:HD11	1.95	0.48
4:A:1116:LEU:HB3	4:A:1308:THR:OG1	2.13	0.48
7:E:31:THR:HB	7:E:34:GLU:HB2	1.96	0.48
4:A:447:GLN:HG2	5:B:1134:GLU:OE2	2.13	0.47
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.14	0.47
4:A:1423:GLY:O	4:A:1427:ASN:ND2	2.47	0.47
5:B:792:MET:SD	5:B:857:ARG:NH2	2.87	0.47
5:B:1030:LEU:O	5:B:1034:VAL:HG23	2.14	0.47
6:C:163:ILE:HD11	12:K:10:PHE:CE1	2.49	0.47
4:A:974:ASP:OD1	4:A:977:LYS:HG2	2.14	0.47
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.96	0.47
5:B:118:ARG:HH21	5:B:194:GLU:CD	2.17	0.47
5:B:60:GLN:NE2	5:B:60:GLN:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:18:GLN:HG2	4:A:228:PHE:CE1	2.49	0.47
5:B:737:THR:OG1	5:B:737:THR:O	2.32	0.47
8:F:86:THR:O	8:F:89:GLU:HG2	2.14	0.47
9:H:104:PHE:HE1	9:H:136:LYS:HB3	1.78	0.47
5:B:334:ILE:HG21	5:B:348:ARG:HB3	1.97	0.47
5:B:365:THR:HG21	5:B:370:PHE:HD1	1.79	0.47
12:K:49:GLU:OE2	12:K:97:LYS:NZ	2.32	0.47
4:A:225:ASN:OD1	4:A:227:VAL:N	2.44	0.47
4:A:768:GLN:HG3	4:A:816:HIS:HA	1.96	0.47
4:A:1060:PRO:HD2	8:F:86:THR:HG21	1.96	0.47
5:B:183:GLU:N	5:B:183:GLU:OE2	2.47	0.47
6:C:254:LYS:O	6:C:257:SER:OG	2.30	0.47
8:F:87:LYS:HE3	8:F:88:TYR:HE1	1.80	0.47
2:T:16:DT:C2	2:T:17:DG:N7	2.82	0.47
4:A:1132:LYS:HD3	4:A:1135:ARG:NH1	2.29	0.47
4:A:1153:TYR:HB2	4:A:1192:LEU:HD23	1.96	0.47
4:A:1168:GLU:HA	4:A:1171:GLN:HB3	1.97	0.47
5:B:115:GLN:O	5:B:119:LEU:HG	2.15	0.47
5:B:408:LEU:HG	5:B:409:ALA:H	1.79	0.47
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.97	0.47
8:F:132:LEU:O	8:F:148:VAL:HG23	2.15	0.47
12:K:24:ASP:OD2	12:K:74:ARG:HD2	2.14	0.47
4:A:42:ASP:N	4:A:49:LYS:HA	2.30	0.47
4:A:268:ASP:HB3	4:A:299:HIS:CE1	2.50	0.47
4:A:457:ALA:O	4:A:507:VAL:HG23	2.14	0.47
4:A:549:MET:HE1	4:A:656:TRP:CD1	2.50	0.47
5:B:634:TYR:HA	5:B:694:ASP:HA	1.96	0.47
5:B:762:ASN:HD21	5:B:1024:ALA:HB3	1.80	0.47
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.48	0.47
5:B:1143:ALA:HB1	5:B:1146:PHE:HB3	1.96	0.47
7:E:28:TYR:CE1	7:E:78:LEU:HG	2.49	0.47
5:B:112:LEU:HD21	5:B:117:ALA:HB2	1.95	0.47
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.96	0.47
6:C:73:GLN:OE1	6:C:75:MET:N	2.42	0.47
4:A:203:SER:O	4:A:207:ILE:HG13	2.15	0.47
4:A:840:ARG:HD2	4:A:1402:PHE:HZ	1.79	0.47
12:K:91:CYS:O	12:K:95:ILE:HG13	2.15	0.47
4:A:117:GLU:O	4:A:123:ARG:HD3	2.15	0.46
4:A:618:GLU:O	4:A:622:VAL:HG12	2.14	0.46
4:A:1030:ARG:NE	4:A:1034:GLU:OE1	2.44	0.46
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:552:MET:HB3	5:B:553:PRO:HD3	1.98	0.46
5:B:816:GLU:N	5:B:816:GLU:OE1	2.48	0.46
5:B:1073:TYR:CD2	5:B:1080:LYS:HG2	2.50	0.46
4:A:592:ASP:O	4:A:595:THR:OG1	2.22	0.46
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	1.98	0.46
4:A:1193:LEU:HB2	4:A:1260:LEU:HD21	1.97	0.46
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.15	0.46
6:C:57:VAL:HG23	6:C:58:LEU:HD23	1.98	0.46
7:E:19:VAL:O	7:E:23:VAL:HG22	2.16	0.46
4:A:122:MET:HE3	4:A:122:MET:HA	1.95	0.46
4:A:537:ARG:HB2	9:H:20:TYR:CE2	2.50	0.46
7:E:93:MET:HB2	7:E:120:ALA:HB1	1.96	0.46
2:T:14:DC:H1'	2:T:15:DA:H1'	1.97	0.46
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.15	0.46
5:B:412:LEU:HB3	5:B:466:TRP:CZ2	2.50	0.46
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.50	0.46
10:I:17:ARG:HG3	10:I:18:GLU:N	2.29	0.46
4:A:343:LYS:HZ3	5:B:1197:PRO:HB3	1.80	0.46
5:B:863:GLU:OE2	5:B:874:PHE:N	2.49	0.46
4:A:42:ASP:HB2	4:A:50:ILE:HG23	1.98	0.46
5:B:872:GLU:HG2	5:B:916:THR:HB	1.97	0.46
5:B:1182:CYS:HB3	5:B:1187:ASN:HB3	1.98	0.46
6:C:59:ALA:O	6:C:63:ILE:HG13	2.16	0.46
12:K:61:TYR:HA	12:K:72:LYS:O	2.15	0.46
3:N:12:DA:H2''	3:N:13:DG:C8	2.51	0.46
5:B:387:LEU:HD23	5:B:387:LEU:HA	1.77	0.46
5:B:542:MET:HB3	5:B:636:PRO:HD2	1.98	0.46
6:C:91:HIS:HB2	6:C:96:SER:OG	2.15	0.46
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.56	0.46
4:A:672:ASP:OD1	4:A:675:THR:OG1	2.21	0.46
4:A:1338:VAL:HG12	4:A:1339:LEU:HD23	1.98	0.46
4:A:1355:VAL:O	4:A:1358:SER:OG	2.34	0.46
5:B:357:GLN:NE2	5:B:368:GLU:HB3	2.31	0.46
6:C:115:SER:OG	6:C:141:GLY:HA3	2.16	0.46
4:A:668:ASP:OD1	6:C:192:TRP:NE1	2.49	0.46
4:A:1437:GLY:HA3	8:F:88:TYR:CD2	2.43	0.46
5:B:1074:ASN:OD1	5:B:1075:GLY:N	2.48	0.46
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.97	0.46
5:B:221:ASN:O	5:B:584:GLY:HA3	2.16	0.46
5:B:770:GLN:OE1	5:B:983:ARG:HA	2.15	0.46
5:B:936:ASP:OD1	5:B:938:SER:OG	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1165:ILE:O	5:B:1217:TYR:OH	2.31	0.46
5:B:652:LYS:HB3	5:B:689:LEU:HD22	1.98	0.45
5:B:661:LEU:HD23	5:B:661:LEU:HA	1.65	0.45
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.51	0.45
5:B:842:ASN:HB2	5:B:999:MET:HE3	1.98	0.45
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.49	0.45
7:E:167:ARG:HA	7:E:167:ARG:HD3	1.68	0.45
11:J:18:TRP:CE2	11:J:22:LEU:HD11	2.51	0.45
13:L:61:THR:HB	13:L:63:ARG:HG3	1.98	0.45
4:A:445:ASN:O	4:A:487:MET:HG2	2.17	0.45
4:A:494:SER:O	4:A:498:ARG:HG3	2.16	0.45
9:H:41:ASP:OD1	9:H:122:LEU:N	2.49	0.45
1:R:1:A:H2'	1:R:2:U:H6	1.80	0.45
4:A:364:VAL:HG12	4:A:458:HIS:HB3	1.97	0.45
4:A:741:ASN:O	4:A:745:GLN:HG3	2.16	0.45
4:A:980:ASP:N	4:A:980:ASP:OD1	2.49	0.45
4:A:1385:THR:CG2	4:A:1386:ARG:H	2.22	0.45
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.98	0.45
5:B:380:TYR:OH	5:B:623:GLU:OE2	2.24	0.45
4:A:279:LEU:HB3	4:A:284:ALA:HB2	1.98	0.45
4:A:1120:LEU:HD22	4:A:1125:ALA:HA	1.97	0.45
5:B:629:ASP:OD2	5:B:630:ALA:N	2.49	0.45
5:B:843:GLN:N	5:B:994:TYR:O	2.37	0.45
5:B:1159:ARG:HH12	5:B:1175:LEU:HD22	1.82	0.45
7:E:46:TYR:CE2	7:E:58:MET:HA	2.52	0.45
4:A:464:PRO:HG2	4:A:465:TYR:CD1	2.52	0.45
4:A:771:GLU:OE2	5:B:510:LYS:NZ	2.48	0.45
5:B:1037:LEU:HD21	11:J:44:TYR:HD2	1.81	0.45
10:I:60:GLN:NE2	10:I:107:SER:OG	2.46	0.45
13:L:64:LEU:HD22	13:L:65:VAL:H	1.82	0.45
4:A:34:LYS:HG2	4:A:83:HIS:HE1	1.82	0.45
4:A:365:GLY:N	4:A:469:ARG:O	2.37	0.45
4:A:1331:SER:OG	4:A:1334:ASP:OD2	2.28	0.45
5:B:898:LEU:HD13	5:B:964:VAL:HG11	1.98	0.45
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.19	0.45
4:A:28:ARG:HH22	4:A:85:ASP:HB3	1.82	0.45
4:A:69:THR:HG22	5:B:1174:LYS:HD3	1.97	0.45
4:A:392:VAL:HG11	4:A:424:ILE:HG12	1.98	0.45
4:A:1263:ILE:O	4:A:1267:MET:HG3	2.17	0.45
5:B:493:SER:OG	5:B:497:ARG:NH2	2.49	0.45
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.51	0.45
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.28	0.45
4:A:1068:ALA:O	4:A:1072:ILE:HG13	2.16	0.45
5:B:554:ILE:O	5:B:558:LEU:N	2.46	0.45
6:C:143:LEU:HD21	6:C:146:LYS:HE3	1.99	0.45
4:A:619:LYS:O	4:A:623:GLY:N	2.35	0.45
4:A:960:ILE:HG21	4:A:1025:ARG:HG2	1.97	0.45
5:B:493:SER:OG	5:B:775:LYS:HE2	2.17	0.45
2:T:22:DT:H2'	2:T:23:DC:H6	1.81	0.45
4:A:28:ARG:HH12	4:A:85:ASP:HB3	1.81	0.45
4:A:94:GLY:HA3	4:A:1410:PHE:CD1	2.51	0.45
4:A:471:ASN:OD1	4:A:472:LEU:N	2.50	0.45
4:A:606:LEU:HB3	4:A:614:PHE:CE1	2.52	0.45
4:A:941:LYS:HA	4:A:941:LYS:HD3	1.54	0.45
4:A:1239:ARG:HH12	4:A:1241:ARG:HH22	1.64	0.45
4:A:1325:THR:HA	7:E:147:HIS:HA	1.97	0.45
5:B:67:SER:HB2	5:B:92:PHE:CD1	2.42	0.45
5:B:325:GLN:HE21	5:B:325:GLN:HB2	1.63	0.45
5:B:936:ASP:OD1	5:B:938:SER:N	2.45	0.45
6:C:82:TYR:CE2	6:C:161:LYS:HG2	2.52	0.45
7:E:184:VAL:HA	7:E:187:TYR:HB3	1.99	0.45
4:A:711:ARG:HH12	10:I:95:THR:HB	1.82	0.44
4:A:841:LEU:HD21	4:A:1105:LEU:CD2	2.46	0.44
5:B:104:GLU:OE1	5:B:120:ARG:NH2	2.47	0.44
5:B:1153:GLU:OE1	5:B:1153:GLU:N	2.51	0.44
6:C:31:ASN:O	6:C:35:ARG:HG3	2.16	0.44
7:E:99:HIS:HD2	7:E:103:LYS:HG3	1.80	0.44
12:K:47:ARG:HD3	12:K:60:ALA:HA	1.98	0.44
13:L:68:GLU:HB2	13:L:70:ARG:HG3	1.99	0.44
4:A:443:LEU:HD11	4:A:455:MET:HE3	1.99	0.44
4:A:951:GLU:O	4:A:954:TRP:NE1	2.30	0.44
5:B:301:ILE:HD13	5:B:382:ILE:HG21	1.99	0.44
5:B:881:ASN:O	5:B:932:HIS:HA	2.17	0.44
7:E:127:ILE:HB	7:E:130:ALA:HB3	1.98	0.44
2:T:10:DT:H2''	2:T:11:DG:C8	2.52	0.44
15:T:101:5N0:O5	4:A:1387:HIS:NE2	2.47	0.44
4:A:571:LEU:HD22	9:H:46:LEU:HD11	1.99	0.44
4:A:714:PHE:O	4:A:718:VAL:HG23	2.17	0.44
4:A:874:ASP:OD1	4:A:875:ALA:N	2.50	0.44
4:A:1267:MET:HA	4:A:1271:ILE:HD13	1.99	0.44
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:282:ILE:HG13	5:B:283:VAL:N	2.32	0.44
6:C:136:ASP:OD1	6:C:137:LYS:N	2.50	0.44
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.58	0.44
2:T:15:DA:H2''	15:T:101:5N0:C22	2.47	0.44
4:A:841:LEU:HD23	4:A:1384:VAL:HG11	1.99	0.44
6:C:115:SER:HB3	6:C:142:VAL:HG22	2.00	0.44
10:I:55:THR:HG22	10:I:55:THR:O	2.17	0.44
5:B:310:MET:HG3	5:B:386:LEU:HD13	2.00	0.44
5:B:770:GLN:HG2	5:B:983:ARG:O	2.17	0.44
5:B:786:ASN:OD1	5:B:967:ARG:NH2	2.50	0.44
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.17	0.44
6:C:99:LEU:HD13	6:C:120:ILE:HA	2.00	0.44
4:A:550:LEU:HD12	4:A:577:ILE:HD13	2.00	0.44
9:H:63:LEU:HB3	9:H:90:ALA:CB	2.47	0.44
9:H:101:ALA:HB2	9:H:116:TYR:HE2	1.83	0.44
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.47	0.44
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.17	0.44
5:B:1159:ARG:HD3	5:B:1161:HIS:HE1	1.83	0.44
4:A:298:PHE:CE2	4:A:314:ALA:HB2	2.52	0.44
4:A:567:LYS:HB3	4:A:568:PRO:HD3	2.00	0.44
4:A:683:ILE:HD13	4:A:683:ILE:HA	1.89	0.44
4:A:1156:PRO:HA	4:A:1190:PRO:HB3	2.00	0.44
12:K:78:THR:HG22	12:K:79:GLU:H	1.83	0.44
4:A:707:GLY:O	4:A:1281:ARG:HD2	2.18	0.43
4:A:993:LEU:HD22	4:A:1046:LEU:HG	2.00	0.43
5:B:751:VAL:HG23	5:B:812:LEU:HD13	2.00	0.43
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.99	0.43
7:E:100:ILE:HD13	7:E:100:ILE:HA	1.85	0.43
2:T:8:DT:H2''	2:T:9:DC:H5'	1.99	0.43
4:A:534:LEU:HD11	4:A:541:ILE:HD11	2.00	0.43
4:A:870:GLU:HG2	7:E:208:TYR:CD2	2.53	0.43
4:A:380:VAL:HG12	4:A:388:LEU:HD13	2.00	0.43
5:B:357:GLN:HE22	5:B:368:GLU:HB3	1.83	0.43
5:B:360:PHE:CE2	5:B:361:LEU:HD13	2.53	0.43
7:E:135:PHE:HD2	7:E:140:LEU:HD11	1.83	0.43
1:R:7:A:H2'	1:R:8:G:H8	1.84	0.43
4:A:608:ILE:HD13	4:A:608:ILE:HA	1.89	0.43
4:A:662:PHE:CE1	4:A:742:ASN:HB3	2.54	0.43
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	2.00	0.43
12:K:8:GLU:O	12:K:37:LYS:HE3	2.19	0.43
2:T:13:DT:H2''	2:T:14:DC:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:689:LYS:HE2	4:A:721:PHE:CZ	2.53	0.43
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.19	0.43
11:J:31:ASP:OD1	11:J:34:THR:OG1	2.24	0.43
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.00	0.43
4:A:881:GLN:OE1	4:A:959:ASN:HA	2.18	0.43
5:B:37:PHE:CE1	5:B:41:LYS:HD2	2.53	0.43
5:B:546:SER:OG	5:B:632:ARG:N	2.50	0.43
5:B:586:TRP:NE1	5:B:588:GLY:O	2.45	0.43
6:C:136:ASP:OD1	6:C:138:GLU:N	2.42	0.43
8:F:87:LYS:HG3	8:F:88:TYR:HD1	1.84	0.43
4:A:765:VAL:CG2	4:A:800:VAL:HB	2.48	0.43
4:A:1355:VAL:HG23	4:A:1356:ILE:CD1	2.49	0.43
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.54	0.43
5:B:972:LYS:NZ	5:B:1101:ASP:OD2	2.38	0.43
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	2.37	0.43
4:A:456:MET:HB2	4:A:478:TYR:OH	2.18	0.43
4:A:1229:SER:OG	4:A:1233:ASP:OD1	2.37	0.43
5:B:334:ILE:HD13	5:B:352:ALA:HB2	2.00	0.43
5:B:759:PRO:CD	5:B:1046:PRO:HG3	2.49	0.43
4:A:538:ASP:HB2	9:H:20:TYR:HD2	1.84	0.43
4:A:1138:ILE:O	4:A:1276:VAL:HG23	2.19	0.43
5:B:567:GLU:OE2	5:B:567:GLU:N	2.48	0.43
5:B:946:ASN:O	5:B:970:THR:OG1	2.31	0.43
7:E:169:ARG:HB3	8:F:140:ASP:HB3	2.01	0.43
9:H:40:LEU:HG	9:H:42:ILE:HG12	2.01	0.43
10:I:80:SER:OG	10:I:103:CYS:SG	2.77	0.43
11:J:17:LYS:HB3	11:J:39:LEU:HD13	2.01	0.43
12:K:13:GLY:H	12:K:16:GLU:HB2	1.83	0.43
15:T:101:5N0:C35	3:N:8:DC:H1'	2.49	0.43
4:A:1001:ARG:HH21	8:F:82:THR:HA	1.83	0.43
5:B:239:GLU:HA	5:B:254:LEU:O	2.19	0.43
7:E:10:SER:O	7:E:14:ARG:HG3	2.18	0.43
7:E:205:SER:O	7:E:207:ARG:N	2.50	0.43
10:I:42:LEU:HD11	10:I:45:ARG:HB2	2.00	0.43
5:B:34:ILE:O	5:B:37:PHE:HB3	2.19	0.42
5:B:401:PHE:HB2	5:B:517:THR:OG1	2.19	0.42
6:C:19:ASP:HB2	6:C:231:ASN:OD1	2.19	0.42
7:E:153:HIS:C	7:E:154:ILE:HD12	2.39	0.42
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.39	0.42
5:B:261:ARG:NE	5:B:262:GLU:OE2	2.48	0.42
5:B:757:PRO:HG2	5:B:984:HIS:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:961:LEU:HD23	5:B:961:LEU:HA	1.77	0.42
6:C:56:THR:HG22	6:C:147:LEU:CD2	2.49	0.42
6:C:60:ASP:OD2	13:L:60:ARG:NH1	2.44	0.42
6:C:92:CYS:SG	6:C:94:LYS:N	2.90	0.42
11:J:57:ILE:O	11:J:61:LEU:HG	2.19	0.42
3:N:11:DG:H2''	3:N:12:DA:H5'	2.00	0.42
4:A:33:ALA:HB2	4:A:58:LEU:HD21	2.02	0.42
4:A:268:ASP:HB3	4:A:299:HIS:NE2	2.34	0.42
4:A:775:ILE:HD13	4:A:775:ILE:HA	1.92	0.42
4:A:899:VAL:HG13	4:A:929:LEU:HD13	2.00	0.42
4:A:42:ASP:N	4:A:48:ALA:O	2.45	0.42
4:A:248:PRO:O	4:A:260:ASP:HB2	2.19	0.42
4:A:298:PHE:CZ	4:A:314:ALA:HB2	2.54	0.42
4:A:711:ARG:NH1	10:I:95:THR:HB	2.35	0.42
5:B:105:SER:HB2	5:B:958:GLN:O	2.19	0.42
6:C:262:LEU:HD11	12:K:87:LEU:HD23	2.00	0.42
9:H:108:SER:HB2	9:H:111:LEU:HB2	2.01	0.42
13:L:30:ILE:HG22	13:L:31:CYS:O	2.19	0.42
4:A:115:LEU:HD12	4:A:119:ASN:HB2	2.02	0.42
4:A:372:LYS:O	4:A:435:HIS:NE2	2.52	0.42
4:A:942:PHE:O	4:A:945:GLU:HG2	2.19	0.42
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.35	0.42
5:B:100:PRO:O	5:B:180:TYR:OH	2.27	0.42
5:B:899:ILE:O	5:B:952:VAL:HG21	2.19	0.42
5:B:1006:ILE:HG23	11:J:45:CYS:HB3	2.02	0.42
6:C:171:GLY:C	6:C:173:ALA:H	2.23	0.42
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.55	0.42
4:A:90:VAL:HG21	4:A:296:LEU:HD12	2.01	0.42
4:A:449:SER:OG	5:B:1134:GLU:HG3	2.20	0.42
5:B:373:ARG:HA	5:B:566:LEU:HD23	2.02	0.42
5:B:405:ARG:NE	5:B:632:ARG:HB3	2.35	0.42
5:B:782:LEU:HD23	5:B:782:LEU:HA	1.82	0.42
7:E:14:ARG:NH1	7:E:141:VAL:HG12	2.28	0.42
9:H:40:LEU:HD13	9:H:123:MET:HB2	2.00	0.42
10:I:113:ASP:OD1	10:I:114:GLN:N	2.53	0.42
4:A:230:ARG:HD3	4:A:233:TRP:CH2	2.55	0.42
4:A:550:LEU:HD23	4:A:556:TRP:CH2	2.55	0.42
4:A:903:ASN:O	4:A:907:THR:OG1	2.20	0.42
5:B:848:ARG:HD2	11:J:8:PHE:HA	2.01	0.42
6:C:73:GLN:OE1	6:C:74:SER:N	2.52	0.42
9:H:27:GLU:OE1	9:H:39:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:900:ALA:HB3	13:L:61:THR:CG2	2.50	0.42
11:J:7:CYS:SG	11:J:9:SER:N	2.92	0.42
11:J:54:VAL:HG12	11:J:56:LEU:HG	2.01	0.42
12:K:77:THR:OG1	12:K:81:TYR:O	2.38	0.42
3:N:12:DA:H4'	3:N:13:DG:OP2	2.16	0.42
4:A:98:LYS:O	4:A:102:VAL:HG12	2.20	0.42
4:A:436:ILE:HD11	4:A:491:VAL:HG11	2.02	0.42
5:B:273:LEU:HD23	5:B:273:LEU:HA	1.87	0.42
6:C:178:PHE:HD2	6:C:179:GLU:N	2.18	0.42
7:E:197:LYS:HE2	7:E:199:ILE:HD11	2.02	0.42
2:T:14:DC:H2''	2:T:15:DA:O4'	2.20	0.41
4:A:30:ILE:HD13	4:A:30:ILE:HA	1.91	0.41
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.41
4:A:1143:LEU:O	4:A:1147:THR:OG1	2.36	0.41
5:B:486:TYR:OH	5:B:794:ASN:ND2	2.52	0.41
5:B:912:ILE:HB	5:B:939:THR:HB	2.01	0.41
6:C:18:VAL:O	6:C:231:ASN:HA	2.20	0.41
8:F:69:LEU:HB3	8:F:70:LYS:H	1.50	0.41
8:F:87:LYS:HG3	8:F:88:TYR:CD1	2.55	0.41
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.59	0.41
13:L:41:SER:N	13:L:44:ASP:OD2	2.52	0.41
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.85	0.41
4:A:853:ASP:OD2	4:A:857:ARG:NH2	2.49	0.41
5:B:258:LEU:HD13	5:B:269:ILE:HG12	2.02	0.41
5:B:526:GLU:OE2	5:B:538:ASN:ND2	2.54	0.41
6:C:14:SER:OG	6:C:15:LYS:N	2.53	0.41
6:C:244:VAL:HG11	12:K:105:PHE:CE2	2.54	0.41
4:A:380:VAL:HG21	4:A:427:GLN:O	2.21	0.41
4:A:573:SER:O	4:A:577:ILE:HG22	2.20	0.41
4:A:1319:VAL:HB	4:A:1322:ILE:HD13	2.02	0.41
5:B:351:TYR:O	5:B:355:ILE:HG13	2.19	0.41
5:B:356:LEU:HD13	5:B:356:LEU:HA	1.82	0.41
5:B:786:ASN:O	5:B:967:ARG:NH2	2.41	0.41
5:B:954:VAL:HG22	5:B:964:VAL:HG13	2.01	0.41
4:A:242:PRO:HB2	4:A:246:VAL:HG21	2.03	0.41
4:A:347:PHE:HB2	5:B:1150:ARG:HH22	1.86	0.41
4:A:569:LYS:HE2	6:C:221:TYR:HB2	2.02	0.41
4:A:1022:LEU:HD12	4:A:1022:LEU:HA	1.91	0.41
4:A:1420:ASP:OD2	4:A:1422:ARG:NH2	2.53	0.41
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.86	0.41
5:B:275:TYR:HE2	5:B:359:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1159:ARG:HD3	5:B:1161:HIS:CE1	2.55	0.41
7:E:23:VAL:O	7:E:28:TYR:HB2	2.20	0.41
2:T:17:DG:C4	2:T:18:DA:C8	3.09	0.41
4:A:273:ASN:O	4:A:277:GLU:HG3	2.19	0.41
4:A:587:HIS:NE2	4:A:969:GLN:HG3	2.36	0.41
4:A:802:ASN:ND2	5:B:729:ILE:O	2.37	0.41
4:A:890:ASP:OD2	4:A:940:ARG:NH1	2.54	0.41
4:A:1121:GLU:HG3	4:A:1122:PRO:HD2	2.01	0.41
5:B:500:THR:HG22	5:B:502:ILE:HG22	2.02	0.41
5:B:666:TYR:O	5:B:668:ASP:N	2.51	0.41
5:B:1060:ARG:NH1	6:C:200:GLU:O	2.54	0.41
6:C:46:ILE:HD13	6:C:67:LEU:O	2.21	0.41
7:E:157:SER:N	7:E:160:GLU:OE1	2.43	0.41
11:J:6:ARG:HD3	11:J:13:VAL:HG12	2.03	0.41
4:A:388:LEU:HD22	4:A:432:VAL:HG11	2.03	0.41
4:A:820:GLY:O	4:A:824:LEU:HG	2.20	0.41
4:A:825:ILE:CD1	5:B:512:ARG:HB2	2.48	0.41
11:J:50:ILE:HD13	11:J:50:ILE:HA	1.88	0.41
4:A:352:VAL:HG21	5:B:1099:VAL:HG22	2.01	0.41
7:E:13:TRP:CE3	7:E:39:LEU:HD13	2.56	0.41
10:I:78:CYS:SG	10:I:80:SER:OG	2.63	0.41
1:R:10:C:H42	2:T:19:DG:H1	1.67	0.41
5:B:46:GLN:H	5:B:46:GLN:HG3	1.65	0.41
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.56	0.41
5:B:394:ASP:OD1	5:B:395:GLN:N	2.50	0.41
5:B:620:ARG:NH1	10:I:68:LEU:HD21	2.36	0.41
9:H:25:ARG:HD2	9:H:39:THR:CG2	2.50	0.41
9:H:26:ILE:HD12	9:H:26:ILE:HA	1.90	0.41
9:H:130:ARG:H	9:H:130:ARG:HE	1.69	0.41
10:I:37:GLU:HG2	10:I:38:ALA:H	1.86	0.41
3:N:11:DG:H2'	3:N:12:DA:H8	1.84	0.41
4:A:184:SER:O	4:A:199:LEU:N	2.53	0.41
4:A:208:LEU:HD23	4:A:235:ILE:HD11	2.02	0.41
4:A:364:VAL:CG1	4:A:458:HIS:HB3	2.50	0.41
4:A:550:LEU:HD12	4:A:577:ILE:CD1	2.50	0.41
4:A:1384:VAL:HA	4:A:1389:PHE:CE2	2.56	0.41
4:A:1441:PHE:HZ	8:F:89:GLU:HA	1.86	0.41
5:B:301:ILE:HG21	5:B:314:LEU:HD11	2.02	0.41
5:B:582:VAL:HA	5:B:626:ILE:O	2.21	0.41
5:B:598:GLU:O	5:B:602:THR:OG1	2.31	0.41
5:B:771:SER:O	5:B:775:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:253:LYS:HB2	6:C:253:LYS:HE3	1.76	0.41
7:E:55:ARG:HD2	7:E:84:ASP:HA	2.02	0.41
7:E:59:SER:HB3	7:E:81:GLU:HA	2.03	0.41
11:J:28:ASP:OD1	11:J:28:ASP:N	2.54	0.41
4:A:1286:LYS:HE2	4:A:1286:LYS:HB2	1.75	0.41
5:B:737:THR:OG1	10:I:66:PRO:O	2.36	0.41
6:C:10:ILE:HD11	12:K:105:PHE:CE1	2.55	0.41
6:C:211:ASP:N	6:C:211:ASP:OD1	2.54	0.41
7:E:116:ILE:HD13	7:E:121:MET:SD	2.61	0.41
8:F:101:ILE:HD13	8:F:120:ILE:HG22	2.02	0.41
2:T:13:DT:H1'	15:T:101:5N0:N6	2.36	0.40
4:A:269:ILE:HD11	4:A:300:VAL:HA	2.03	0.40
4:A:825:ILE:O	4:A:829:VAL:HG23	2.22	0.40
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.21	0.40
4:A:1105:LEU:HD23	4:A:1384:VAL:HG21	2.03	0.40
5:B:512:ARG:H	5:B:512:ARG:HG3	1.55	0.40
5:B:760:ASP:OD1	5:B:760:ASP:N	2.50	0.40
5:B:975:GLN:HG2	5:B:976:ILE:H	1.86	0.40
5:B:1015:HIS:O	5:B:1018:PRO:HD2	2.21	0.40
9:H:95:TYR:CE1	9:H:97:MET:HG3	2.56	0.40
13:L:49:LYS:HG3	13:L:50:ASP:OD1	2.22	0.40
2:T:19:DG:H5'	4:A:832:ALA:O	2.21	0.40
4:A:356:ASP:HB2	4:A:469:ARG:HE	1.86	0.40
4:A:442:VAL:HG12	4:A:491:VAL:HG22	2.03	0.40
4:A:598:LEU:O	9:H:122:LEU:HD12	2.20	0.40
5:B:299:GLU:OE1	5:B:572:HIS:N	2.47	0.40
5:B:1010:LEU:HD23	5:B:1010:LEU:HA	1.89	0.40
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.95	0.40
13:L:31:CYS:SG	13:L:32:ALA:N	2.94	0.40
2:T:3:DT:H2''	2:T:4:DT:H71	2.03	0.40
4:A:279:LEU:HD13	4:A:279:LEU:HA	1.93	0.40
4:A:335:ARG:HE	4:A:335:ARG:HB2	1.61	0.40
4:A:526:ASP:HB2	5:B:835:GLN:CD	2.41	0.40
5:B:726:ALA:HB2	5:B:1053:GLU:HG3	2.03	0.40
5:B:801:LYS:HE2	11:J:52:THR:HA	2.04	0.40
5:B:821:GLN:HB2	5:B:851:PHE:CE2	2.56	0.40
9:H:89:LEU:HB2	9:H:91:ASP:OD2	2.21	0.40
4:A:543:LEU:O	4:A:547:LEU:HG	2.22	0.40
4:A:853:ASP:OD1	4:A:855:THR:OG1	2.33	0.40
4:A:1436:ILE:O	4:A:1439:GLY:N	2.54	0.40
6:C:40:GLU:OE2	6:C:254:LYS:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:15:ALA:HA	7:E:140:LEU:O	2.22	0.40
8:F:97:ARG:HA	8:F:97:ARG:HD2	1.89	0.40
10:I:61:ASP:OD1	10:I:61:ASP:N	2.54	0.40
4:A:1327:ILE:O	7:E:147:HIS:NE2	2.52	0.40
5:B:373:ARG:NE	5:B:567:GLU:OE2	2.54	0.40
5:B:825:VAL:HG21	5:B:1092:TYR:CE1	2.56	0.40
5:B:847:ASP:O	5:B:852:ARG:NH2	2.54	0.40
5:B:977:GLY:HA2	5:B:989:THR:OG1	2.21	0.40
6:C:26:ASP:N	6:C:26:ASP:OD1	2.53	0.40
6:C:55:THR:OG1	6:C:152:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
4	A	1370/1733 (79%)	1264 (92%)	106 (8%)	0	100	100
5	B	1103/1224 (90%)	1030 (93%)	73 (7%)	0	100	100
6	C	265/318 (83%)	245 (92%)	20 (8%)	0	100	100
7	E	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
8	F	84/155 (54%)	78 (93%)	6 (7%)	0	100	100
9	H	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	I	116/122 (95%)	104 (90%)	12 (10%)	0	100	100
11	J	63/70 (90%)	57 (90%)	6 (10%)	0	100	100
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3239 (93%)	254 (7%)	0	100	100

There are no Ramachandran outliers to report.

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 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	
4	A	1194/1520 (79%)	1137 (95%)	57 (5%)	25	56
5	B	955/1061 (90%)	919 (96%)	36 (4%)	33	61
6	C	235/274 (86%)	225 (96%)	10 (4%)	29	58
7	E	193/197 (98%)	188 (97%)	5 (3%)	46	69
8	F	73/137 (53%)	69 (94%)	4 (6%)	21	53
9	H	116/128 (91%)	109 (94%)	7 (6%)	19	50
10	I	110/116 (95%)	102 (93%)	8 (7%)	14	44
11	J	60/65 (92%)	58 (97%)	2 (3%)	38	64
12	K	99/102 (97%)	96 (97%)	3 (3%)	41	66
13	L	37/57 (65%)	32 (86%)	5 (14%)	4	21
All	All	3072/3657 (84%)	2935 (96%)	137 (4%)	27	57

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	7	SER
4	A	22	PHE
4	A	23	SER
4	A	36	ARG
4	A	67	CYS
4	A	68	GLN
4	A	74	MET
4	A	83	HIS
4	A	113	LEU
4	A	167	CYS
4	A	184	SER
4	A	185	TRP
4	A	238	CYS
4	A	261	ASP

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Mol	Chain	Res	Type
4	A	265	LYS
4	A	270	LEU
4	A	286	HIS
4	A	291	GLU
4	A	335	ARG
4	A	383	TYR
4	A	408	ASP
4	A	445	ASN
4	A	446	ARG
4	A	517	ASN
4	A	551	TYR
4	A	573	SER
4	A	593	GLU
4	A	599	SER
4	A	603	ASN
4	A	618	GLU
4	A	629	LEU
4	A	663	SER
4	A	688	LYS
4	A	742	ASN
4	A	821	ARG
4	A	884	ASP
4	A	905	ASP
4	A	906	HIS
4	A	918	GLU
4	A	978	PRO
4	A	979	SER
4	A	1029	ARG
4	A	1100	ARG
4	A	1105	LEU
4	A	1140	HIS
4	A	1174	PHE
4	A	1204	ASP
4	A	1215	ARG
4	A	1218	GLN
4	A	1223	ASP
4	A	1234	GLU
4	A	1274	ARG
4	A	1331	SER
4	A	1359	ASP
4	A	1366	ARG
4	A	1373	ASP

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Mol	Chain	Res	Type
4	A	1400	CYS
5	B	46	GLN
5	B	65	GLU
5	B	133	LYS
5	B	215	GLN
5	B	232	SER
5	B	241	ARG
5	B	245	GLU
5	B	267	ARG
5	B	302	CYS
5	B	351	TYR
5	B	370	PHE
5	B	401	PHE
5	B	404	LYS
5	B	497	ARG
5	B	604	ARG
5	B	608	ASP
5	B	621	GLU
5	B	679	TYR
5	B	738	PHE
5	B	853	SER
5	B	894	ASP
5	B	931	TYR
5	B	941	LEU
5	B	963	PHE
5	B	996	ARG
5	B	1029	CYS
5	B	1072	MET
5	B	1084	GLN
5	B	1092	TYR
5	B	1155	SER
5	B	1156	ASP
5	B	1158	PHE
5	B	1161	HIS
5	B	1163	CYS
5	B	1177	HIS
5	B	1220	ARG
6	C	34	ARG
6	C	62	PHE
6	C	88	CYS
6	C	94	LYS
6	C	178	PHE

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Mol	Chain	Res	Type
6	C	187	LYS
6	C	221	TYR
6	C	231	ASN
6	C	241	ASP
6	C	264	GLN
7	E	33	GLU
7	E	110	PHE
7	E	121	MET
7	E	146	HIS
7	E	205	SER
8	F	71	GLU
8	F	111	LEU
8	F	128	LYS
8	F	147	SER
9	H	36	CYS
9	H	38	LEU
9	H	94	ASP
9	H	102	TYR
9	H	117	SER
9	H	130	ARG
9	H	131	ASN
10	I	4	PHE
10	I	7	CYS
10	I	8	ARG
10	I	17	ARG
10	I	29	CYS
10	I	61	ASP
10	I	71	SER
10	I	83	ASN
11	J	28	ASP
11	J	55	ASP
12	K	65	HIS
12	K	81	TYR
12	K	108	GLU
13	L	31	CYS
13	L	33	GLU
13	L	51	CYS
13	L	54	ARG
13	L	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	92	HIS
4	A	394	ASN
4	A	397	ASN
4	A	650	GLN
4	A	660	ASN
4	A	717	ASN
4	A	1009	ASN
4	A	1140	HIS
4	A	1427	ASN
5	B	60	GLN
5	B	357	GLN
5	B	538	ASN
5	B	794	ASN
5	B	835	GLN
5	B	1117	GLN
5	B	1161	HIS
5	B	1177	HIS
6	C	264	GLN
7	E	99	HIS
9	H	128	ASN
9	H	131	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/11 (90%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	C
1	R	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
15	5N0	T	101	-	91,107,107	2.46	31 (34%)	91,153,153	1.58	10 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	5N0	T	101	-	-	6/47/92/92	0/9/9/9

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C59-C63	7.37	1.54	1.47
15	T	101	5N0	C49-N23	6.38	1.47	1.33
15	T	101	5N0	C56-N25	6.27	1.47	1.33
15	T	101	5N0	C22-N10	6.08	1.47	1.33
15	T	101	5N0	C26-N14	5.33	1.47	1.35
15	T	101	5N0	C5-N3	4.80	1.48	1.35
15	T	101	5N0	C37-N19	4.54	1.47	1.35
15	T	101	5N0	C10-N6	4.45	1.47	1.35
15	T	101	5N0	C43-N21	4.43	1.47	1.35
15	T	101	5N0	C30-C31	4.33	1.56	1.53
15	T	101	5N0	C31-N17	4.30	1.47	1.35
15	T	101	5N0	C16-N8	4.25	1.47	1.35
15	T	101	5N0	C6-C10	4.13	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C4-C5	3.84	1.56	1.53
15	T	101	5N0	C9-N3	3.84	1.49	1.40
15	T	101	5N0	C42-N19	3.53	1.48	1.41
15	T	101	5N0	C21-N8	3.35	1.48	1.41
15	T	101	5N0	C14-N6	3.34	1.48	1.41
15	T	101	5N0	C29-N14	3.31	1.47	1.40
15	T	101	5N0	C36-N17	3.26	1.48	1.41
15	T	101	5N0	C48-N21	3.07	1.47	1.41
15	T	101	5N0	C2-N1	-2.67	1.33	1.37
15	T	101	5N0	C57-C56	2.28	1.55	1.50
15	T	101	5N0	O5-C26	-2.28	1.18	1.23
15	T	101	5N0	O8-C43	-2.15	1.18	1.23
15	T	101	5N0	O1-C5	-2.11	1.19	1.23
15	T	101	5N0	O10-C56	-2.09	1.19	1.23
15	T	101	5N0	O7-C37	-2.09	1.19	1.23
15	T	101	5N0	O3-C16	-2.05	1.19	1.23
15	T	101	5N0	O9-C49	-2.05	1.19	1.23
15	T	101	5N0	O2-C10	-2.04	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	5N0	C4-C5-N3	6.97	121.26	113.69
15	T	101	5N0	C6-C10-N6	5.45	119.60	113.69
15	T	101	5N0	C29-N14-C26	-5.18	120.21	127.55
15	T	101	5N0	C24-C25-C26	-4.84	100.38	110.85
15	T	101	5N0	C19-N9-C17	2.55	111.36	108.65
15	T	101	5N0	C48-N21-C43	-2.34	120.51	126.58
15	T	101	5N0	C9-N3-C5	-2.16	122.10	128.07
15	T	101	5N0	C3-N2-C4	2.08	109.11	104.01
15	T	101	5N0	O4-C22-N10	-2.05	118.53	122.61
15	T	101	5N0	O8-C43-N21	-2.04	119.06	123.71

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C23-C24-C25-C26
15	T	101	5N0	C47-C44-C49-O9
15	T	101	5N0	C50-C51-C52-N24
15	T	101	5N0	C53-C54-C55-N25
15	T	101	5N0	N24-C53-C54-C55

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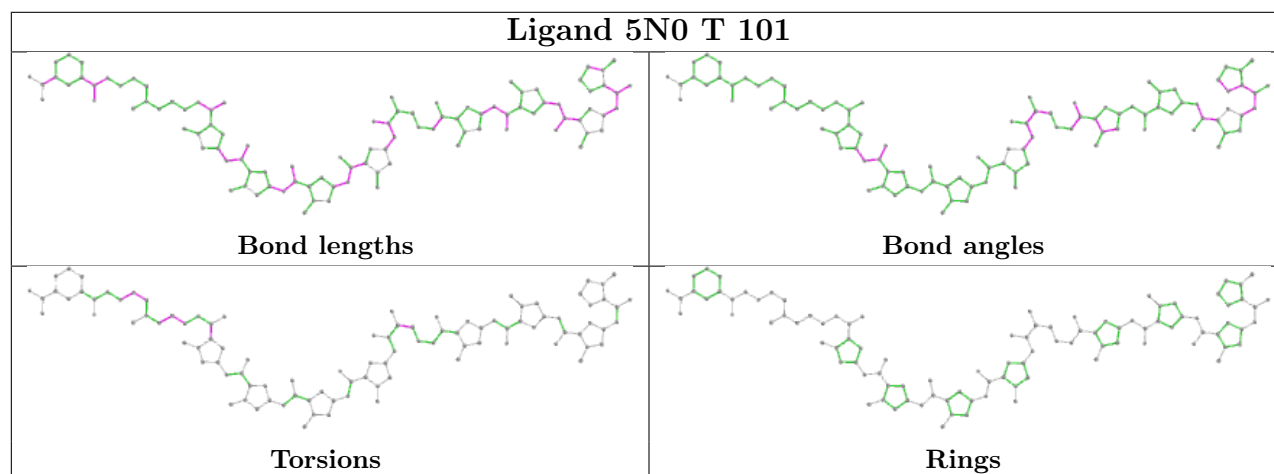
Mol	Chain	Res	Type	Atoms
15	T	101	5N0	N23-C50-C51-C52

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	101	5N0	5	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 [i](#)

There are no such residues in this entry.





























5.8 Polymer linkage issues [i](#)

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, 95th 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	R	11/11 (100%)	0.04	0  	116, 132, 191, 198	0
2	T	26/30 (86%)	-0.14	0  	118, 225, 252, 258	0
3	N	14/20 (70%)	0.01	0  	229, 244, 260, 264	0
4	A	1384/1733 (79%)	-0.08	29 (2%)  	52, 113, 188, 236	0
5	B	1123/1224 (91%)	-0.13	12 (1%)  	55, 99, 153, 196	0
6	C	267/318 (83%)	-0.30	0  	67, 99, 136, 165	0
7	E	212/215 (98%)	-0.06	6 (2%)  	96, 154, 209, 231	0
8	F	86/155 (55%)	-0.36	1 (1%)  	82, 114, 147, 186	0
9	H	133/146 (91%)	0.17	3 (2%)  	106, 137, 170, 202	0
10	I	118/122 (96%)	-0.25	0  	83, 117, 150, 162	0
11	J	65/70 (92%)	-0.32	0  	73, 93, 151, 161	0
12	K	114/120 (95%)	-0.18	0  	78, 105, 131, 153	0
13	L	43/70 (61%)	0.10	2 (4%)  	92, 158, 222, 258	0
All	All	3596/4234 (84%)	-0.12	53 (1%)  	52, 111, 185, 264	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	144	THR	5.3
7	E	83	CYS	4.9
5	B	106	ASP	3.7
4	A	69	THR	3.7
7	E	110	PHE	3.4
9	H	139	ASN	3.4
4	A	143	LYS	3.3
4	A	103	CYS	3.3
4	A	1257	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
4	A	150	THR	3.1
4	A	106	VAL	3.1
4	A	114	LEU	3.0
7	E	93	MET	3.0
5	B	1172	ILE	2.9
5	B	869	SER	2.9
4	A	91	PHE	2.8
13	L	45	ALA	2.8
4	A	149	GLU	2.7
5	B	92	PHE	2.6
5	B	1181	GLU	2.6
5	B	132	VAL	2.5
4	A	186	LYS	2.5
4	A	386	ASP	2.5
7	E	82	PHE	2.4
4	A	660	ASN	2.4
4	A	145	LYS	2.4
5	B	1161	HIS	2.3
9	H	134	ASN	2.3
7	E	126	SER	2.3
4	A	3	GLY	2.2
4	A	166	GLY	2.2
4	A	167	CYS	2.2
13	L	46	VAL	2.2
7	E	44	ALA	2.2
4	A	118	HIS	2.2
4	A	163	SER	2.2
4	A	258	GLY	2.1
5	B	134	LYS	2.1
5	B	913	GLY	2.1
4	A	181	LEU	2.1
4	A	84	ILE	2.1
4	A	200	ARG	2.1
4	A	44	THR	2.1
9	H	86	ASP	2.0
4	A	65	LEU	2.0
4	A	1126	ALA	2.0
5	B	69	LEU	2.0
4	A	259	GLU	2.0
5	B	248	SER	2.0
4	A	105	CYS	2.0
8	F	104	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	168	GLY	2.0
5	B	468	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

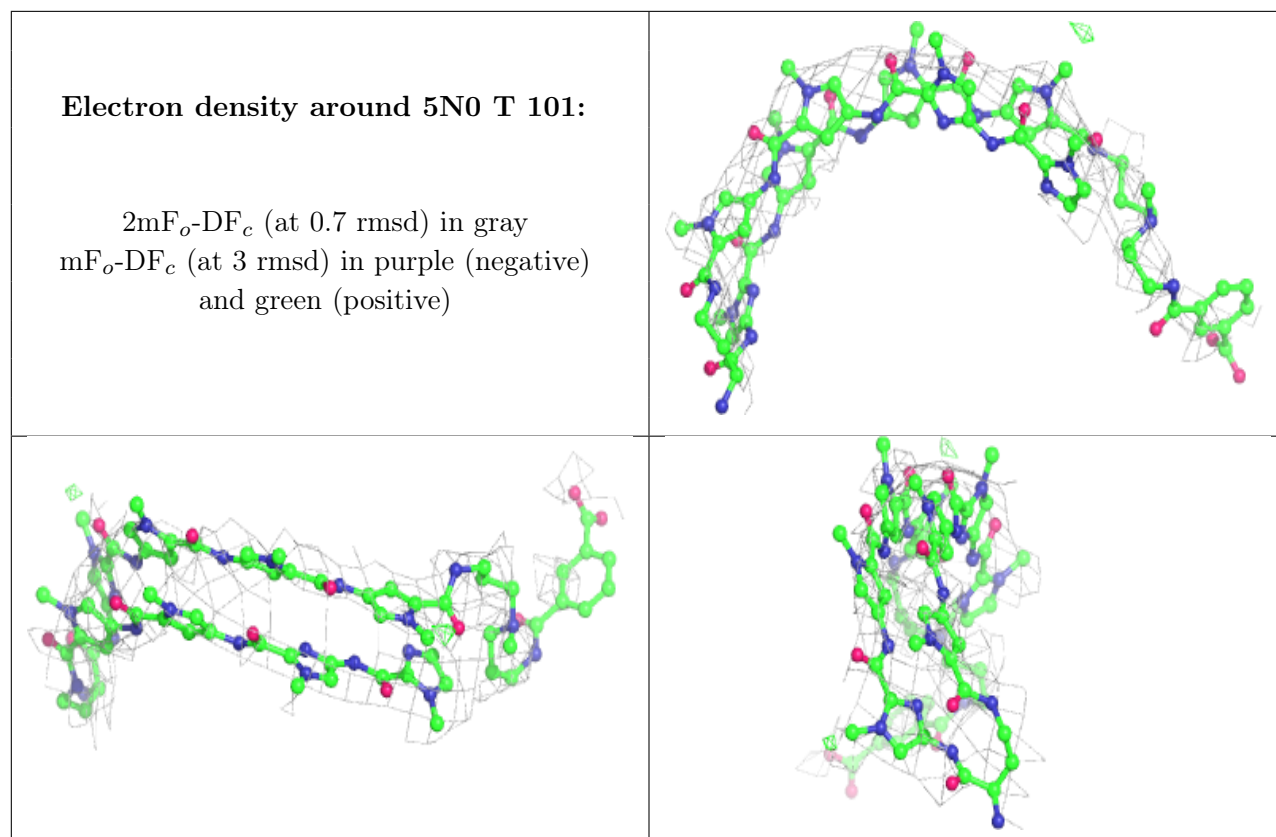
There are no monosaccharides in this entry.

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, 95th 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(\AA^2)	Q<0.9
15	5N0	T	101	99/99	0.82	0.36	198,236,262,264	0
16	ZN	A	1802	1/1	0.88	0.10	167,167,167,167	0
16	ZN	B	1301	1/1	0.90	0.08	195,195,195,195	0
16	ZN	A	1801	1/1	0.91	0.17	242,242,242,242	0
14	MG	R	2001	1/1	0.92	0.35	141,141,141,141	0
16	ZN	L	101	1/1	0.92	0.06	182,182,182,182	0
16	ZN	J	101	1/1	0.96	0.22	90,90,90,90	0
16	ZN	C	401	1/1	0.98	0.10	108,108,108,108	0
16	ZN	I	201	1/1	0.99	0.12	99,99,99,99	0
16	ZN	I	202	1/1	1.00	0.12	110,110,110,110	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.