



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 AM UTC

PDB ID : 2NVQ / pdb_00002nvq
Title : RNA Polymerase II Elongation Complex in 150 mM Mg+2 with 2'dUTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-13
Resolution : 2.90 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

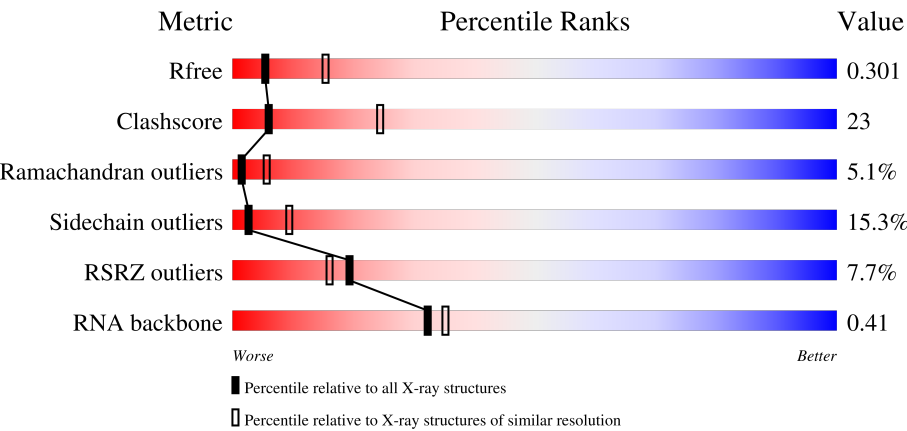
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	10	40% 40% 20%
2	T	28	14% 50% 39% 11%
3	N	14	29% 29% 57% 14%
4	A	1733	6% 44% 28% 7% 19%

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	DUT	T	29[B]	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29425 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 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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 13.6 kDa polypeptide.

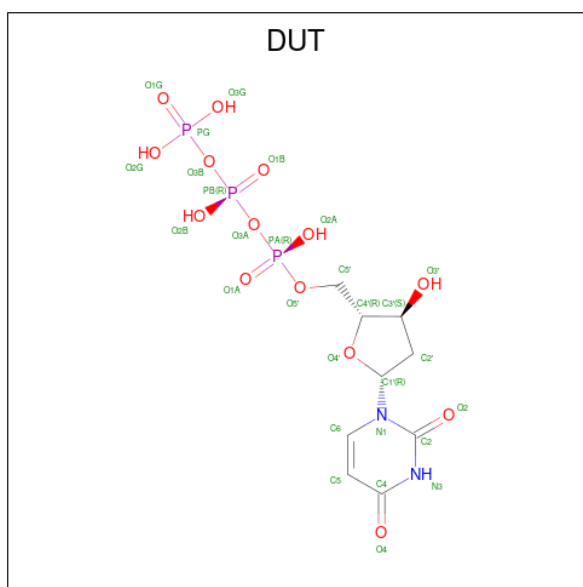
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 14 is DEOXYURIDINE-5'-TRIPHOSPHATE (CCD ID: DUT) (formula: $C_9H_{15}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	1
			56	18	4	28	6		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

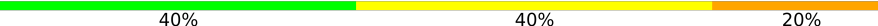
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 3	Mg 3	0	1

3 Residue-property plots [i](#)

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

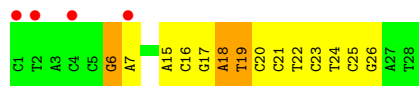
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R: 



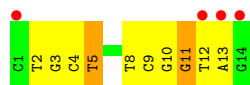
- Molecule 2: 28-MER DNA template strand

Chain T: 



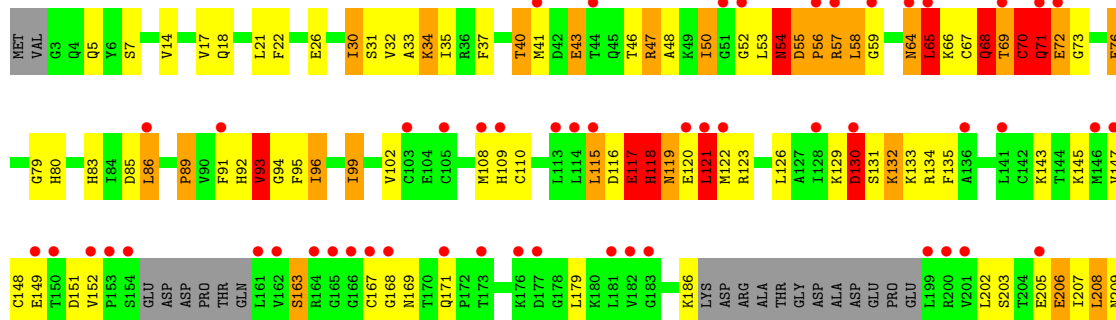
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

Chain N: 

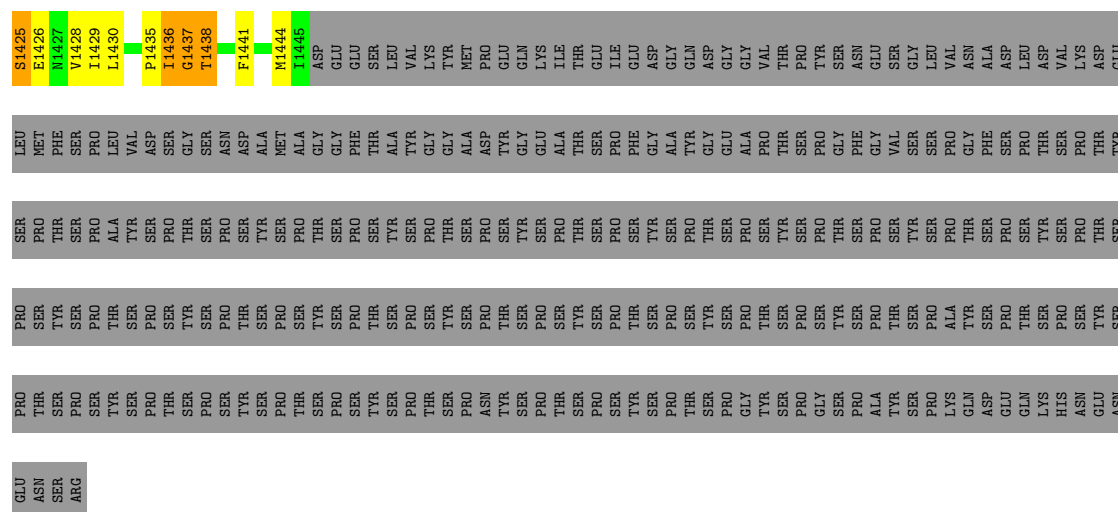


- Molecule 4: DNA-directed RNA polymerase II largest subunit

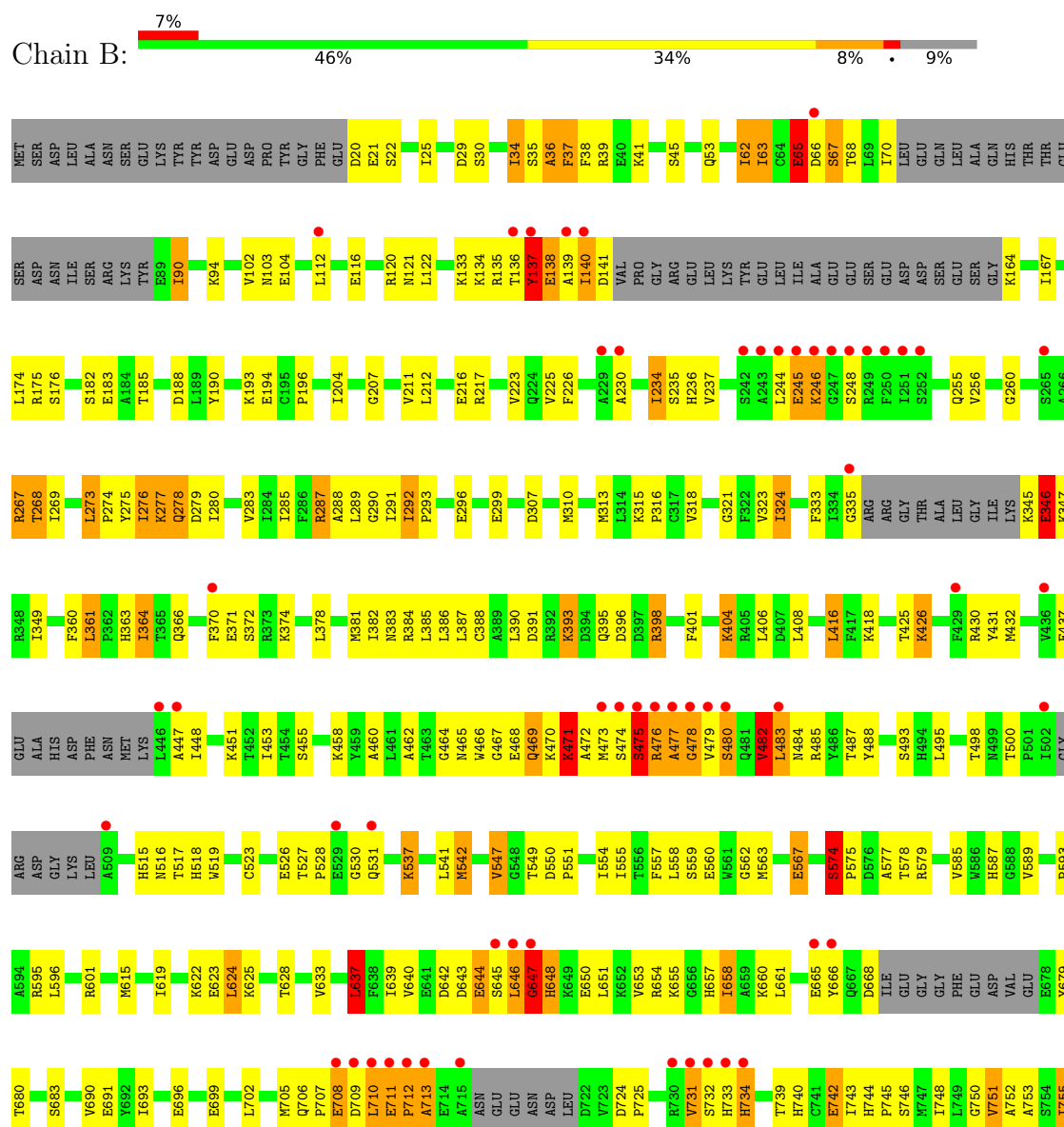
Chain A: 

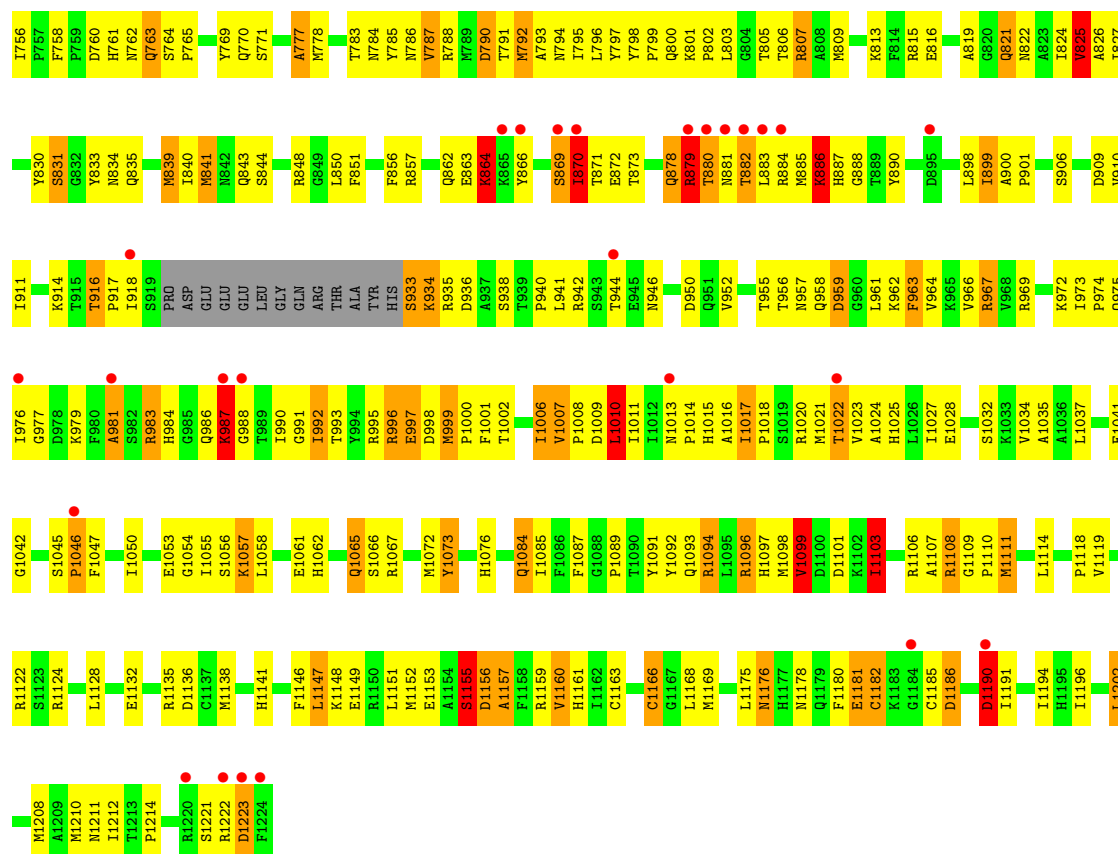






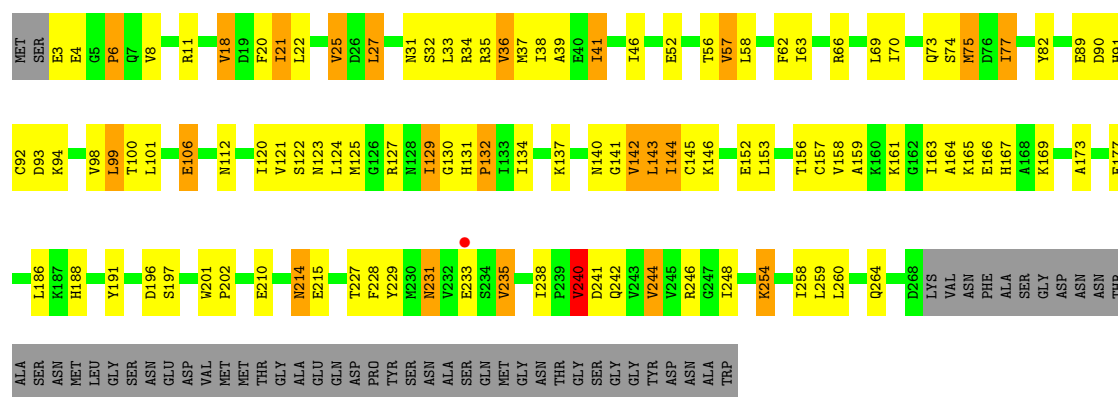
- Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide





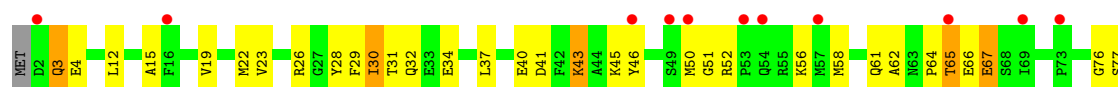
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 49% 28% 7% 16%

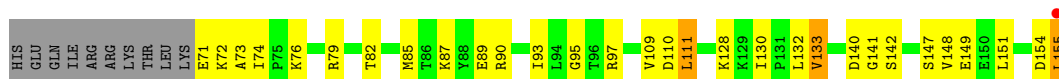
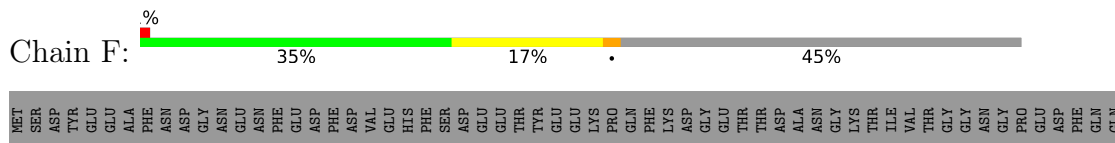


• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

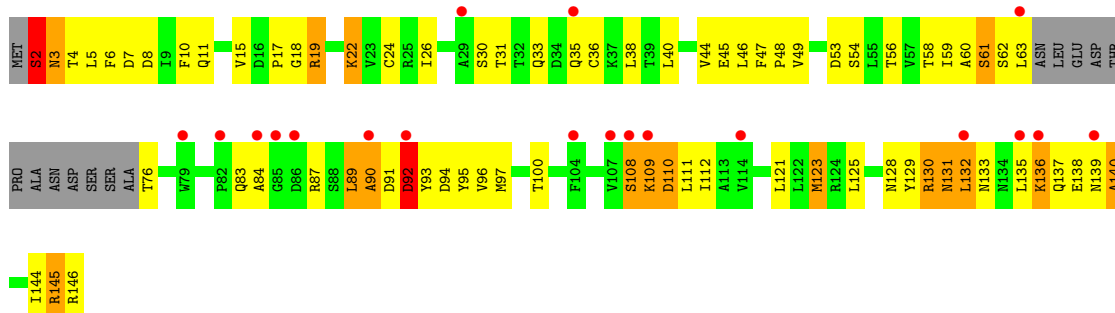
Chain E: 17% 57% 34% 7%



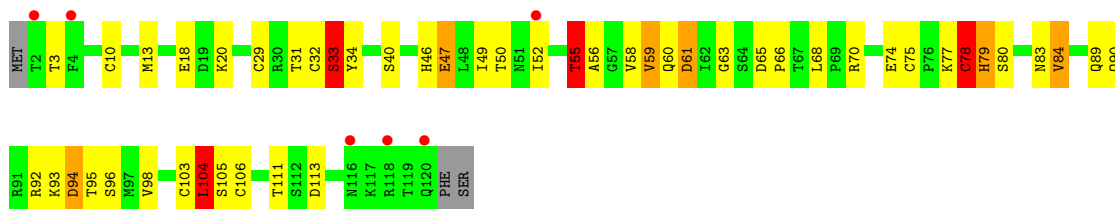
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



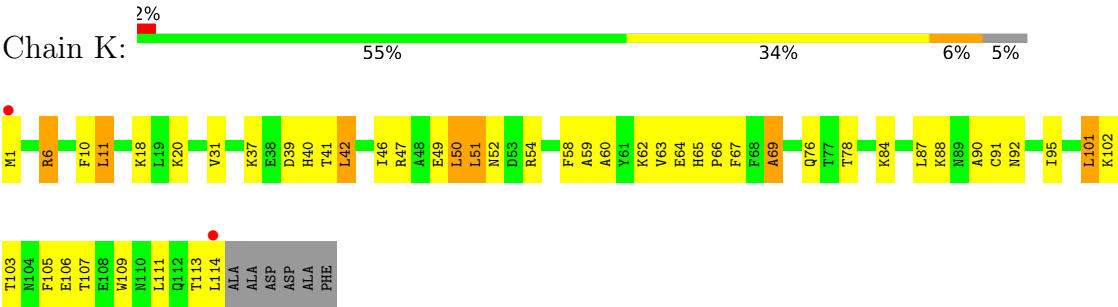
- Molecule 10: DNA-directed RNA polymerase II subunit 9



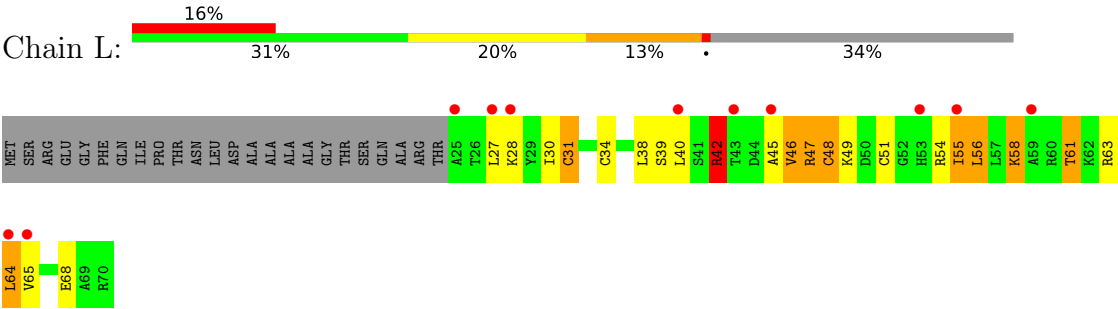
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



● Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.65Å 222.76Å 195.28Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	48.45 – 2.90 48.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (48.45-2.90) 92.7 (48.45-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.229 , 0.283 0.262 , 0.301	Depositor DCC
R_{free} test set	4429 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29425	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DUT, 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	R	0.88	0/243	1.66	7/378 (1.9%)
2	T	0.54	0/634	1.24	3/975 (0.3%)
3	N	0.60	0/317	1.34	2/488 (0.4%)
4	A	0.94	3/11241 (0.0%)	1.12	39/15199 (0.3%)
5	B	1.05	7/9033 (0.1%)	1.18	29/12181 (0.2%)
6	C	0.98	0/2133	1.19	9/2891 (0.3%)
7	E	0.81	0/1788	1.02	1/2406 (0.0%)
8	F	0.82	0/700	0.92	0/945
9	H	0.82	0/1086	1.05	3/1470 (0.2%)
10	I	0.95	0/989	1.11	3/1331 (0.2%)
11	J	1.09	0/541	1.21	2/727 (0.3%)
12	K	0.95	0/937	1.11	3/1265 (0.2%)
13	L	1.17	0/365	1.30	2/485 (0.4%)
All	All	0.96	10/30007 (0.0%)	1.15	103/40741 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	11
5	B	0	8
6	C	0	2
All	All	0	21

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1055	ILE	CA-CB	8.99	1.63	1.54
4	A	423	ASP	N-CA	-6.48	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	777	ALA	CA-CB	6.15	1.62	1.53
4	A	1089	VAL	CA-CB	6.00	1.61	1.54
5	B	34	ILE	CA-CB	-5.79	1.47	1.54
5	B	268	THR	CA-CB	5.63	1.62	1.53
5	B	1073	TYR	CA-C	5.30	1.59	1.52
5	B	230	ALA	CA-C	5.12	1.59	1.52
5	B	870	ILE	CA-CB	5.10	1.61	1.54
4	A	463	ILE	CA-CB	5.03	1.60	1.54

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	140	ILE	N-CA-C	11.83	120.97	111.62
1	R	8	G	C4'-C3'-C2'	-9.14	93.46	102.60
4	A	886	ILE	N-CA-C	8.96	118.95	110.53
4	A	921	GLY	N-CA-C	-8.34	104.00	111.67
4	A	626	ASN	N-CA-C	7.92	119.61	110.97
1	R	6	G	C4'-C3'-O3'	-7.92	101.12	113.00
11	J	3	VAL	CB-CA-C	-7.66	102.62	110.89
4	A	474	VAL	N-CA-C	-7.62	105.29	112.83
4	A	313	GLN	N-CA-C	7.50	118.42	108.07
11	J	27	GLU	N-CA-C	7.05	118.61	111.07
1	R	9	G	C4'-C3'-O3'	-6.97	102.54	113.00
5	B	1006	ILE	CB-CA-C	-6.89	103.74	111.45
4	A	491	VAL	N-CA-C	6.74	115.32	107.77
5	B	835	GLN	N-CA-C	6.58	119.43	110.55
4	A	460	VAL	N-CA-C	6.56	118.05	109.58
5	B	287	ARG	N-CA-C	-6.52	103.79	111.03
4	A	513	SER	CA-C-N	6.43	126.11	119.56
4	A	513	SER	C-N-CA	6.43	126.11	119.56
6	C	41	ILE	CA-C-N	6.43	126.46	119.90
6	C	41	ILE	C-N-CA	6.43	126.46	119.90
3	N	5	DT	P-O3'-C3'	6.38	129.77	120.20
1	R	6	G	C4'-C3'-C2'	-6.37	96.23	102.60
9	H	92	ASP	N-CA-C	-6.35	105.11	112.92
4	A	244	PRO	N-CA-C	6.35	118.44	110.70
4	A	525	GLN	CB-CA-C	-6.25	109.35	116.54
5	B	637	LEU	N-CA-C	6.23	118.54	109.07
12	K	69	ALA	N-CA-C	6.22	119.03	111.82
13	L	31	CYS	CA-CB-SG	6.18	128.61	114.40
4	A	1346	ALA	N-CA-C	6.11	117.94	111.28
5	B	574	SER	CA-C-N	6.10	127.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	574	SER	C-N-CA	6.10	127.47	119.84
5	B	1186	ASP	N-CA-C	6.03	119.71	111.39
5	B	475	SER	N-CA-C	-5.98	105.09	112.38
4	A	152	VAL	CA-C-N	5.89	127.20	119.84
4	A	152	VAL	C-N-CA	5.89	127.20	119.84
4	A	507	VAL	CB-CA-C	-5.88	108.11	113.70
5	B	90	ILE	CB-CA-C	-5.85	102.53	110.42
6	C	144	ILE	CB-CA-C	-5.85	104.36	112.02
6	C	38	ILE	CB-CA-C	-5.83	104.40	112.04
4	A	487	MET	N-CA-C	5.81	119.02	109.72
5	B	787	VAL	CB-CA-C	-5.74	105.23	110.63
10	I	78	CYS	N-CA-CB	5.73	120.17	110.49
5	B	204	ILE	CB-CA-C	-5.72	103.89	110.41
6	C	143	LEU	CA-C-N	5.72	127.88	120.56
6	C	143	LEU	C-N-CA	5.72	127.88	120.56
6	C	197	SER	N-CA-C	5.70	117.95	111.11
5	B	732	SER	N-CA-C	5.63	116.80	108.86
5	B	1155	SER	CB-CA-C	-5.62	110.08	116.54
4	A	288	ALA	N-CA-C	-5.62	107.07	114.31
4	A	993	LEU	N-CA-C	-5.56	105.12	111.07
7	E	150	VAL	N-CA-C	5.56	112.62	107.56
4	A	411	ASP	N-CA-C	5.53	118.25	109.96
9	H	2	SER	CA-C-N	5.53	131.65	121.70
9	H	2	SER	C-N-CA	5.53	131.65	121.70
6	C	21	ILE	N-CA-C	-5.50	101.96	109.55
4	A	351	THR	N-CA-C	5.49	116.62	108.60
4	A	70	CYS	N-CA-C	-5.48	105.31	111.28
1	R	8	G	C1'-O4'-C4'	-5.47	104.43	109.90
4	A	670	ILE	CB-CA-C	-5.45	104.35	111.81
4	A	423	ASP	N-CA-C	-5.44	104.32	108.78
4	A	816	HIS	N-CA-C	-5.43	105.44	111.36
4	A	417	TYR	N-CA-C	-5.42	101.64	109.29
13	L	58	LYS	N-CA-C	5.40	119.17	112.59
5	B	825	VAL	N-CA-C	5.39	117.00	109.55
10	I	55	THR	N-CA-C	-5.39	101.66	109.59
5	B	764	SER	N-CA-C	5.38	120.88	113.77
4	A	719	VAL	N-CA-C	5.38	116.75	110.62
5	B	839	MET	N-CA-C	5.37	117.42	108.99
5	B	821	GLN	N-CA-C	5.37	117.98	109.50
6	C	20	PHE	N-CA-C	5.32	117.35	108.99
4	A	242	PRO	CA-C-N	5.31	125.85	120.38
4	A	242	PRO	C-N-CA	5.31	125.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	6	G	O4'-C1'-C2'	-5.31	102.29	107.60
2	T	19	DT	N1-C1'-C2'	-5.29	105.56	113.50
5	B	1010	LEU	N-CA-C	5.28	116.98	108.32
10	I	78	CYS	CA-CB-SG	5.25	126.48	114.40
5	B	1084	GLN	CA-C-N	-5.22	116.31	123.14
5	B	1084	GLN	C-N-CA	-5.22	116.31	123.14
4	A	375	THR	N-CA-C	5.21	117.74	109.50
5	B	755	ILE	CB-CA-C	-5.20	104.31	111.65
2	T	18	DA	P-O5'-C5'	-5.16	112.26	120.00
4	A	499	ALA	CA-C-N	5.14	127.69	120.28
4	A	499	ALA	C-N-CA	5.14	127.69	120.28
4	A	351	THR	CB-CA-C	-5.14	101.10	111.17
1	R	8	G	O4'-C4'-C3'	-5.12	98.88	104.00
12	K	64	GLU	N-CA-C	5.12	116.86	111.28
5	B	278	GLN	N-CA-C	5.11	114.36	108.49
5	B	1099	VAL	CB-CA-C	-5.09	105.36	111.88
4	A	356	ASP	CB-CA-C	-5.09	104.97	110.98
4	A	1113	THR	CA-C-N	-5.09	114.71	119.85
4	A	1113	THR	C-N-CA	-5.09	114.71	119.85
3	N	11	DG	P-O3'-C3'	5.08	127.82	120.20
4	A	507	VAL	O-C-N	5.08	123.67	120.42
5	B	1103	ILE	CA-C-N	-5.07	113.81	122.33
5	B	1103	ILE	C-N-CA	-5.07	113.81	122.33
5	B	1114	LEU	N-CA-C	5.07	116.49	111.07
4	A	574	GLY	N-CA-C	-5.06	106.66	112.73
4	A	566	ILE	CB-CA-C	-5.04	105.17	110.62
2	T	6	DG	P-O3'-C3'	5.04	127.76	120.20
5	B	448	ILE	CB-CA-C	-5.04	104.18	111.19
12	K	6	ARG	N-CA-C	5.02	117.49	111.71
4	A	613	ILE	N-CA-C	5.01	116.11	111.45
5	B	934	LYS	N-CA-C	5.01	116.93	108.96

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1082	ASN	Peptide
4	A	115	LEU	Peptide
4	A	117	GLU	Peptide
4	A	218	ASP	Peptide
4	A	297	GLN	Peptide
4	A	298	PHE	Peptide

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Mol	Chain	Res	Type	Group
4	A	400	PRO	Peptide
4	A	402	ALA	Peptide
4	A	450	LEU	Peptide
4	A	671	ALA	Peptide
4	A	85	ASP	Peptide
5	B	1155	SER	Peptide
5	B	137	TYR	Peptide
5	B	138	GLU	Peptide
5	B	36	ALA	Peptide
5	B	478	GLY	Peptide
5	B	647	GLY	Peptide
5	B	886	LYS	Peptide
5	B	981	ALA	Peptide
6	C	3	GLU	Peptide
6	C	4	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	4	0
2	T	566	0	316	22	0
3	N	284	0	161	8	0
4	A	11043	0	11133	570	0
5	B	8861	0	8884	485	0
6	C	2095	0	2051	94	0
7	E	1752	0	1776	58	0
8	F	688	0	707	20	0
9	H	1068	0	1040	54	0
10	I	971	0	927	31	0
11	J	532	0	542	39	0
12	K	919	0	929	43	0
13	L	363	0	386	14	0
14	T	56	0	22	16	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	3	0	0	0	0
All	All	29425	0	28983	1332	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 23.

All (1332) 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:B:647:GLY:HA3	5:B:648:HIS:CB	1.51	1.34
5:B:800:GLN:HB3	11:J:52:THR:CG2	1.58	1.32
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.51	1.25
4:A:672:ASP:OD2	4:A:736:ASN:ND2	1.73	1.21
4:A:116:ASP:CB	4:A:117:GLU:HB2	1.73	1.17
4:A:672:ASP:CG	4:A:675:THR:OG1	1.87	1.17
5:B:906:SER:HB3	5:B:946:ASN:HB2	1.25	1.16
4:A:399:HIS:CB	4:A:400:PRO:HD3	1.74	1.16
5:B:647:GLY:HA3	5:B:648:HIS:HB2	1.21	1.16
2:T:18:DA:N1	14:T:29[B]:DUT:O2	1.78	1.15
4:A:399:HIS:HB3	4:A:400:PRO:CD	1.76	1.14
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.28	1.13
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.14	1.13
4:A:1029:ARG:HG2	4:A:1029:ARG:HH11	1.13	1.13
4:A:672:ASP:OD1	4:A:674:PRO:HG2	1.49	1.12
4:A:672:ASP:HB3	4:A:675:THR:CB	1.80	1.12
4:A:1123:GLY:HA3	4:A:1124:HIS:HB2	1.19	1.11
4:A:590:ARG:HG3	4:A:590:ARG:HH11	1.16	1.10
5:B:1094:ARG:HH11	5:B:1094:ARG:CG	1.65	1.09
5:B:345:LYS:HA	5:B:347:LYS:H	0.97	1.08
4:A:116:ASP:HB3	4:A:117:GLU:HB2	1.29	1.08
5:B:647:GLY:HA3	5:B:648:HIS:HB3	1.30	1.08
5:B:1094:ARG:HG2	5:B:1094:ARG:NH1	1.54	1.08
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.36	1.08
4:A:672:ASP:HB3	4:A:675:THR:HB	1.13	1.08
4:A:249:SER:O	4:A:250:ILE:HG13	1.55	1.06
4:A:116:ASP:CA	4:A:117:GLU:HB2	1.84	1.06
4:A:672:ASP:CB	4:A:675:THR:HB	1.85	1.05
5:B:800:GLN:HB3	11:J:52:THR:HG21	1.31	1.03
2:T:18:DA:C2	14:T:29[B]:DUT:O2	2.11	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:565:ILE:HG23	4:A:567:LYS:CE	1.88	1.02
4:A:913:LEU:HD11	4:A:981:LEU:O	1.59	1.01
4:A:567:LYS:HB3	9:H:96:VAL:H	1.22	1.01
4:A:399:HIS:CG	4:A:400:PRO:HD3	1.95	1.00
5:B:709:ASP:O	5:B:710:LEU:HD23	1.60	1.00
5:B:647:GLY:CA	5:B:648:HIS:CB	2.36	1.00
5:B:708:GLU:O	5:B:712:PRO:HD3	1.60	1.00
4:A:53:LEU:HG	4:A:54:ASN:H	1.27	1.00
2:T:18:DA:N6	14:T:29[B]:DUT:HN3	1.60	0.99
5:B:801:LYS:O	11:J:52:THR:HG23	1.60	0.99
4:A:323:LYS:HG2	4:A:324:SER:H	1.26	0.99
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.93	0.99
4:A:299:HIS:O	4:A:301:ALA:N	1.94	0.99
5:B:313:MET:HE2	5:B:390:LEU:HG	1.42	0.98
4:A:315:LEU:HG	4:A:320:ARG:HH21	1.28	0.98
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.43	0.98
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.02	0.98
4:A:472:LEU:O	4:A:475:THR:HB	1.63	0.97
4:A:672:ASP:CB	4:A:675:THR:CB	2.42	0.97
6:C:235:VAL:HG11	11:J:6:ARG:HH21	1.29	0.97
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.45	0.97
2:T:18:DA:H61	14:T:29[B]:DUT:HN3	1.12	0.96
4:A:116:ASP:HB3	4:A:117:GLU:CB	1.94	0.96
6:C:167:HIS:HD2	6:C:169:LYS:H	1.13	0.96
5:B:345:LYS:HA	5:B:347:LYS:N	1.80	0.96
4:A:56:PRO:C	4:A:57:ARG:HG3	1.90	0.95
4:A:56:PRO:O	4:A:57:ARG:HG3	1.65	0.94
7:E:64:PRO:HD3	7:E:76:GLY:HA2	1.49	0.93
4:A:609:ASP:O	4:A:611:GLN:N	2.01	0.92
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.34	0.92
5:B:647:GLY:CA	5:B:648:HIS:HB3	1.98	0.92
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.34	0.91
5:B:313:MET:CE	5:B:390:LEU:HG	1.99	0.91
4:A:1110:ASN:H	4:A:1110:ASN:HD22	1.18	0.91
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.36	0.91
4:A:590:ARG:HG3	4:A:590:ARG:NH1	1.78	0.90
6:C:56:THR:HG22	6:C:57:VAL:H	1.35	0.90
5:B:744:HIS:HD2	5:B:746:SER:H	1.15	0.90
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.12	0.89
4:A:116:ASP:HA	4:A:117:GLU:HB2	1.52	0.89
4:A:943:LEU:O	4:A:945:GLU:N	2.05	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:68:GLN:O	4:A:68:GLN:NE2	2.05	0.88
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.08	0.88
4:A:565:ILE:CG2	4:A:567:LYS:HE3	1.98	0.87
4:A:129:LYS:O	4:A:130:ASP:HB2	1.73	0.87
4:A:565:ILE:HG12	4:A:567:LYS:HZ1	1.37	0.87
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.37	0.87
5:B:710:LEU:O	5:B:711:GLU:HB3	1.72	0.86
4:A:1029:ARG:HH11	4:A:1029:ARG:CG	1.88	0.86
4:A:218:ASP:HB2	4:A:219:PHE:HB2	1.55	0.86
5:B:260:GLY:O	5:B:267:ARG:HD3	1.76	0.85
4:A:567:LYS:HB3	9:H:96:VAL:N	1.90	0.85
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.59	0.85
4:A:265:LYS:HG2	4:A:303:TYR:HB2	1.57	0.85
5:B:1094:ARG:HH11	5:B:1094:ARG:HG2	0.74	0.85
2:T:18:DA:N1	14:T:29[B]:DUT:C2	2.40	0.84
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.40	0.84
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.60	0.84
5:B:957:ASN:HD22	5:B:959:ASP:HB2	1.43	0.83
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.08	0.83
4:A:567:LYS:HG3	4:A:568:PRO:HD2	1.61	0.83
5:B:140:ILE:HB	5:B:141:ASP:HB2	1.61	0.83
4:A:324:SER:O	4:A:326:ARG:N	2.12	0.83
4:A:672:ASP:OD1	4:A:675:THR:OG1	1.89	0.83
5:B:805:THR:HG21	5:B:815:ARG:HH21	1.44	0.83
4:A:134:ARG:HD3	4:A:221:SER:O	1.79	0.82
4:A:218:ASP:H	4:A:219:PHE:HB3	1.43	0.82
4:A:399:HIS:CB	4:A:400:PRO:CD	2.40	0.82
4:A:855:THR:HG21	4:A:857:ARG:HE	1.44	0.82
12:K:65:HIS:HD2	12:K:67:PHE:H	1.25	0.82
13:L:46:VAL:HG12	13:L:47:ARG:H	1.42	0.82
4:A:306:ASN:HD21	4:A:313:GLN:HB2	1.45	0.82
4:A:590:ARG:HH11	4:A:590:ARG:CG	1.93	0.81
10:I:103:CYS:O	10:I:105:SER:N	2.13	0.81
5:B:90:ILE:CD1	5:B:134:LYS:HG2	2.10	0.81
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.62	0.81
7:E:175:LEU:HD12	7:E:176:PRO:HD2	1.63	0.81
4:A:65:LEU:HD23	4:A:65:LEU:H	1.46	0.81
5:B:287:ARG:NH1	5:B:324:ILE:O	2.14	0.81
4:A:672:ASP:CB	4:A:675:THR:OG1	2.29	0.80
4:A:754:SER:H	4:A:757:ASN:HD22	1.30	0.80
4:A:1444:MET:HB2	8:F:133:VAL:HG12	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.10	0.80
5:B:1084:GLN:NE2	6:C:191:TYR:HA	1.97	0.80
5:B:744:HIS:CD2	5:B:746:SER:H	1.99	0.80
5:B:63:ILE:O	5:B:67:SER:HB3	1.81	0.79
4:A:249:SER:O	4:A:250:ILE:CG1	2.30	0.79
5:B:176:SER:O	5:B:182:SER:HB3	1.82	0.79
5:B:363:HIS:O	5:B:364:ILE:HB	1.83	0.79
4:A:961:ARG:HG2	4:A:961:ARG:HH11	1.48	0.79
4:A:253:ASN:H	4:A:253:ASN:HD22	1.31	0.79
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	1.64	0.79
5:B:906:SER:HB3	5:B:946:ASN:CB	2.10	0.79
4:A:269:ILE:HG22	4:A:299:HIS:HB2	1.66	0.78
5:B:476:ARG:O	5:B:478:GLY:N	2.17	0.78
4:A:855:THR:CG2	4:A:857:ARG:HE	1.96	0.78
5:B:1006:ILE:HD11	11:J:43:ARG:HB2	1.65	0.78
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	1.66	0.78
4:A:298:PHE:C	4:A:298:PHE:CD2	2.59	0.78
4:A:332:LYS:O	4:A:333:GLU:HG2	1.82	0.77
4:A:596:THR:O	4:A:598:LEU:N	2.17	0.77
5:B:800:GLN:CB	11:J:52:THR:HG21	2.14	0.77
4:A:456:MET:HE2	4:A:510:GLN:HB2	1.66	0.77
5:B:882:THR:HB	5:B:934:LYS:O	1.83	0.77
5:B:167:ILE:HG22	5:B:167:ILE:O	1.84	0.77
5:B:1107:ALA:O	5:B:1108:ARG:HB3	1.85	0.77
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.66	0.77
7:E:108:GLY:HA3	7:E:132:ILE:HG22	1.65	0.77
5:B:879:ARG:NE	5:B:879:ARG:H	1.83	0.77
5:B:825:VAL:HG23	5:B:1010:LEU:HB3	1.65	0.76
5:B:864:LYS:HG2	5:B:871:THR:HG23	1.67	0.76
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.66	0.76
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.13	0.76
5:B:102:VAL:HG23	5:B:112:LEU:HB2	1.66	0.76
4:A:378:GLU:OE2	4:A:434:ARG:HD3	1.86	0.76
4:A:901:LEU:HA	4:A:907:THR:HG23	1.68	0.76
4:A:961:ARG:HG2	4:A:961:ARG:NH1	1.99	0.76
5:B:211:VAL:CG2	5:B:483:LEU:HD13	2.15	0.76
5:B:137:TYR:O	5:B:138:GLU:HB2	1.85	0.76
4:A:208:LEU:O	4:A:208:LEU:HD22	1.86	0.75
5:B:906:SER:CB	5:B:946:ASN:HB2	2.13	0.75
5:B:1163:CYS:SG	5:B:1166:CYS:N	2.56	0.75
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:3:GLN:HG2	7:E:4:GLU:H	1.51	0.75
5:B:1168:LEU:HD22	5:B:1208:MET:HE2	1.68	0.75
5:B:398:ARG:HB3	5:B:398:ARG:NH1	2.02	0.74
5:B:984:HIS:CE1	5:B:1025:HIS:HA	2.22	0.74
4:A:31:SER:OG	4:A:83:HIS:HD2	1.71	0.74
5:B:223:VAL:O	5:B:384:ARG:NH2	2.20	0.74
6:C:98:VAL:H	6:C:122:SER:HB2	1.51	0.74
4:A:567:LYS:HG3	4:A:568:PRO:CD	2.18	0.74
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.34	0.74
5:B:30:SER:O	5:B:34:ILE:HD12	1.88	0.74
5:B:225:VAL:HG11	5:B:385:LEU:HA	1.69	0.74
5:B:797:TYR:O	11:J:1:MET:HG2	1.86	0.74
4:A:47:ARG:HA	4:A:47:ARG:CZ	2.18	0.74
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.69	0.73
5:B:313:MET:HE2	5:B:390:LEU:CG	2.18	0.73
4:A:1029:ARG:HG2	4:A:1029:ARG:NH1	1.94	0.73
4:A:1123:GLY:HA3	4:A:1124:HIS:CB	2.08	0.73
5:B:278:GLN:HG2	5:B:279:ASP:H	1.52	0.73
5:B:426:LYS:HE2	5:B:430:ARG:HH22	1.52	0.73
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.22	0.73
4:A:471:ASN:O	4:A:474:VAL:HG12	1.88	0.73
4:A:596:THR:C	4:A:598:LEU:H	1.94	0.73
5:B:647:GLY:CA	5:B:648:HIS:HB2	2.11	0.73
4:A:298:PHE:HD2	4:A:299:HIS:HA	1.52	0.73
11:J:3:VAL:CG2	11:J:18:TRP:HB2	2.17	0.72
5:B:25:ILE:HG23	5:B:29:ASP:HB2	1.70	0.72
5:B:216:GLU:OE1	5:B:537:LYS:HE2	1.90	0.72
5:B:1160:VAL:HG11	5:B:1169:MET:HG2	1.71	0.72
4:A:567:LYS:CB	4:A:568:PRO:CD	2.66	0.72
4:A:1333:ILE:O	4:A:1337:GLU:HG3	1.89	0.72
4:A:208:LEU:HD22	4:A:208:LEU:C	2.14	0.72
4:A:399:HIS:CG	4:A:400:PRO:CD	2.72	0.72
5:B:801:LYS:O	11:J:52:THR:CG2	2.35	0.72
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.72	0.72
7:E:65:THR:HB	7:E:67:GLU:HB2	1.71	0.72
5:B:346:GLU:HA	5:B:349:ILE:CD1	2.20	0.72
5:B:979:LYS:HE2	5:B:987:LYS:HG2	1.72	0.72
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.01	0.72
4:A:1110:ASN:H	4:A:1110:ASN:ND2	1.86	0.72
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.25	0.72
4:A:666:ILE:CD1	5:B:1027:ILE:HG12	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:515:HIS:H	5:B:518:HIS:CD2	2.08	0.71
7:E:22:MET:CE	7:E:26:ARG:HH21	2.03	0.71
5:B:800:GLN:CB	11:J:52:THR:HG22	2.14	0.71
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.71	0.71
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.72	0.71
12:K:65:HIS:CD2	12:K:67:PHE:H	2.08	0.71
5:B:426:LYS:HE2	5:B:430:ARG:NH2	2.06	0.71
5:B:864:LYS:HB3	5:B:872:GLU:H	1.55	0.71
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.73	0.71
12:K:40:HIS:HE1	12:K:63:VAL:HG22	1.56	0.70
5:B:1211:ASN:O	5:B:1212:ILE:HG13	1.91	0.70
4:A:1063:MET:SD	4:A:1436:ILE:HG13	2.31	0.70
5:B:879:ARG:H	5:B:879:ARG:CZ	2.05	0.70
5:B:955:THR:HG22	5:B:956:THR:H	1.57	0.70
5:B:1175:LEU:O	5:B:1176:ASN:HB3	1.90	0.70
4:A:741:ASN:HD22	4:A:744:LYS:H	1.39	0.70
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.74	0.70
5:B:705:MET:H	5:B:710:LEU:HD12	1.55	0.70
4:A:399:HIS:CD2	4:A:400:PRO:HD3	2.26	0.69
12:K:102:LYS:O	12:K:106:GLU:HG3	1.91	0.69
5:B:976:ILE:HG23	5:B:977:GLY:N	2.06	0.69
5:B:563:MET:HE1	5:B:587:HIS:HB2	1.74	0.69
6:C:11:ARG:HD3	6:C:21:ILE:HD11	1.75	0.69
4:A:117:GLU:C	4:A:118:HIS:O	2.34	0.69
4:A:249:SER:C	4:A:250:ILE:CG1	2.66	0.69
4:A:553:VAL:HG13	4:A:648:ASN:ND2	2.08	0.69
4:A:605:MET:HE3	4:A:614:PHE:O	1.93	0.69
4:A:800:VAL:O	4:A:802:ASN:N	2.25	0.69
4:A:1161:THR:HG22	4:A:1163:ILE:N	2.06	0.69
6:C:56:THR:HG22	6:C:57:VAL:N	2.08	0.69
9:H:47:PHE:HB3	9:H:95:TYR:HD1	1.58	0.69
7:E:19:VAL:O	7:E:23:VAL:HG23	1.92	0.69
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.73	0.69
13:L:46:VAL:HG12	13:L:47:ARG:N	2.07	0.68
4:A:298:PHE:HA	4:A:299:HIS:O	1.92	0.68
4:A:456:MET:HE1	4:A:521:MET:HE3	1.73	0.68
2:T:18:DA:N1	14:T:29[B]:DUT:N3	2.42	0.68
4:A:31:SER:OG	4:A:83:HIS:CD2	2.46	0.68
4:A:265:LYS:C	4:A:267:ALA:H	2.01	0.68
5:B:802:PRO:HB3	5:B:1091:TYR:CG	2.29	0.68
4:A:117:GLU:H	4:A:118:HIS:C	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:535:THR:HG21	4:A:617:VAL:H	1.59	0.68
4:A:553:VAL:HG13	4:A:648:ASN:HD22	1.58	0.68
4:A:568:PRO:O	4:A:569:LYS:CB	2.41	0.68
4:A:219:PHE:HE1	4:A:226:GLU:HA	1.59	0.68
4:A:319:GLY:HA2	4:A:320:ARG:NH1	2.09	0.67
9:H:26:ILE:HG22	9:H:40:LEU:HB3	1.75	0.67
6:C:242:GLN:HB3	6:C:246:ARG:HE	1.59	0.67
4:A:593:GLU:OE2	4:A:593:GLU:HA	1.94	0.67
5:B:712:PRO:O	5:B:713:ALA:HB3	1.94	0.67
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.75	0.67
12:K:40:HIS:HE1	12:K:63:VAL:CG2	2.07	0.67
14:T:29[A]:DUT:H5'2	14:T:29[A]:DUT:O1B	1.94	0.67
5:B:841:MET:HE2	5:B:1010:LEU:HD11	1.77	0.67
5:B:1023:VAL:O	5:B:1027:ILE:HG13	1.94	0.67
4:A:251:SER:HB3	4:A:258:GLY:HA3	1.75	0.67
4:A:423:ASP:CG	4:A:424:ILE:H	2.01	0.67
4:A:901:LEU:H	4:A:926:GLN:NE2	1.93	0.67
5:B:37:PHE:O	5:B:38:PHE:HB2	1.93	0.67
5:B:136:THR:O	5:B:137:TYR:C	2.34	0.67
5:B:63:ILE:O	5:B:67:SER:CB	2.43	0.67
5:B:624:LEU:HD12	5:B:625:LYS:N	2.10	0.67
5:B:1006:ILE:HG22	5:B:1007:VAL:N	2.07	0.67
4:A:351:THR:HG22	4:A:352:VAL:H	1.59	0.66
4:A:351:THR:HG21	4:A:466:SER:O	1.94	0.66
4:A:423:ASP:OD2	4:A:424:ILE:N	2.20	0.66
7:E:12:LEU:HD11	7:E:58:MET:HE1	1.76	0.66
4:A:116:ASP:CA	4:A:117:GLU:CB	2.63	0.66
4:A:407:ARG:HD2	4:A:413:ILE:HD11	1.77	0.66
5:B:90:ILE:HD13	5:B:134:LYS:HG2	1.77	0.66
4:A:707:GLY:HA3	4:A:1281:ARG:HG3	1.77	0.66
5:B:957:ASN:ND2	5:B:959:ASP:HB2	2.10	0.66
10:I:78:CYS:C	10:I:80:SER:H	2.04	0.66
11:J:48:ARG:HG3	11:J:48:ARG:HH11	1.61	0.66
4:A:56:PRO:C	4:A:57:ARG:CG	2.67	0.65
4:A:866:PHE:C	4:A:867:ILE:HG13	2.20	0.65
4:A:943:LEU:O	4:A:946:VAL:N	2.27	0.65
4:A:869:GLY:O	7:E:204:THR:HG21	1.95	0.65
9:H:137:GLN:C	9:H:139:ASN:H	2.03	0.65
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.77	0.65
4:A:1383:SER:O	4:A:1388:GLY:HA3	1.96	0.65
5:B:848:ARG:HH22	5:B:996:ARG:NH1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:32:CYS:SG	10:I:33:SER:N	2.69	0.65
9:H:109:LYS:NZ	9:H:111:LEU:HD12	2.12	0.65
5:B:346:GLU:HA	5:B:349:ILE:HD12	1.79	0.65
5:B:476:ARG:C	5:B:478:GLY:H	2.05	0.65
5:B:879:ARG:O	5:B:882:THR:HG22	1.97	0.65
4:A:679:ILE:HG23	4:A:729:ALA:HB1	1.78	0.65
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.77	0.65
4:A:116:ASP:HA	4:A:117:GLU:CB	2.18	0.65
5:B:20:ASP:CG	5:B:21:GLU:H	2.05	0.65
5:B:984:HIS:CD2	5:B:1024:ALA:HB3	2.31	0.65
5:B:1156:ASP:O	5:B:1157:ALA:HB3	1.96	0.65
6:C:258:ILE:CD1	12:K:42:LEU:HD21	2.26	0.64
10:I:63:GLY:HA3	10:I:104:LEU:HD11	1.77	0.64
4:A:68:GLN:O	4:A:70:CYS:N	2.26	0.64
4:A:117:GLU:H	4:A:118:HIS:CA	2.10	0.64
5:B:549:THR:HG22	5:B:550:ASP:H	1.62	0.64
5:B:1007:VAL:HG13	5:B:1008:PRO:HD2	1.78	0.64
4:A:47:ARG:HA	4:A:47:ARG:NE	2.12	0.64
5:B:398:ARG:CB	5:B:398:ARG:HH11	2.11	0.64
5:B:800:GLN:CB	11:J:52:THR:CG2	2.55	0.64
5:B:911:ILE:HD11	5:B:941:LEU:HD12	1.80	0.64
5:B:223:VAL:HG13	5:B:384:ARG:HH21	1.63	0.64
5:B:976:ILE:CG2	5:B:977:GLY:N	2.60	0.63
4:A:1174:PHE:C	4:A:1174:PHE:CD1	2.76	0.63
9:H:47:PHE:HB3	9:H:95:TYR:CD1	2.33	0.63
2:T:15:DA:H2''	2:T:16:DC:O5'	1.98	0.63
4:A:567:LYS:HD3	9:H:95:TYR:CG	2.33	0.63
7:E:77:SER:HB3	7:E:105:PHE:HA	1.79	0.63
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.34	0.63
4:A:65:LEU:HD23	4:A:65:LEU:N	2.14	0.63
5:B:211:VAL:HG23	5:B:483:LEU:HD13	1.80	0.63
6:C:167:HIS:CD2	6:C:169:LYS:H	2.05	0.63
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.64	0.63
9:H:24:CYS:HB2	9:H:44:VAL:HG21	1.81	0.63
4:A:34:LYS:HE2	4:A:57:ARG:HH21	1.63	0.63
5:B:624:LEU:HD12	5:B:624:LEU:C	2.24	0.63
5:B:1190:ASP:O	5:B:1191:ILE:HG13	1.99	0.63
7:E:62:ALA:HB3	7:E:78:LEU:HD22	1.80	0.63
4:A:636:GLU:OE2	4:A:962:ARG:HD2	1.97	0.63
10:I:103:CYS:C	10:I:105:SER:H	2.05	0.63
4:A:399:HIS:NE2	4:A:462:VAL:HG11	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:277:LYS:HZ1	5:B:335:GLY:H	1.47	0.62
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.32	0.62
6:C:142:VAL:H	11:J:16:ASP:HB3	1.64	0.62
4:A:1084:PHE:CZ	4:A:1093:LYS:HA	2.33	0.62
5:B:1111:MET:HE2	5:B:1118:PRO:N	2.14	0.62
3:N:4:DC:H2"	3:N:5:DT:OP2	1.99	0.62
4:A:345:VAL:HG22	5:B:1128:LEU:O	1.99	0.62
13:L:30:ILE:O	13:L:56:LEU:HA	1.99	0.62
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.63	0.62
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.99	0.62
6:C:70:ILE:HD11	6:C:144:ILE:CD1	2.30	0.62
4:A:1174:PHE:C	4:A:1174:PHE:HD1	2.07	0.62
5:B:911:ILE:HD11	5:B:941:LEU:HA	1.80	0.62
4:A:218:ASP:H	4:A:219:PHE:CB	2.11	0.62
5:B:712:PRO:O	5:B:713:ALA:CB	2.47	0.62
9:H:2:SER:CB	9:H:3:ASN:HB2	2.28	0.62
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.35	0.62
4:A:1325:THR:HG22	4:A:1326:ARG:HG3	1.80	0.62
4:A:72:GLU:HB3	4:A:76:GLU:CG	2.30	0.62
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	1.99	0.62
5:B:710:LEU:O	5:B:711:GLU:CB	2.47	0.62
4:A:1129:GLU:HA	4:A:1132:LYS:HE3	1.82	0.61
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.81	0.61
5:B:976:ILE:O	5:B:990:ILE:O	2.17	0.61
4:A:673:GLY:N	4:A:674:PRO:HD2	2.15	0.61
3:N:2:DT:H1'	3:N:3:DG:N7	2.15	0.61
4:A:565:ILE:HG12	4:A:567:LYS:NZ	2.15	0.61
6:C:73:GLN:HE21	6:C:74:SER:H	1.48	0.61
4:A:323:LYS:CG	4:A:324:SER:H	2.09	0.61
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	1.99	0.61
4:A:315:LEU:HG	4:A:320:ARG:NH2	2.09	0.61
12:K:91:CYS:O	12:K:95:ILE:HG13	2.00	0.61
4:A:351:THR:HG22	4:A:352:VAL:N	2.15	0.61
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.00	0.61
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.82	0.61
5:B:753:ALA:HA	5:B:756:ILE:HD12	1.83	0.61
8:F:72:LYS:HD3	8:F:142:SER:HB3	1.83	0.61
5:B:35:SER:HB3	5:B:39:ARG:HH21	1.64	0.61
6:C:131:HIS:O	6:C:132:PRO:C	2.42	0.61
4:A:323:LYS:HG2	4:A:324:SER:N	2.06	0.61
5:B:516:ASN:H	5:B:516:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:115:LEU:O	4:A:122:MET:HG2	2.01	0.60
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.83	0.60
5:B:398:ARG:HB3	5:B:398:ARG:HH11	1.64	0.60
5:B:711:GLU:CG	5:B:711:GLU:O	2.50	0.60
4:A:247:ARG:N	4:A:248:PRO:HD3	2.16	0.60
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.83	0.60
5:B:465:ASN:HA	5:B:476:ARG:HA	1.83	0.60
4:A:1189:SER:OG	4:A:1190:PRO:HD2	2.01	0.60
6:C:173:ALA:O	6:C:233:GLU:O	2.18	0.60
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.82	0.60
4:A:58:LEU:C	4:A:58:LEU:HD23	2.27	0.60
4:A:962:ARG:HA	4:A:965:GLN:HE21	1.67	0.60
5:B:487:THR:OG1	5:B:777:ALA:O	2.20	0.60
5:B:706:GLN:O	5:B:710:LEU:HB2	2.02	0.60
4:A:1080:THR:HG22	4:A:1081:LEU:N	2.17	0.59
5:B:955:THR:HG22	5:B:956:THR:N	2.18	0.59
7:E:28:TYR:HA	7:E:64:PRO:HA	1.84	0.59
9:H:2:SER:CA	9:H:3:ASN:HB2	2.32	0.59
4:A:65:LEU:H	4:A:65:LEU:CD2	2.16	0.59
4:A:93:VAL:HG22	4:A:304:MET:HE3	1.85	0.59
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.84	0.59
5:B:886:LYS:HB3	5:B:887:HIS:HA	1.82	0.59
4:A:1193:LEU:HD21	4:A:1267:MET:HE2	1.83	0.59
4:A:117:GLU:H	4:A:118:HIS:CB	2.15	0.59
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.14	0.59
5:B:475:SER:C	5:B:477:ALA:H	2.11	0.59
5:B:882:THR:HG23	5:B:883:LEU:H	1.68	0.59
5:B:1099:VAL:C	5:B:1103:ILE:HD11	2.27	0.59
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.84	0.59
5:B:879:ARG:NE	5:B:879:ARG:N	2.51	0.59
7:E:94:LYS:HE2	7:E:94:LYS:HA	1.84	0.59
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.32	0.59
4:A:870:GLU:HG2	7:E:208:TYR:CD2	2.38	0.59
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.38	0.59
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.85	0.58
5:B:848:ARG:HA	6:C:69:LEU:HD21	1.84	0.58
7:E:41:ASP:O	7:E:45:LYS:HG2	2.03	0.58
4:A:115:LEU:HD22	4:A:119:ASN:HD22	1.67	0.58
4:A:218:ASP:O	4:A:221:SER:HB2	2.03	0.58
4:A:218:ASP:CB	4:A:219:PHE:HB2	2.29	0.58
5:B:287:ARG:HD3	5:B:292:ILE:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:313:MET:HE1	5:B:390:LEU:HG	1.85	0.58
10:I:63:GLY:CA	10:I:104:LEU:HD11	2.34	0.58
4:A:64:ASN:HB3	4:A:66:LYS:HG2	1.84	0.58
4:A:452:LYS:HD3	4:A:510:GLN:OE1	2.03	0.58
5:B:802:PRO:HB3	5:B:1091:TYR:CD2	2.39	0.58
4:A:299:HIS:HA	4:A:302:THR:HG22	1.84	0.58
4:A:1435:PRO:C	4:A:1436:ILE:HD12	2.28	0.58
5:B:318:VAL:HG21	10:I:13:MET:HE2	1.86	0.58
5:B:986:GLN:NE2	5:B:1022:THR:HG21	2.18	0.58
6:C:166:GLU:HG2	12:K:10:PHE:CZ	2.38	0.58
4:A:167:CYS:O	4:A:169:ASN:N	2.37	0.58
4:A:102:VAL:HG12	4:A:211:PHE:HE1	1.68	0.58
4:A:423:ASP:O	4:A:424:ILE:HB	2.04	0.58
4:A:1435:PRO:O	4:A:1436:ILE:HD12	2.03	0.58
5:B:869:SER:O	5:B:870:ILE:HG13	2.03	0.58
5:B:1111:MET:HE2	5:B:1118:PRO:CA	2.34	0.58
4:A:273:ASN:HA	4:A:296:LEU:HD12	1.85	0.58
5:B:1149:GLU:HA	5:B:1153:GLU:OE2	2.04	0.57
6:C:73:GLN:HE21	6:C:75:MET:H	1.51	0.57
4:A:672:ASP:HB2	4:A:736:ASN:OD1	2.04	0.57
4:A:853:ASP:OD1	4:A:855:THR:HG22	2.03	0.57
4:A:93:VAL:CG1	4:A:301:ALA:HB1	2.27	0.57
4:A:1029:ARG:CG	4:A:1029:ARG:NH1	2.54	0.57
4:A:53:LEU:HG	4:A:54:ASN:N	2.09	0.57
5:B:307:ASP:OD2	5:B:310:MET:HE2	2.05	0.57
5:B:834:ASN:HB3	5:B:840:ILE:HD12	1.86	0.57
5:B:1013:ASN:C	5:B:1015:HIS:H	2.12	0.57
5:B:345:LYS:N	5:B:346:GLU:HG3	2.20	0.57
6:C:73:GLN:HE21	6:C:74:SER:N	2.03	0.57
6:C:242:GLN:HE21	6:C:246:ARG:HE	1.52	0.57
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.85	0.57
5:B:370:PHE:O	5:B:372:SER:N	2.37	0.57
9:H:129:TYR:C	9:H:131:ASN:H	2.11	0.57
4:A:364:VAL:O	4:A:364:VAL:HG13	2.04	0.57
4:A:567:LYS:CG	4:A:568:PRO:CD	2.80	0.57
4:A:756:ILE:O	4:A:760:GLN:HG3	2.03	0.57
5:B:886:LYS:HB3	5:B:887:HIS:CA	2.34	0.57
5:B:291:ILE:HD12	5:B:291:ILE:H	1.68	0.57
10:I:103:CYS:C	10:I:105:SER:N	2.60	0.57
4:A:276:LEU:CD1	4:A:292:ALA:HB1	2.34	0.57
7:E:175:LEU:CD1	7:E:176:PRO:HD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.70	0.57
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.87	0.57
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.87	0.56
4:A:590:ARG:NH2	4:A:621:THR:OG1	2.37	0.56
5:B:784:ASN:OD1	5:B:788:ARG:HD2	2.05	0.56
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.87	0.56
5:B:1182:CYS:SG	5:B:1185:CYS:HB3	2.44	0.56
13:L:28:LYS:HB2	13:L:39:SER:HB2	1.87	0.56
5:B:831:SER:HB2	5:B:833:TYR:HD1	1.70	0.56
7:E:40:GLU:HA	7:E:43:LYS:HZ2	1.70	0.56
10:I:10:CYS:SG	10:I:32:CYS:HB3	2.45	0.56
5:B:705:MET:N	5:B:710:LEU:HD12	2.21	0.56
5:B:783:THR:HG22	11:J:63:TYR:HE1	1.69	0.56
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.87	0.56
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.86	0.56
10:I:75:CYS:HB3	10:I:78:CYS:O	2.05	0.56
3:N:12:DT:H5"	7:E:119:SER:CB	2.35	0.56
4:A:549:MET:SD	4:A:577:ILE:CD1	2.94	0.56
4:A:55:ASP:H	4:A:56:PRO:HD2	1.70	0.56
5:B:122:LEU:HD22	5:B:958:GLN:HB2	1.86	0.56
5:B:274:PRO:O	5:B:275:TYR:HB2	2.06	0.56
5:B:637:LEU:HD13	5:B:740:HIS:HB3	1.88	0.56
9:H:89:LEU:C	9:H:91:ASP:H	2.13	0.56
4:A:885:THR:O	4:A:940:ARG:HD2	2.04	0.56
7:E:111:VAL:HG12	7:E:137:GLU:HG2	1.88	0.56
4:A:901:LEU:H	4:A:926:GLN:HE21	1.53	0.56
5:B:25:ILE:HD12	5:B:653:VAL:HG23	1.88	0.56
5:B:41:LYS:O	5:B:45:SER:HB3	2.06	0.56
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.89	0.56
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.41	0.56
4:A:870:GLU:HB2	7:E:204:THR:HG21	1.86	0.56
5:B:850:LEU:HD21	5:B:1009:ASP:HB3	1.88	0.56
5:B:487:THR:HG22	5:B:488:TYR:N	2.20	0.55
5:B:523:CYS:HB2	5:B:750:GLY:N	2.22	0.55
5:B:639:ILE:CD1	5:B:691:GLU:HB2	2.33	0.55
6:C:235:VAL:HG11	11:J:6:ARG:NH2	2.12	0.55
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.40	0.55
5:B:516:ASN:H	5:B:516:ASN:ND2	2.04	0.55
5:B:785:TYR:CD1	5:B:785:TYR:C	2.83	0.55
7:E:56:LYS:HB2	7:E:84:ASP:OD1	2.06	0.55
7:E:172:GLU:HG3	7:E:213:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:197:LYS:HE3	7:E:199:ILE:HD11	1.88	0.55
9:H:63:LEU:C	9:H:90:ALA:H	2.14	0.55
5:B:245:GLU:HG2	5:B:246:LYS:N	2.22	0.55
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.89	0.55
5:B:909:ASP:O	5:B:940:PRO:HA	2.06	0.55
6:C:233:GLU:OE1	11:J:43:ARG:NH2	2.40	0.55
4:A:306:ASN:O	4:A:307:ASP:HB3	2.07	0.55
6:C:56:THR:CG2	6:C:57:VAL:H	2.13	0.55
5:B:778:MET:HG2	5:B:794:ASN:HB3	1.87	0.55
4:A:72:GLU:HB3	4:A:76:GLU:HG3	1.89	0.55
4:A:672:ASP:OD1	4:A:674:PRO:CG	2.40	0.55
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.88	0.55
5:B:711:GLU:O	5:B:711:GLU:HG3	2.06	0.55
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.89	0.55
4:A:117:GLU:N	4:A:118:HIS:C	2.64	0.55
4:A:246:VAL:HG12	4:A:246:VAL:O	2.07	0.55
4:A:1211:GLN:O	4:A:1215:ARG:HB2	2.06	0.55
5:B:807:ARG:HH11	5:B:807:ARG:CG	2.20	0.55
5:B:986:GLN:HE21	5:B:1022:THR:HG21	1.71	0.55
7:E:40:GLU:HA	7:E:43:LYS:NZ	2.21	0.55
4:A:304:MET:O	4:A:326:ARG:HB2	2.06	0.55
4:A:1076:ALA:HA	4:A:1079:MET:HE2	1.89	0.55
5:B:770:GLN:OE1	5:B:983:ARG:HA	2.05	0.55
5:B:976:ILE:CG2	5:B:977:GLY:H	2.20	0.55
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.87	0.55
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.89	0.55
6:C:166:GLU:HG2	12:K:10:PHE:HZ	1.71	0.55
14:T:29[A]:DUT:O1B	14:T:29[A]:DUT:H4'	2.07	0.54
4:A:71:GLN:C	4:A:73:GLY:H	2.16	0.54
4:A:707:GLY:CA	4:A:1281:ARG:HG3	2.37	0.54
5:B:451:LYS:HG2	5:B:455:SER:HB2	1.88	0.54
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.21	0.54
10:I:32:CYS:O	10:I:33:SER:HB2	2.06	0.54
4:A:35:ILE:O	4:A:35:ILE:HG22	2.06	0.54
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.89	0.54
5:B:212:LEU:HD23	5:B:480:SER:HB2	1.87	0.54
6:C:66:ARG:NH2	11:J:3:VAL:O	2.40	0.54
9:H:129:TYR:HA	9:H:131:ASN:ND2	2.23	0.54
14:T:29[A]:DUT:O1B	14:T:29[A]:DUT:C5'	2.55	0.54
4:A:253:ASN:O	4:A:254:GLU:HB2	2.05	0.54
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:474:VAL:HG22	4:A:478:TYR:CE1	2.43	0.54
4:A:58:LEU:HG	4:A:58:LEU:O	2.07	0.54
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.72	0.54
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.06	0.54
5:B:1006:ILE:CD1	11:J:43:ARG:HB2	2.36	0.54
6:C:57:VAL:HG11	11:J:57:ILE:HD12	1.88	0.54
5:B:558:LEU:C	5:B:560:GLU:H	2.16	0.54
5:B:886:LYS:HD2	5:B:890:TYR:OH	2.07	0.54
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.41	0.54
9:H:2:SER:HB2	9:H:3:ASN:HB2	1.88	0.54
9:H:22:LYS:HD2	9:H:45:GLU:OE1	2.07	0.54
12:K:10:PHE:CD1	12:K:11:LEU:HD13	2.43	0.54
4:A:372:LYS:HA	4:A:435:HIS:CD2	2.43	0.54
4:A:403:LYS:HB2	4:A:404:TYR:CD1	2.42	0.54
4:A:800:VAL:C	4:A:802:ASN:H	2.14	0.54
5:B:62:ILE:HD12	5:B:418:LYS:HG3	1.89	0.54
10:I:78:CYS:SG	10:I:106:CYS:N	2.81	0.54
2:T:16:DC:H2'	2:T:17:DG:H8	1.71	0.54
4:A:70:CYS:O	4:A:72:GLU:HG2	2.08	0.54
4:A:1082:ASN:H	4:A:1082:ASN:ND2	2.06	0.54
4:A:1138:ILE:HG21	4:A:1316:VAL:HG13	1.89	0.54
5:B:1017:ILE:H	5:B:1018:PRO:HD3	1.73	0.54
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.89	0.54
2:T:20:DC:H2'	2:T:21:DC:O4'	2.08	0.54
5:B:886:LYS:CB	5:B:887:HIS:HA	2.37	0.54
4:A:92:HIS:HE1	5:B:1210:MET:O	1.91	0.54
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.90	0.54
4:A:477:PRO:HG3	4:A:521:MET:CE	2.38	0.54
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.90	0.54
5:B:515:HIS:N	5:B:518:HIS:CD2	2.76	0.54
12:K:40:HIS:CE1	12:K:63:VAL:CG2	2.90	0.54
4:A:567:LYS:NZ	9:H:95:TYR:CZ	2.75	0.54
4:A:575:LYS:HD3	4:A:612:ILE:HD11	1.90	0.54
5:B:278:GLN:CG	5:B:279:ASP:H	2.16	0.54
5:B:361:LEU:HD11	5:B:381:MET:CE	2.38	0.53
12:K:65:HIS:CD2	12:K:66:PRO:CD	2.91	0.53
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.08	0.53
4:A:93:VAL:HG13	4:A:301:ALA:CB	2.28	0.53
5:B:363:HIS:O	5:B:364:ILE:CB	2.53	0.53
4:A:848:ILE:HD13	4:A:858:ASN:HB3	1.90	0.53
4:A:1333:ILE:O	4:A:1333:ILE:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:645:SER:C	5:B:647:GLY:H	2.17	0.53
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	1.91	0.53
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.91	0.53
4:A:1130:GLN:HE21	4:A:1134:ILE:HD11	1.73	0.53
5:B:292:ILE:H	5:B:293:PRO:HD2	1.74	0.53
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.73	0.53
7:E:30:ILE:HG23	7:E:34:GLU:OE1	2.08	0.53
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.91	0.53
6:C:100:THR:HG22	6:C:101:LEU:N	2.22	0.53
2:T:16:DC:C6	2:T:17:DG:C8	2.97	0.53
4:A:381:THR:HG22	4:A:383:TYR:H	1.74	0.53
5:B:563:MET:HA	5:B:589:VAL:O	2.09	0.53
5:B:567:GLU:H	5:B:567:GLU:CD	2.16	0.53
6:C:167:HIS:HD2	6:C:169:LYS:N	1.95	0.53
10:I:78:CYS:O	10:I:80:SER:N	2.40	0.53
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.41	0.53
4:A:901:LEU:HA	4:A:907:THR:CG2	2.38	0.53
4:A:1329:THR:HG22	4:A:1331:SER:N	2.24	0.53
5:B:235:SER:OG	5:B:236:HIS:ND1	2.39	0.53
5:B:515:HIS:N	5:B:518:HIS:HD2	2.07	0.53
5:B:872:GLU:HG2	5:B:916:THR:HB	1.90	0.53
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.44	0.52
5:B:643:ASP:O	5:B:644:GLU:HB3	2.09	0.52
5:B:1045:SER:O	5:B:1046:PRO:C	2.52	0.52
2:T:18:DA:H2'	2:T:19:DT:C6	2.43	0.52
4:A:102:VAL:HG12	4:A:211:PHE:CE1	2.44	0.52
4:A:451:HIS:HB3	4:A:454:SER:H	1.74	0.52
4:A:871:ASP:HB3	7:E:205:SER:HB3	1.90	0.52
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.75	0.52
5:B:898:LEU:HB2	13:L:58:LYS:HE3	1.92	0.52
6:C:92:CYS:SG	6:C:94:LYS:HB2	2.50	0.52
9:H:26:ILE:CG2	9:H:40:LEU:HB3	2.39	0.52
4:A:1436:ILE:O	4:A:1438:THR:N	2.43	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.24	0.52
5:B:346:GLU:HA	5:B:349:ILE:HD13	1.91	0.52
4:A:456:MET:HE2	4:A:510:GLN:CB	2.36	0.52
4:A:1110:ASN:HD22	4:A:1110:ASN:N	1.90	0.52
4:A:249:SER:C	4:A:250:ILE:HG12	2.35	0.52
4:A:313:GLN:HG2	4:A:322:VAL:HG22	1.91	0.52
4:A:1425:SER:O	4:A:1429:ILE:HG13	2.10	0.52
9:H:131:ASN:O	9:H:133:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:58:LEU:HB2	4:A:80:HIS:O	2.10	0.52
4:A:534:LEU:O	4:A:574:GLY:HA3	2.10	0.52
4:A:568:PRO:O	4:A:569:LYS:HB2	2.09	0.52
4:A:786:HIS:HE1	5:B:742:GLU:OE1	1.93	0.52
5:B:211:VAL:HG21	5:B:483:LEU:HD13	1.88	0.52
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.91	0.52
3:N:8:DT:H2''	3:N:9:DC:OP2	2.09	0.52
4:A:55:ASP:O	4:A:57:ARG:N	2.43	0.52
4:A:297:GLN:HG3	4:A:298:PHE:N	2.25	0.52
5:B:1006:ILE:CG2	5:B:1007:VAL:N	2.73	0.52
1:R:2:U:H2'	1:R:3:C:H6	1.74	0.52
4:A:95:PHE:O	4:A:96:ILE:C	2.52	0.52
5:B:601:ARG:HA	5:B:615:MET:HE1	1.92	0.52
5:B:794:ASN:C	5:B:795:ILE:HD12	2.35	0.52
5:B:801:LYS:HG2	11:J:52:THR:O	2.09	0.52
11:J:45:CYS:O	11:J:48:ARG:HG3	2.10	0.52
4:A:57:ARG:HB3	4:A:68:GLN:HB3	1.92	0.52
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.45	0.52
4:A:365:GLY:O	4:A:468:PHE:HA	2.10	0.51
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.39	0.51
4:A:456:MET:HE1	4:A:521:MET:CE	2.40	0.51
4:A:590:ARG:NH2	4:A:620:LYS:HB2	2.26	0.51
4:A:821:ARG:O	4:A:825:ILE:HG12	2.10	0.51
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.91	0.51
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.91	0.51
9:H:128:ASN:O	9:H:131:ASN:OD1	2.27	0.51
5:B:102:VAL:HG12	5:B:103:ASN:N	2.24	0.51
5:B:957:ASN:ND2	5:B:959:ASP:H	2.09	0.51
9:H:100:THR:HG23	9:H:138:GLU:HA	1.91	0.51
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.11	0.51
1:R:3:C:H42	2:T:26:DG:H1	1.57	0.51
4:A:34:LYS:HE2	4:A:57:ARG:NH2	2.26	0.51
4:A:67:CYS:C	4:A:68:GLN:HG3	2.35	0.51
5:B:287:ARG:HA	5:B:291:ILE:O	2.10	0.51
5:B:542:MET:HE1	5:B:743:ILE:HG13	1.92	0.51
5:B:770:GLN:HG2	5:B:983:ARG:O	2.11	0.51
5:B:807:ARG:HG3	5:B:807:ARG:NH1	2.24	0.51
4:A:117:GLU:CA	4:A:118:HIS:O	2.59	0.51
4:A:324:SER:C	4:A:326:ARG:N	2.69	0.51
5:B:640:VAL:HG22	5:B:651:LEU:CD2	2.41	0.51
5:B:863:GLU:OE1	5:B:962:LYS:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:248:ILE:HG12	12:K:101:LEU:HD12	1.92	0.51
7:E:100:ILE:O	7:E:101:GLN:C	2.52	0.51
4:A:56:PRO:O	4:A:57:ARG:CG	2.51	0.51
5:B:794:ASN:N	5:B:794:ASN:HD22	2.07	0.51
5:B:844:SER:O	5:B:848:ARG:HG3	2.11	0.51
6:C:165:LYS:O	12:K:6:ARG:NH1	2.43	0.51
4:A:709:THR:HG21	10:I:93:LYS:O	2.11	0.51
5:B:879:ARG:NE	5:B:879:ARG:CA	2.74	0.51
12:K:49:GLU:HA	12:K:52:ASN:ND2	2.25	0.51
4:A:130:ASP:O	4:A:132:LYS:N	2.35	0.51
4:A:135:PHE:HD1	4:A:222:LEU:HB2	1.75	0.51
5:B:193:LYS:NZ	11:J:65:PRO:HG3	2.26	0.51
5:B:857:ARG:HH21	5:B:942:ARG:NH2	2.09	0.51
5:B:1107:ALA:O	5:B:1108:ARG:CB	2.58	0.51
4:A:549:MET:SD	4:A:577:ILE:HD11	2.50	0.51
5:B:140:ILE:H	5:B:141:ASP:C	2.19	0.51
5:B:803:LEU:HG	5:B:822:ASN:ND2	2.26	0.51
5:B:1073:TYR:N	5:B:1073:TYR:CD1	2.79	0.51
8:F:111:LEU:HD12	8:F:111:LEU:H	1.76	0.51
4:A:115:LEU:HD12	4:A:122:MET:HE2	1.93	0.50
4:A:1110:ASN:ND2	4:A:1110:ASN:N	2.52	0.50
5:B:906:SER:CB	5:B:946:ASN:CB	2.83	0.50
4:A:320:ARG:CZ	4:A:320:ARG:H	2.24	0.50
4:A:323:LYS:O	4:A:324:SER:CB	2.59	0.50
5:B:884:ARG:O	5:B:936:ASP:HB3	2.12	0.50
6:C:46:ILE:HA	6:C:159:ALA:HA	1.92	0.50
9:H:44:VAL:HG12	9:H:44:VAL:O	2.10	0.50
12:K:40:HIS:CE1	12:K:63:VAL:HG21	2.46	0.50
12:K:62:LYS:HG3	12:K:62:LYS:O	2.10	0.50
4:A:71:GLN:O	4:A:73:GLY:N	2.44	0.50
4:A:1295:THR:OG1	4:A:1297:GLU:OE1	2.29	0.50
5:B:665:GLU:O	5:B:668:ASP:HB3	2.10	0.50
6:C:167:HIS:CD2	6:C:169:LYS:HB3	2.46	0.50
7:E:144:ILE:O	7:E:150:VAL:HG21	2.11	0.50
4:A:130:ASP:C	4:A:132:LYS:H	2.18	0.50
4:A:535:THR:HG22	4:A:616:VAL:HA	1.93	0.50
4:A:754:SER:N	4:A:757:ASN:HD22	2.04	0.50
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.47	0.50
7:E:15:ALA:O	7:E:19:VAL:HG23	2.12	0.50
9:H:5:LEU:HD12	9:H:60:ALA:O	2.11	0.50
4:A:541:ILE:HG13	4:A:546:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:O	4:A:569:LYS:N	2.45	0.50
4:A:647:GLY:O	4:A:651:LYS:HG3	2.11	0.50
4:A:800:VAL:O	4:A:800:VAL:HG12	2.11	0.50
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.93	0.50
11:J:42:LYS:HG3	11:J:43:ARG:H	1.77	0.50
12:K:47:ARG:HH11	12:K:47:ARG:HB3	1.75	0.50
4:A:253:ASN:CG	4:A:254:GLU:H	2.19	0.50
4:A:276:LEU:HD11	4:A:292:ALA:CB	2.42	0.50
4:A:381:THR:HG23	4:A:382:PRO:HD2	1.92	0.50
5:B:843:GLN:HB2	5:B:993:THR:HB	1.94	0.50
4:A:32:VAL:O	4:A:57:ARG:NH1	2.44	0.50
4:A:608:ILE:C	4:A:609:ASP:O	2.53	0.50
5:B:563:MET:HE1	5:B:587:HIS:CB	2.40	0.50
4:A:826:ASP:HA	4:A:829:VAL:HB	1.93	0.50
5:B:1072:MET:HE1	5:B:1087:PHE:CD1	2.47	0.50
4:A:244:PRO:HB2	4:A:245:PRO:CD	2.42	0.50
4:A:496:GLU:HB2	8:F:95:GLY:HA3	1.94	0.50
4:A:779:PHE:CE2	5:B:517:THR:HG22	2.47	0.50
6:C:163:ILE:HD12	6:C:165:LYS:HB2	1.93	0.50
4:A:545:GLN:HB3	4:A:549:MET:HE3	1.93	0.49
4:A:775:ILE:O	4:A:797:LYS:HE2	2.12	0.49
5:B:464:GLY:HA3	5:B:478:GLY:HA2	1.94	0.49
5:B:981:ALA:O	5:B:1093:GLN:N	2.31	0.49
9:H:139:ASN:O	9:H:140:ALA:HB3	2.12	0.49
2:T:18:DA:H2	14:T:29[B]:DUT:O2	1.86	0.49
4:A:203:SER:O	4:A:207:ILE:HG13	2.12	0.49
4:A:1123:GLY:CA	4:A:1124:HIS:HB2	2.13	0.49
4:A:1436:ILE:O	4:A:1437:GLY:C	2.54	0.49
4:A:273:ASN:C	4:A:275:SER:H	2.20	0.49
4:A:298:PHE:HA	4:A:299:HIS:C	2.35	0.49
4:A:367:PRO:HG2	4:A:370:ILE:HG13	1.93	0.49
4:A:754:SER:H	4:A:757:ASN:ND2	2.05	0.49
4:A:1444:MET:O	8:F:133:VAL:N	2.42	0.49
5:B:62:ILE:HG23	5:B:418:LYS:HG3	1.93	0.49
7:E:3:GLN:HG2	7:E:4:GLU:N	2.21	0.49
4:A:552:TRP:NE1	4:A:655:PHE:CD1	2.81	0.49
5:B:873:THR:O	5:B:914:LYS:HG3	2.12	0.49
9:H:56:THR:O	9:H:144:ILE:HA	2.12	0.49
9:H:83:GLN:HG3	12:K:54:ARG:HB3	1.95	0.49
11:J:3:VAL:CG2	11:J:18:TRP:CB	2.83	0.49
2:T:18:DA:H61	14:T:29[B]:DUT:C4	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:219:PHE:HZ	4:A:230:ARG:HD3	1.78	0.49
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.95	0.49
5:B:416:LEU:HD12	5:B:466:TRP:CZ2	2.47	0.49
5:B:488:TYR:CE2	5:B:813:LYS:HB2	2.48	0.49
5:B:705:MET:HE3	5:B:705:MET:HA	1.94	0.49
9:H:137:GLN:C	9:H:139:ASN:N	2.70	0.49
4:A:290:GLU:OE1	4:A:293:GLU:HG3	2.13	0.49
4:A:341:MET:HE1	4:A:1425:SER:HB3	1.95	0.49
4:A:455:MET:O	5:B:1141:HIS:HE1	1.95	0.49
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	3.00	0.49
5:B:185:THR:OG1	5:B:188:ASP:OD2	2.29	0.49
5:B:979:LYS:CE	5:B:987:LYS:HG2	2.42	0.49
4:A:64:ASN:HB3	4:A:66:LYS:CG	2.43	0.49
5:B:190:TYR:CZ	5:B:196:PRO:HG3	2.47	0.49
5:B:287:ARG:O	5:B:289:LEU:N	2.46	0.49
5:B:526:GLU:HG3	5:B:771:SER:HB3	1.94	0.49
5:B:793:ALA:C	5:B:794:ASN:HD22	2.21	0.49
5:B:975:GLN:HG2	5:B:976:ILE:H	1.78	0.49
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.27	0.49
11:J:48:ARG:CZ	11:J:49:MET:HE1	2.42	0.49
13:L:42:ARG:HD2	13:L:42:ARG:H	1.77	0.49
4:A:265:LYS:C	4:A:267:ALA:N	2.69	0.49
5:B:234:ILE:HD13	5:B:234:ILE:H	1.76	0.49
6:C:57:VAL:HG12	6:C:58:LEU:HD23	1.93	0.49
10:I:10:CYS:SG	10:I:31:THR:HB	2.52	0.49
4:A:770:VAL:HA	4:A:822:GLU:OE1	2.13	0.49
5:B:882:THR:HG23	5:B:883:LEU:N	2.28	0.49
5:B:1111:MET:HE2	5:B:1118:PRO:HA	1.94	0.49
6:C:260:LEU:HG	6:C:264:GLN:HE22	1.78	0.49
7:E:109:ILE:HD13	7:E:109:ILE:N	2.28	0.49
9:H:92:ASP:OD2	9:H:92:ASP:N	2.45	0.49
4:A:91:PHE:HD2	4:A:297:GLN:OE1	1.96	0.49
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.94	0.49
5:B:911:ILE:HD11	5:B:941:LEU:CA	2.43	0.49
5:B:1190:ASP:C	5:B:1191:ILE:HG13	2.38	0.49
9:H:7:ASP:O	9:H:8:ASP:HB2	2.12	0.49
4:A:89:PRO:HG2	4:A:205:GLU:HG3	1.93	0.48
4:A:871:ASP:HB3	7:E:204:THR:HG23	1.93	0.48
10:I:55:THR:HG23	10:I:58:VAL:HG21	1.94	0.48
4:A:693:VAL:O	4:A:696:GLU:HB3	2.14	0.48
4:A:855:THR:HG23	4:A:857:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1195:LEU:HD11	4:A:1267:MET:CE	2.40	0.48
5:B:696:GLU:O	5:B:699:GLU:HB2	2.13	0.48
4:A:335:ARG:NH1	5:B:1202:LEU:HD12	2.28	0.48
4:A:1111:MET:HG3	4:A:1114:PRO:HG3	1.94	0.48
4:A:1356:ILE:O	4:A:1359:ASP:HB3	2.13	0.48
5:B:1037:LEU:HD13	5:B:1062:HIS:HB3	1.94	0.48
6:C:27:LEU:HA	6:C:228:PHE:CZ	2.48	0.48
8:F:109:VAL:HG22	8:F:110:ASP:N	2.28	0.48
4:A:148:CYS:HB3	4:A:169:ASN:H	1.78	0.48
5:B:574:SER:N	5:B:575:PRO:HD3	2.28	0.48
5:B:783:THR:HG21	11:J:59:LYS:HB3	1.96	0.48
6:C:70:ILE:HD11	6:C:144:ILE:HD12	1.94	0.48
3:N:12:DT:H5"	7:E:119:SER:HB2	1.95	0.48
4:A:306:ASN:O	4:A:307:ASP:CB	2.61	0.48
5:B:744:HIS:HD2	5:B:746:SER:N	1.97	0.48
4:A:1166:ASP:O	4:A:1168:GLU:N	2.47	0.48
5:B:918:ILE:HG13	5:B:935:ARG:NH1	2.28	0.48
6:C:238:ILE:HG22	6:C:242:GLN:HB2	1.95	0.48
5:B:291:ILE:HD12	5:B:291:ILE:N	2.28	0.48
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.48	0.48
9:H:40:LEU:HD13	9:H:123:MET:HG3	1.95	0.48
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.47	0.48
6:C:73:GLN:HE21	6:C:75:MET:N	2.12	0.48
4:A:151:ASP:CG	4:A:163:SER:HA	2.38	0.48
4:A:695:LYS:HA	4:A:695:LYS:HD2	1.56	0.48
4:A:1080:THR:CG2	4:A:1081:LEU:N	2.77	0.48
6:C:22:LEU:HD21	6:C:25:VAL:HG21	1.95	0.48
4:A:414:ASP:OD1	4:A:416:ARG:HG2	2.14	0.48
4:A:1004:ASN:O	4:A:1008:GLN:HG2	2.13	0.48
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.95	0.48
5:B:1016:ALA:HB1	5:B:1020:ARG:NH1	2.29	0.48
6:C:77:ILE:HD12	6:C:161:LYS:HG3	1.96	0.48
4:A:672:ASP:OD1	4:A:675:THR:N	2.47	0.47
5:B:1054:GLY:HA2	5:B:1057:LYS:NZ	2.29	0.47
8:F:71:GLU:HA	8:F:72:LYS:C	2.39	0.47
4:A:1004:ASN:CG	7:E:167:ARG:HD2	2.39	0.47
4:A:1329:THR:CG2	4:A:1331:SER:H	2.26	0.47
5:B:841:MET:O	5:B:993:THR:HA	2.14	0.47
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.47	0.47
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:O1A	2.13	0.47
4:A:381:THR:CG2	4:A:382:PRO:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:919:ILE:O	4:A:922:ASP:HB2	2.14	0.47
5:B:22:SER:O	5:B:654:ARG:HD2	2.14	0.47
5:B:841:MET:HE2	5:B:1010:LEU:CD1	2.42	0.47
9:H:137:GLN:HB3	9:H:139:ASN:HB2	1.96	0.47
4:A:26:GLU:O	4:A:30:ILE:HB	2.14	0.47
4:A:457:ALA:HB2	4:A:501:LEU:HD13	1.97	0.47
4:A:1154:TYR:HE1	10:I:18:GLU:HG3	1.79	0.47
5:B:470:LYS:C	5:B:472:ALA:H	2.22	0.47
5:B:752:ALA:O	5:B:755:ILE:HG12	2.14	0.47
5:B:805:THR:HG22	5:B:809:MET:SD	2.54	0.47
5:B:881:ASN:HB2	5:B:933:SER:OG	2.14	0.47
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.47	0.47
5:B:1180:PHE:O	5:B:1181:GLU:HG2	2.15	0.47
4:A:208:LEU:C	4:A:208:LEU:CD2	2.85	0.47
4:A:507:VAL:HB	4:A:508:PRO:HD3	1.95	0.47
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.15	0.47
5:B:660:LYS:HE2	5:B:679:TYR:CD1	2.49	0.47
6:C:6:PRO:HB2	12:K:101:LEU:HD23	1.96	0.47
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.77	0.47
12:K:49:GLU:C	12:K:51:LEU:H	2.20	0.47
4:A:117:GLU:O	4:A:123:ARG:HG2	2.14	0.47
4:A:800:VAL:C	4:A:802:ASN:N	2.70	0.47
4:A:1193:LEU:HB2	4:A:1260:LEU:HD11	1.96	0.47
5:B:53:GLN:HG2	5:B:547:VAL:HG13	1.95	0.47
5:B:378:LEU:O	5:B:382:ILE:HG12	2.15	0.47
5:B:745:PRO:O	5:B:748:ILE:HG12	2.15	0.47
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.96	0.47
5:B:1094:ARG:CG	5:B:1094:ARG:NH1	2.38	0.47
7:E:64:PRO:CD	7:E:76:GLY:HA2	2.33	0.47
7:E:172:GLU:CG	7:E:213:ILE:HD12	2.45	0.47
10:I:46:HIS:O	10:I:47:GLU:O	2.33	0.47
11:J:1:MET:O	11:J:2:ILE:HB	2.13	0.47
4:A:672:ASP:OD2	4:A:736:ASN:CG	2.52	0.47
4:A:800:VAL:HG13	4:A:812:GLU:HG2	1.96	0.47
5:B:474:SER:C	5:B:476:ARG:N	2.70	0.47
5:B:778:MET:HB3	5:B:796:LEU:HD13	1.95	0.47
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.49	0.47
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.49	0.47
5:B:821:GLN:HB2	5:B:851:PHE:CE2	2.50	0.47
8:F:140:ASP:OD1	8:F:141:GLY:N	2.48	0.47
14:T:29[B]:DUT:C3'	14:T:29[B]:DUT:C6	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:64:ASN:O	4:A:66:LYS:N	2.48	0.47
4:A:312:PRO:O	4:A:313:GLN:NE2	2.48	0.47
4:A:320:ARG:H	4:A:320:ARG:NE	2.13	0.47
4:A:455:MET:O	5:B:1141:HIS:CE1	2.68	0.47
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.15	0.47
6:C:69:LEU:HD12	6:C:69:LEU:N	2.30	0.47
4:A:746:MET:HG2	5:B:1015:HIS:HE1	1.80	0.46
5:B:406:LEU:HD12	5:B:633:VAL:HG22	1.97	0.46
5:B:470:LYS:O	5:B:471:LYS:HG3	2.15	0.46
5:B:562:GLY:O	5:B:563:MET:HB3	2.15	0.46
5:B:890:TYR:CE2	5:B:910:VAL:HG21	2.50	0.46
5:B:1175:LEU:O	5:B:1176:ASN:CB	2.63	0.46
1:R:9:G:H2'	1:R:10:A:C8	2.50	0.46
4:A:14:VAL:HB	4:A:1430:LEU:HD13	1.97	0.46
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.97	0.46
4:A:43:GLU:OE1	4:A:46:THR:HB	2.16	0.46
4:A:55:ASP:O	4:A:58:LEU:N	2.48	0.46
4:A:253:ASN:O	4:A:254:GLU:CB	2.63	0.46
4:A:443:LEU:HD23	4:A:443:LEU:HA	1.73	0.46
4:A:495:GLU:O	4:A:498:ARG:HG3	2.14	0.46
5:B:798:TYR:OH	6:C:62:PHE:HE2	1.99	0.46
7:E:86:PRO:O	7:E:114:ASN:HB2	2.15	0.46
9:H:135:LEU:C	9:H:137:GLN:H	2.22	0.46
12:K:46:ILE:O	12:K:50:LEU:HB2	2.15	0.46
4:A:298:PHE:O	4:A:298:PHE:CG	2.68	0.46
4:A:650:GLN:O	4:A:654:ASN:HB2	2.16	0.46
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.49	0.46
6:C:231:ASN:HD22	6:C:231:ASN:C	2.23	0.46
7:E:102:GLU:C	7:E:104:ASN:H	2.23	0.46
4:A:499:ALA:O	4:A:503:GLN:HG2	2.14	0.46
5:B:680:THR:O	5:B:683:SER:HB2	2.15	0.46
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.48	0.46
4:A:116:ASP:HB3	4:A:117:GLU:HB3	1.87	0.46
4:A:523:ILE:HG23	4:A:527:THR:HB	1.97	0.46
4:A:532:ARG:HG3	4:A:616:VAL:HG11	1.98	0.46
4:A:1158:PRO:HB3	4:A:1188:GLN:OE1	2.16	0.46
4:A:1188:GLN:HB3	4:A:1189:SER:H	1.59	0.46
5:B:237:VAL:HG11	5:B:255:GLN:HE21	1.81	0.46
9:H:109:LYS:HZ2	9:H:111:LEU:HD12	1.81	0.46
4:A:68:GLN:C	4:A:70:CYS:H	2.18	0.46
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:LEU:HD12	4:A:808:LEU:N	2.30	0.46
5:B:1021:MET:HE3	5:B:1021:MET:HB2	1.71	0.46
5:B:1106:ARG:HG2	5:B:1107:ALA:N	2.31	0.46
5:B:1106:ARG:NH2	5:B:1111:MET:HE3	2.29	0.46
14:T:29[B]:DUT:C6	14:T:29[B]:DUT:H3'	2.46	0.46
4:A:949:ASP:OD1	4:A:949:ASP:N	2.45	0.46
5:B:475:SER:C	5:B:477:ALA:N	2.72	0.46
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.81	0.46
6:C:98:VAL:C	6:C:99:LEU:HD22	2.40	0.46
6:C:254:LYS:HD3	12:K:42:LEU:HD13	1.98	0.46
4:A:323:LYS:O	4:A:324:SER:HB3	2.16	0.46
4:A:873:MET:HE3	4:A:957:PRO:HG3	1.98	0.46
5:B:273:LEU:HD21	5:B:360:PHE:CD1	2.51	0.46
7:E:124:VAL:HA	7:E:132:ILE:HD11	1.97	0.46
11:J:5:VAL:O	11:J:6:ARG:O	2.33	0.46
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:H3'	1.97	0.46
4:A:351:THR:C	4:A:486:GLU:HG3	2.41	0.46
4:A:847:ASP:OD2	4:A:858:ASN:HB2	2.16	0.46
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.46	0.46
5:B:386:LEU:C	5:B:388:CYS:H	2.23	0.46
5:B:1110:PRO:O	5:B:1119:VAL:HG13	2.16	0.46
4:A:567:LYS:HD3	9:H:95:TYR:CD1	2.50	0.46
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.98	0.46
1:R:2:U:H2'	1:R:3:C:C6	2.51	0.45
4:A:671:ALA:O	4:A:672:ASP:O	2.35	0.45
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.16	0.45
5:B:25:ILE:HD12	5:B:653:VAL:CG2	2.46	0.45
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.97	0.45
5:B:956:THR:HB	13:L:46:VAL:HG21	1.98	0.45
5:B:1076:HIS:CG	12:K:40:HIS:CD2	3.04	0.45
5:B:1156:ASP:O	5:B:1157:ALA:CB	2.61	0.45
12:K:51:LEU:CD1	12:K:59:ALA:HB3	2.46	0.45
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.98	0.45
4:A:800:VAL:HA	4:A:812:GLU:HG2	1.97	0.45
4:A:1171:GLN:H	4:A:1171:GLN:HG3	1.50	0.45
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.99	0.45
4:A:1277:GLU:O	4:A:1278:ASN:CB	2.64	0.45
4:A:120:GLU:O	4:A:121:LEU:HB2	2.15	0.45
4:A:711:ARG:NH1	10:I:95:THR:O	2.50	0.45
5:B:651:LEU:HD11	5:B:707:PRO:HG3	1.98	0.45
3:N:11:DG:H1'	3:N:12:DT:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:575:LYS:HB3	4:A:612:ILE:HG12	1.98	0.45
4:A:705:LYS:O	4:A:706:HIS:C	2.60	0.45
5:B:709:ASP:C	5:B:710:LEU:HD23	2.35	0.45
5:B:1155:SER:O	5:B:1156:ASP:O	2.34	0.45
7:E:127:ILE:HD13	7:E:127:ILE:H	1.82	0.45
4:A:99:ILE:HD11	4:A:234:MET:CB	2.47	0.45
4:A:115:LEU:HD21	4:A:145:LYS:HE3	1.99	0.45
7:E:128:PRO:HA	7:E:129:PRO:C	2.41	0.45
7:E:192:ARG:O	7:E:192:ARG:HG3	2.16	0.45
9:H:6:PHE:CG	9:H:7:ASP:N	2.84	0.45
9:H:89:LEU:O	9:H:91:ASP:N	2.50	0.45
9:H:108:SER:O	9:H:110:ASP:N	2.50	0.45
4:A:1341:ILE:HG22	7:E:182:ASP:OD2	2.16	0.45
5:B:465:ASN:OD1	5:B:476:ARG:HB2	2.15	0.45
5:B:643:ASP:OD2	5:B:644:GLU:N	2.50	0.45
5:B:1106:ARG:HG2	5:B:1108:ARG:H	1.82	0.45
5:B:1111:MET:CE	5:B:1118:PRO:HA	2.47	0.45
6:C:124:LEU:O	6:C:127:ARG:HG2	2.17	0.45
4:A:446:ARG:HB2	4:A:487:MET:SD	2.57	0.45
4:A:826:ASP:N	4:A:826:ASP:OD1	2.49	0.45
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	1.98	0.45
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.52	0.45
5:B:102:VAL:HG22	5:B:112:LEU:HD22	1.99	0.45
5:B:1013:ASN:C	5:B:1015:HIS:N	2.72	0.45
5:B:1221:SER:C	5:B:1223:ASP:H	2.24	0.45
6:C:70:ILE:HD11	6:C:144:ILE:HD11	1.99	0.45
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.51	0.45
4:A:567:LYS:HB2	9:H:95:TYR:HA	1.99	0.45
4:A:897:TYR:CD2	4:A:936:LEU:HD13	2.52	0.45
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.98	0.45
5:B:211:VAL:O	5:B:480:SER:HA	2.17	0.45
5:B:276:ILE:HD13	5:B:277:LYS:HE3	1.98	0.45
6:C:124:LEU:CD2	6:C:129:ILE:HG22	2.46	0.45
4:A:343:LYS:HE2	5:B:1151:LEU:HG	1.98	0.45
4:A:450:LEU:O	4:A:450:LEU:CD1	2.64	0.45
4:A:474:VAL:O	4:A:478:TYR:HD1	1.99	0.45
5:B:527:THR:OG1	5:B:528:PRO:HD2	2.16	0.45
2:T:16:DC:H2'	2:T:17:DG:C8	2.50	0.45
4:A:108:MET:HE3	4:A:202:LEU:HD21	1.99	0.45
4:A:115:LEU:HD12	4:A:122:MET:CE	2.46	0.45
4:A:403:LYS:O	4:A:404:TYR:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:474:VAL:HG22	4:A:478:TYR:HE1	1.82	0.45
4:A:901:LEU:HD23	4:A:907:THR:HG22	1.98	0.45
5:B:226:PHE:HA	5:B:395:GLN:HG3	1.98	0.45
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.47	0.45
5:B:802:PRO:HB3	5:B:1091:TYR:CD1	2.51	0.45
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.52	0.45
6:C:152:GLU:HG2	6:C:153:LEU:N	2.32	0.45
7:E:127:ILE:N	7:E:128:PRO:HD3	2.32	0.45
4:A:50:ILE:O	4:A:56:PRO:HD3	2.16	0.44
4:A:571:LEU:HD22	9:H:46:LEU:HD11	1.98	0.44
4:A:1148:ILE:HD13	10:I:49:ILE:HD12	1.98	0.44
4:A:1172:LEU:HD23	4:A:1172:LEU:H	1.82	0.44
8:F:132:LEU:O	8:F:148:VAL:HG23	2.16	0.44
4:A:265:LYS:HE3	4:A:302:THR:HG23	1.99	0.44
4:A:299:HIS:CA	4:A:302:THR:HG22	2.47	0.44
5:B:102:VAL:CG2	5:B:112:LEU:HB2	2.42	0.44
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.53	0.44
12:K:84:LYS:O	12:K:88:LYS:HG3	2.16	0.44
4:A:115:LEU:HD13	4:A:119:ASN:ND2	2.31	0.44
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.98	0.44
5:B:393:LYS:HE3	5:B:393:LYS:HA	1.99	0.44
5:B:558:LEU:C	5:B:560:GLU:N	2.75	0.44
5:B:637:LEU:HD11	5:B:693:ILE:HG13	2.00	0.44
5:B:654:ARG:H	5:B:657:HIS:HD2	1.65	0.44
5:B:911:ILE:CD1	5:B:941:LEU:HA	2.47	0.44
8:F:71:GLU:HA	8:F:72:LYS:HA	1.84	0.44
12:K:46:ILE:HG22	12:K:50:LEU:HD12	1.99	0.44
4:A:86:LEU:CB	4:A:237:THR:O	2.66	0.44
4:A:353:ILE:HD13	4:A:487:MET:CE	2.47	0.44
4:A:1349:TYR:HA	4:A:1372:VAL:HG21	1.98	0.44
6:C:99:LEU:HD22	6:C:99:LEU:N	2.32	0.44
6:C:123:ASN:ND2	6:C:125:MET:HG3	2.32	0.44
10:I:68:LEU:HD13	10:I:84:VAL:HG11	1.98	0.44
4:A:332:LYS:C	4:A:333:GLU:HG2	2.41	0.44
4:A:605:MET:HE1	4:A:612:ILE:HD12	1.99	0.44
4:A:1115:SER:HB3	4:A:1330:ASN:ND2	2.32	0.44
5:B:287:ARG:C	5:B:289:LEU:N	2.75	0.44
5:B:416:LEU:HD11	5:B:460:ALA:CB	2.47	0.44
5:B:1096:ARG:O	5:B:1097:HIS:CB	2.66	0.44
7:E:213:ILE:HG12	7:E:214:CYS:H	1.82	0.44
11:J:53:HIS:HE1	11:J:55:ASP:OD1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:40:THR:HG22	4:A:54:ASN:HD21	1.82	0.44
4:A:224:PHE:O	4:A:225:ASN:C	2.61	0.44
4:A:404:TYR:HA	4:A:413:ILE:O	2.17	0.44
4:A:568:PRO:O	4:A:569:LYS:HB3	2.17	0.44
4:A:645:LEU:O	4:A:649:ILE:HG13	2.18	0.44
4:A:845:LEU:O	4:A:846:GLU:C	2.60	0.44
5:B:333:PHE:HD1	5:B:333:PHE:O	2.00	0.44
5:B:826:ALA:O	5:B:1011:ILE:HA	2.18	0.44
8:F:73:ALA:O	8:F:74:ILE:HG13	2.18	0.44
4:A:1059:HIS:CE1	8:F:87:LYS:H	2.36	0.44
4:A:1279:ILE:O	4:A:1279:ILE:HG22	2.18	0.44
5:B:167:ILE:O	5:B:167:ILE:CG2	2.52	0.44
6:C:33:LEU:HG	6:C:37:MET:HE3	1.99	0.44
6:C:240:VAL:O	6:C:241:ASP:C	2.61	0.44
12:K:113:THR:O	12:K:114:LEU:CB	2.65	0.44
4:A:43:GLU:HG3	4:A:50:ILE:HG12	1.99	0.44
4:A:55:ASP:N	4:A:56:PRO:HD2	2.33	0.44
5:B:383:ASN:HD21	5:B:387:LEU:HD22	1.81	0.44
5:B:557:PHE:CD2	5:B:557:PHE:C	2.96	0.44
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.49	0.44
5:B:1122:ARG:C	5:B:1124:ARG:H	2.26	0.44
4:A:313:GLN:HG3	4:A:314:ALA:H	1.82	0.44
4:A:830:LYS:HE2	4:A:1082:ASN:ND2	2.33	0.44
4:A:902:LEU:HG	4:A:926:GLN:HG3	2.00	0.44
4:A:943:LEU:O	4:A:944:ARG:C	2.61	0.44
5:B:515:HIS:H	5:B:518:HIS:HD2	1.56	0.44
5:B:950:ASP:HB3	5:B:967:ARG:HG2	1.99	0.44
4:A:132:LYS:HB3	4:A:132:LYS:HE2	1.85	0.43
4:A:670:ILE:HD12	5:B:1067:ARG:NH1	2.33	0.43
5:B:382:ILE:O	5:B:383:ASN:C	2.59	0.43
5:B:702:LEU:HD12	5:B:702:LEU:HA	1.81	0.43
5:B:879:ARG:HB3	5:B:880:THR:H	1.55	0.43
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.33	0.43
13:L:42:ARG:HD2	13:L:42:ARG:N	2.33	0.43
3:N:12:DT:H2"	3:N:13:DA:OP2	2.18	0.43
4:A:230:ARG:HG3	4:A:233:TRP:CZ3	2.52	0.43
4:A:567:LYS:CB	9:H:95:TYR:HA	2.48	0.43
4:A:771:GLU:N	4:A:822:GLU:OE1	2.39	0.43
4:A:984:LYS:O	4:A:988:LEU:HB3	2.18	0.43
5:B:65:GLU:HB3	5:B:66:ASP:H	1.54	0.43
5:B:645:SER:O	5:B:647:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:770:GLN:CD	5:B:983:ARG:HA	2.43	0.43
5:B:1017:ILE:H	5:B:1018:PRO:CD	2.31	0.43
6:C:69:LEU:HB3	11:J:6:ARG:HD2	2.00	0.43
6:C:82:TYR:CE2	6:C:161:LYS:HD3	2.53	0.43
9:H:2:SER:N	9:H:3:ASN:HB2	2.33	0.43
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.99	0.43
9:H:93:TYR:HD2	9:H:145:ARG:HB3	1.82	0.43
12:K:107:THR:O	12:K:111:LEU:HG	2.19	0.43
4:A:315:LEU:HB3	4:A:316:GLN:H	1.55	0.43
4:A:1091:SER:C	4:A:1093:LYS:H	2.26	0.43
5:B:431:TYR:CE2	5:B:447:ALA:HB3	2.53	0.43
5:B:760:ASP:OD1	5:B:760:ASP:N	2.48	0.43
5:B:1084:GLN:HG2	6:C:201:TRP:CH2	2.53	0.43
5:B:1099:VAL:O	5:B:1103:ILE:CD1	2.66	0.43
4:A:99:ILE:HD13	4:A:234:MET:HE3	1.99	0.43
5:B:762:ASN:OD1	5:B:984:HIS:HD2	2.01	0.43
5:B:785:TYR:CD1	5:B:786:ASN:N	2.87	0.43
11:J:38:ARG:HE	11:J:38:ARG:HB2	1.69	0.43
4:A:215:SER:HB3	4:A:218:ASP:CG	2.43	0.43
4:A:341:MET:HB3	5:B:1132:GLU:HB3	2.00	0.43
4:A:904:THR:HG23	4:A:905:ASP:OD1	2.18	0.43
4:A:1043:ASP:N	4:A:1043:ASP:OD1	2.51	0.43
5:B:839:MET:CE	5:B:1010:LEU:HD21	2.48	0.43
5:B:955:THR:HG23	13:L:54:ARG:O	2.18	0.43
5:B:1096:ARG:O	5:B:1097:HIS:HB2	2.19	0.43
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.00	0.43
7:E:179:GLN:C	7:E:181:ALA:N	2.73	0.43
8:F:71:GLU:HA	8:F:72:LYS:O	2.19	0.43
10:I:94:ASP:OD2	10:I:94:ASP:N	2.51	0.43
4:A:269:ILE:C	4:A:269:ILE:HD12	2.43	0.43
4:A:272:ALA:HA	4:A:275:SER:HB3	2.00	0.43
4:A:477:PRO:HG3	4:A:521:MET:HE3	1.99	0.43
4:A:666:ILE:HD11	5:B:1027:ILE:HG12	2.00	0.43
4:A:1293:SER:HB2	4:A:1299:VAL:CG2	2.48	0.43
5:B:798:TYR:N	5:B:799:PRO:HD3	2.33	0.43
5:B:806:THR:HG23	5:B:1045:SER:HA	2.00	0.43
5:B:911:ILE:HD11	5:B:941:LEU:CB	2.49	0.43
5:B:1016:ALA:HB1	5:B:1020:ARG:HH12	1.83	0.43
5:B:1106:ARG:NH2	5:B:1109:GLY:H	2.17	0.43
7:E:32:GLN:O	7:E:32:GLN:HG3	2.18	0.43
9:H:10:PHE:HA	9:H:30:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:224:PHE:HD2	4:A:229:SER:O	2.01	0.43
6:C:37:MET:HE3	6:C:37:MET:HB2	1.73	0.43
8:F:85:MET:O	8:F:155:LEU:HD21	2.19	0.43
4:A:673:GLY:N	4:A:674:PRO:CD	2.81	0.43
4:A:845:LEU:O	4:A:848:ILE:HG12	2.19	0.43
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.33	0.43
4:A:1171:GLN:O	4:A:1174:PHE:CD2	2.71	0.43
5:B:785:TYR:C	5:B:787:VAL:H	2.27	0.43
5:B:991:GLY:O	5:B:992:ILE:HB	2.17	0.43
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.54	0.43
12:K:37:LYS:HA	12:K:69:ALA:HB1	2.01	0.43
12:K:39:ASP:HB2	12:K:40:HIS:H	1.65	0.43
2:T:17:DG:N3	2:T:17:DG:H2'	2.34	0.43
4:A:1025:ARG:O	4:A:1035:TYR:OH	2.35	0.43
5:B:1032:SER:HB3	5:B:1089:PRO:HG2	2.00	0.43
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.48	0.43
12:K:10:PHE:CE1	12:K:11:LEU:HD13	2.54	0.43
4:A:22:PHE:HB2	5:B:1211:ASN:CG	2.42	0.43
5:B:916:THR:HA	5:B:917:PRO:HD2	1.90	0.43
9:H:17:PRO:O	9:H:19:ARG:N	2.51	0.43
9:H:95:TYR:HE2	9:H:97:MET:HE2	1.84	0.43
4:A:7:SER:OG	5:B:1161:HIS:HE1	2.01	0.42
4:A:43:GLU:HG2	4:A:50:ILE:HG23	2.01	0.42
4:A:398:GLU:O	4:A:399:HIS:O	2.36	0.42
4:A:599:SER:C	4:A:601:LYS:H	2.27	0.42
5:B:493:SER:HA	5:B:751:VAL:HG11	2.01	0.42
8:F:76:LYS:HA	8:F:79:ARG:HD3	2.01	0.42
4:A:516:SER:HB2	4:A:518:LYS:HG2	2.01	0.42
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.53	0.42
4:A:784:LEU:HB3	4:A:786:HIS:HD2	1.85	0.42
4:A:1400:CYS:O	4:A:1405:THR:HG23	2.18	0.42
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	2.01	0.42
5:B:813:LYS:HA	5:B:816:GLU:OE1	2.18	0.42
4:A:35:ILE:HA	4:A:52:GLY:O	2.19	0.42
5:B:398:ARG:NH1	5:B:398:ARG:CB	2.72	0.42
5:B:558:LEU:O	5:B:560:GLU:N	2.53	0.42
5:B:758:PHE:HB3	5:B:761:HIS:CD2	2.54	0.42
5:B:883:LEU:N	5:B:883:LEU:HD23	2.34	0.42
5:B:956:THR:HA	5:B:961:LEU:O	2.19	0.42
6:C:8:VAL:HG11	12:K:105:PHE:HD1	1.85	0.42
7:E:113:GLN:HA	7:E:137:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:709:THR:HG22	4:A:711:ARG:H	1.85	0.42
5:B:778:MET:O	5:B:819:ALA:HB1	2.19	0.42
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.49	0.42
6:C:201:TRP:HA	6:C:202:PRO:HD3	1.79	0.42
2:T:22:DT:H2'	2:T:23:DC:C6	2.54	0.42
4:A:206:GLU:O	4:A:210:ILE:HG12	2.19	0.42
4:A:384:ASN:O	4:A:387:ARG:N	2.52	0.42
4:A:424:ILE:O	4:A:424:ILE:HG22	2.20	0.42
4:A:828:ALA:HB1	5:B:530:GLY:HA2	2.02	0.42
4:A:1064:VAL:O	4:A:1064:VAL:HG12	2.19	0.42
4:A:1301:GLU:HA	4:A:1302:PRO:HD3	1.89	0.42
4:A:1403:GLU:O	4:A:1404:GLU:C	2.61	0.42
5:B:174:LEU:O	5:B:175:ARG:HB3	2.18	0.42
5:B:870:ILE:O	5:B:870:ILE:HG22	2.19	0.42
6:C:22:LEU:HD23	6:C:22:LEU:O	2.19	0.42
6:C:70:ILE:CD1	6:C:144:ILE:HD11	2.49	0.42
8:F:72:LYS:O	8:F:73:ALA:HB3	2.20	0.42
13:L:58:LYS:O	13:L:58:LYS:HG2	2.20	0.42
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.84	0.42
4:A:1116:LEU:HD22	4:A:1329:THR:OG1	2.20	0.42
5:B:36:ALA:HB2	5:B:661:LEU:HD22	2.02	0.42
5:B:116:GLU:HG2	5:B:120:ARG:HD3	2.00	0.42
5:B:471:LYS:O	5:B:476:ARG:HD3	2.18	0.42
5:B:1111:MET:HE2	5:B:1118:PRO:CD	2.50	0.42
6:C:244:VAL:HG21	12:K:105:PHE:CE1	2.54	0.42
9:H:129:TYR:C	9:H:131:ASN:N	2.78	0.42
4:A:265:LYS:CG	4:A:303:TYR:HB2	2.40	0.42
4:A:351:THR:CG2	4:A:352:VAL:N	2.82	0.42
4:A:535:THR:HG21	4:A:617:VAL:N	2.32	0.42
4:A:1187:GLN:HG3	4:A:1188:GLN:H	1.84	0.42
4:A:1206:ASP:N	4:A:1274:ARG:HH12	2.18	0.42
5:B:458:LYS:O	5:B:462:ALA:N	2.52	0.42
4:A:68:GLN:C	4:A:70:CYS:N	2.75	0.42
4:A:909:ASP:HA	4:A:910:PRO:HD2	1.84	0.42
4:A:1373:ASP:HA	4:A:1376:THR:HG22	2.02	0.42
5:B:848:ARG:HD2	11:J:8:PHE:O	2.20	0.42
5:B:1065:GLN:HE21	5:B:1065:GLN:HB2	1.63	0.42
10:I:111:THR:HG23	10:I:113:ASP:H	1.85	0.42
11:J:48:ARG:HH11	11:J:48:ARG:CG	2.29	0.42
2:T:22:DT:H2'	2:T:23:DC:H6	1.85	0.42
4:A:886:ILE:HG22	4:A:887:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1084:PHE:HZ	4:A:1093:LYS:HA	1.79	0.42
5:B:787:VAL:O	5:B:787:VAL:HG12	2.19	0.42
6:C:73:GLN:NE2	6:C:74:SER:H	2.15	0.42
6:C:99:LEU:N	6:C:99:LEU:CD2	2.83	0.42
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.01	0.42
4:A:132:LYS:NZ	4:A:133:LYS:HE3	2.35	0.42
4:A:598:LEU:O	4:A:599:SER:C	2.63	0.42
4:A:1174:PHE:CD1	4:A:1175:SER:HB2	2.55	0.42
4:A:1385:THR:C	4:A:1387:HIS:N	2.78	0.42
5:B:333:PHE:C	5:B:333:PHE:CD1	2.98	0.42
5:B:595:ARG:O	5:B:596:LEU:C	2.63	0.42
5:B:878:GLN:O	5:B:879:ARG:C	2.63	0.42
8:F:97:ARG:HD3	8:F:130:ILE:HG23	2.01	0.42
4:A:276:LEU:HD11	4:A:292:ALA:O	2.20	0.41
4:A:470:LEU:HD21	4:A:487:MET:HE3	2.01	0.41
5:B:622:LYS:HE2	10:I:59:VAL:HG11	2.02	0.41
5:B:654:ARG:H	5:B:657:HIS:CD2	2.38	0.41
5:B:744:HIS:CD2	5:B:746:SER:OG	2.73	0.41
5:B:769:TYR:CD2	5:B:769:TYR:N	2.87	0.41
5:B:911:ILE:HD11	5:B:941:LEU:CD1	2.48	0.41
5:B:1098:MET:HE3	5:B:1098:MET:HB2	1.82	0.41
6:C:242:GLN:HB3	6:C:246:ARG:NE	2.32	0.41
14:T:29[B]:DUT:H6	14:T:29[B]:DUT:C3'	2.49	0.41
4:A:92:HIS:CD2	4:A:92:HIS:C	2.97	0.41
4:A:323:LYS:HZ3	4:A:324:SER:N	2.18	0.41
4:A:894:GLU:C	4:A:896:ARG:N	2.78	0.41
4:A:1017:LEU:HB2	7:E:206:GLY:N	2.35	0.41
5:B:273:LEU:HD11	5:B:285:ILE:HD12	2.02	0.41
5:B:796:LEU:HD12	5:B:796:LEU:HA	1.67	0.41
5:B:910:VAL:HG13	5:B:938:SER:HB3	2.02	0.41
5:B:972:LYS:HZ2	5:B:1098:MET:HE1	1.86	0.41
4:A:148:CYS:HB3	4:A:167:CYS:O	2.20	0.41
4:A:512:VAL:HA	4:A:519:PRO:HA	2.01	0.41
5:B:1053:GLU:O	5:B:1057:LYS:HE3	2.19	0.41
5:B:1058:LEU:HA	5:B:1061:GLU:OE2	2.19	0.41
7:E:29:PHE:C	7:E:30:ILE:HD12	2.44	0.41
7:E:122:LYS:HE3	7:E:122:LYS:HA	2.02	0.41
9:H:44:VAL:HG13	9:H:48:PRO:HA	2.02	0.41
4:A:92:HIS:O	4:A:94:GLY:N	2.53	0.41
4:A:399:HIS:HB3	4:A:400:PRO:HD2	1.85	0.41
4:A:579:SER:OG	4:A:612:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:676:MET:SD	4:A:679:ILE:HD12	2.61	0.41
4:A:761:MET:CG	5:B:1021:MET:HG2	2.46	0.41
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.17	0.41
4:A:1086:PHE:H	4:A:1086:PHE:HD1	1.69	0.41
5:B:176:SER:O	5:B:182:SER:CB	2.62	0.41
5:B:273:LEU:O	5:B:276:ILE:HG22	2.20	0.41
5:B:712:PRO:HD2	5:B:733:HIS:CE1	2.55	0.41
6:C:106:GLU:OE2	6:C:106:GLU:HA	2.19	0.41
13:L:48:CYS:HB3	13:L:51:CYS:H	1.85	0.41
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.21	0.41
4:A:406:ILE:HD11	4:A:433:GLU:OE2	2.21	0.41
4:A:702:LEU:HD22	4:A:702:LEU:HA	1.85	0.41
4:A:1407:GLU:OE1	4:A:1407:GLU:N	2.47	0.41
5:B:274:PRO:C	5:B:276:ILE:H	2.28	0.41
5:B:795:ILE:HD12	5:B:795:ILE:N	2.36	0.41
4:A:33:ALA:O	4:A:83:HIS:CD2	2.73	0.41
4:A:71:GLN:HB2	4:A:72:GLU:H	1.69	0.41
4:A:298:PHE:CD2	4:A:298:PHE:O	2.71	0.41
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.55	0.41
5:B:542:MET:HE3	5:B:542:MET:HB3	1.84	0.41
5:B:886:LYS:CB	5:B:887:HIS:CA	2.96	0.41
5:B:1007:VAL:HG13	5:B:1008:PRO:CD	2.49	0.41
2:T:25:DC:H5"	5:B:482:VAL:HG11	2.02	0.41
4:A:65:LEU:O	4:A:65:LEU:HG	2.21	0.41
4:A:284:ALA:HA	4:A:285:PRO:HD3	1.89	0.41
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.51	0.41
4:A:855:THR:HG21	4:A:857:ARG:NE	2.21	0.41
4:A:1013:ASP:C	4:A:1015:VAL:H	2.29	0.41
5:B:360:PHE:HE2	5:B:374:LYS:HB3	1.84	0.41
5:B:815:ARG:HE	5:B:815:ARG:HB3	1.71	0.41
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.56	0.41
4:A:92:HIS:O	4:A:93:VAL:C	2.63	0.41
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	2.20	0.41
5:B:135:ARG:HH11	5:B:137:TYR:HA	1.85	0.41
5:B:386:LEU:C	5:B:388:CYS:N	2.78	0.41
5:B:784:ASN:HB3	11:J:63:TYR:CZ	2.55	0.41
5:B:984:HIS:CD2	5:B:1024:ALA:CB	3.03	0.41
6:C:41:ILE:HD13	6:C:41:ILE:HG21	1.78	0.41
7:E:198:ILE:CD1	7:E:212:ARG:HG3	2.50	0.41
4:A:58:LEU:O	4:A:58:LEU:CG	2.68	0.41
4:A:71:GLN:C	4:A:73:GLY:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LYS:O	4:A:267:ALA:N	2.52	0.41
4:A:409:SER:O	4:A:411:ASP:N	2.54	0.41
4:A:899:VAL:HB	4:A:929:LEU:HD13	2.02	0.41
4:A:901:LEU:HB2	4:A:926:GLN:CG	2.51	0.41
4:A:1293:SER:HB2	4:A:1299:VAL:HG21	2.02	0.41
5:B:487:THR:CG2	5:B:488:TYR:N	2.83	0.41
5:B:640:VAL:HG22	5:B:651:LEU:HD23	2.03	0.41
5:B:1002:THR:CG2	5:B:1006:ILE:H	2.33	0.41
6:C:134:ILE:HD12	6:C:141:GLY:H	1.85	0.41
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.51	0.41
10:I:77:LYS:O	10:I:79:HIS:N	2.54	0.41
4:A:567:LYS:HG3	4:A:568:PRO:CG	2.51	0.41
4:A:830:LYS:HE2	4:A:1082:ASN:HD22	1.85	0.41
4:A:974:ASP:OD1	4:A:974:ASP:C	2.64	0.41
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.60	0.41
4:A:1385:THR:C	4:A:1387:HIS:H	2.29	0.41
5:B:744:HIS:HA	5:B:745:PRO:HD3	1.85	0.41
5:B:841:MET:HE3	5:B:990:ILE:HD11	2.03	0.41
5:B:885:MET:HB3	5:B:886:LYS:H	1.68	0.41
5:B:1006:ILE:HG22	5:B:1007:VAL:H	1.83	0.41
6:C:177:GLU:HG3	6:C:231:ASN:HB3	2.03	0.41
6:C:229:TYR:CD1	6:C:229:TYR:N	2.89	0.41
10:I:55:THR:HG23	10:I:58:VAL:CG2	2.50	0.41
4:A:894:GLU:C	4:A:896:ARG:H	2.29	0.40
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	2.03	0.40
4:A:1345:ARG:HG2	4:A:1372:VAL:CG1	2.51	0.40
5:B:136:THR:O	5:B:137:TYR:O	2.39	0.40
6:C:74:SER:O	6:C:77:ILE:HB	2.22	0.40
8:F:128:LYS:HD3	8:F:149:GLU:O	2.21	0.40
9:H:146:ARG:HA	9:H:146:ARG:HD3	1.97	0.40
10:I:96:SER:OG	10:I:98:VAL:HG23	2.21	0.40
2:T:24:DT:OP1	5:B:792:MET:HE1	2.22	0.40
4:A:265:LYS:HD3	4:A:322:VAL:HG21	2.03	0.40
4:A:1402:PHE:CD2	4:A:1403:GLU:HB2	2.56	0.40
5:B:724:ASP:OD1	5:B:725:PRO:HD2	2.20	0.40
5:B:1153:GLU:OE2	5:B:1153:GLU:N	2.50	0.40
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.36	0.40
12:K:87:LEU:O	12:K:90:ALA:HB3	2.21	0.40
4:A:1138:ILE:H	4:A:1138:ILE:HG13	1.77	0.40
4:A:1215:ARG:NE	4:A:1218:GLN:HE21	2.19	0.40
5:B:850:LEU:CD2	5:B:1009:ASP:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:996:ARG:HH22	6:C:173:ALA:HB3	1.85	0.40
5:B:1106:ARG:CG	5:B:1107:ALA:N	2.85	0.40
6:C:63:ILE:HA	6:C:66:ARG:HG3	2.02	0.40
7:E:161:LYS:C	7:E:163:GLU:N	2.77	0.40
8:F:147:SER:O	8:F:151:LEU:HD12	2.22	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.87	0.40
2:T:6:DG:N2	3:N:10:DG:N2	2.70	0.40
2:T:7:DA:OP2	2:T:7:DA:H2'	2.21	0.40
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.62	0.40
4:A:303:TYR:HD2	4:A:304:MET:HG3	1.86	0.40
4:A:343:LYS:NZ	5:B:1156:ASP:HB2	2.37	0.40
4:A:545:GLN:O	4:A:549:MET:HG3	2.21	0.40
4:A:779:PHE:CZ	5:B:517:THR:HA	2.56	0.40
5:B:705:MET:CE	5:B:742:GLU:HG2	2.52	0.40
5:B:706:GLN:O	5:B:707:PRO:C	2.64	0.40
5:B:711:GLU:H	5:B:712:PRO:HD3	1.87	0.40
5:B:762:ASN:HD22	5:B:762:ASN:HA	1.64	0.40
5:B:792:MET:HE2	5:B:857:ARG:HG3	2.03	0.40
5:B:1034:VAL:O	5:B:1035:ALA:C	2.64	0.40
5:B:1046:PRO:HB2	5:B:1047:PHE:H	1.80	0.40
6:C:62:PHE:C	6:C:62:PHE:CD2	3.00	0.40
10:I:56:ALA:HB3	10:I:89:GLN:HG3	2.02	0.40
10:I:59:VAL:O	10:I:61:ASP:N	2.54	0.40
4:A:247:ARG:HD3	4:A:262:LEU:HD23	2.03	0.40
4:A:323:LYS:HZ2	4:A:323:LYS:N	2.19	0.40
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.98	0.40
5:B:121:ASN:HA	5:B:207:GLY:HA3	2.04	0.40
5:B:216:GLU:HB3	5:B:500:THR:HG23	2.02	0.40
5:B:278:GLN:CG	5:B:279:ASP:N	2.84	0.40
5:B:796:LEU:HB3	5:B:799:PRO:HG3	2.04	0.40
9:H:60:ALA:O	9:H:61:SER:CB	2.69	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 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	1395/1733 (80%)	1153 (83%)	158 (11%)	84 (6%)	1	4
5	B	1096/1224 (90%)	938 (86%)	108 (10%)	50 (5%)	2	7
6	C	264/318 (83%)	229 (87%)	27 (10%)	8 (3%)	3	14
7	E	212/215 (99%)	177 (84%)	28 (13%)	7 (3%)	3	13
8	F	83/155 (54%)	71 (86%)	11 (13%)	1 (1%)	10	34
9	H	129/146 (88%)	94 (73%)	22 (17%)	13 (10%)	0	1
10	I	117/122 (96%)	94 (80%)	14 (12%)	9 (8%)	1	2
11	J	63/70 (90%)	58 (92%)	2 (3%)	3 (5%)	2	7
12	K	112/120 (93%)	104 (93%)	8 (7%)	0	100	100
13	L	44/70 (63%)	28 (64%)	10 (23%)	6 (14%)	0	0
All	All	3515/4173 (84%)	2946 (84%)	388 (11%)	181 (5%)	1	6

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	55	ASP
4	A	56	PRO
4	A	65	LEU
4	A	69	THR
4	A	93	VAL
4	A	118	HIS
4	A	121	LEU
4	A	130	ASP
4	A	131	SER
4	A	168	GLY
4	A	250	ILE
4	A	254	GLU
4	A	300	VAL
4	A	315	LEU
4	A	323	LYS
4	A	324	SER
4	A	399	HIS
4	A	451	HIS
4	A	567	LYS
4	A	593	GLU
4	A	597	LEU

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Mol	Chain	Res	Type
4	A	609	ASP
4	A	610	GLY
4	A	672	ASP
4	A	846	GLU
4	A	923	LEU
4	A	944	ARG
4	A	1123	GLY
4	A	1166	ASP
4	A	1221	LYS
5	B	65	GLU
5	B	67	SER
5	B	137	TYR
5	B	469	GLN
5	B	477	ALA
5	B	484	ASN
5	B	531	GLN
5	B	648	HIS
5	B	711	GLU
5	B	713	ALA
5	B	731	VAL
5	B	879	ARG
5	B	1046	PRO
5	B	1156	ASP
7	E	50	MET
7	E	172	GLU
9	H	3	ASN
9	H	61	SER
9	H	62	SER
9	H	108	SER
9	H	109	LYS
9	H	131	ASN
9	H	132	LEU
10	I	33	SER
10	I	47	GLU
10	I	60	GLN
10	I	79	HIS
10	I	104	LEU
13	L	64	LEU
4	A	68	GLN
4	A	76	GLU
4	A	79	GLY
4	A	117	GLU

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Mol	Chain	Res	Type
4	A	119	ASN
4	A	214	ILE
4	A	215	SER
4	A	266	LEU
4	A	283	GLY
4	A	297	GLN
4	A	307	ASP
4	A	312	PRO
4	A	404	TYR
4	A	408	ASP
4	A	410	GLY
4	A	424	ILE
4	A	568	PRO
4	A	569	LYS
4	A	853	ASP
4	A	943	LEU
4	A	1278	ASN
4	A	1437	GLY
5	B	288	ALA
5	B	471	LYS
5	B	473	MET
5	B	864	LYS
5	B	870	ILE
5	B	888	GLY
5	B	987	LYS
7	E	206	GLY
9	H	18	GLY
9	H	54	SER
9	H	90	ALA
10	I	3	THR
11	J	2	ILE
11	J	6	ARG
13	L	45	ALA
4	A	40	THR
4	A	48	ALA
4	A	72	GLU
4	A	149	GLU
4	A	248	PRO
4	A	308	ILE
4	A	310	GLY
4	A	958	VAL
4	A	1083	THR

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Mol	Chain	Res	Type
4	A	1093	LYS
5	B	37	PHE
5	B	104	GLU
5	B	290	GLY
5	B	364	ILE
5	B	371	GLU
5	B	476	ARG
5	B	559	SER
5	B	644	GLU
5	B	647	GLY
5	B	712	PRO
5	B	992	ILE
5	B	1223	ASP
6	C	227	THR
7	E	51	GLY
8	F	154	ASP
9	H	130	ARG
9	H	136	LYS
4	A	71	GLN
4	A	109	HIS
4	A	126	LEU
4	A	249	SER
4	A	332	LYS
4	A	400	PRO
4	A	418	SER
4	A	979	SER
4	A	1014	ALA
4	A	1084	PHE
5	B	139	ALA
5	B	248	SER
5	B	467	GLY
5	B	646	LEU
5	B	734	HIS
5	B	1190	ASP
6	C	90	ASP
6	C	214	ASN
10	I	78	CYS
13	L	56	LEU
4	A	325	ILE
4	A	801	GLU
4	A	1081	LEU
5	B	346	GLU

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Mol	Chain	Res	Type
5	B	480	SER
5	B	1017	ILE
5	B	1108	ARG
5	B	1157	ALA
6	C	130	GLY
6	C	142	VAL
6	C	240	VAL
7	E	124	VAL
9	H	140	ALA
13	L	42	ARG
13	L	46	VAL
13	L	55	ILE
4	A	225	ASN
4	A	1127	ASP
5	B	483	LEU
5	B	901	PRO
6	C	6	PRO
6	C	132	PRO
7	E	3	GLN
7	E	86	PRO
10	I	20	LYS
10	I	34	TYR
11	J	15	GLY
4	A	96	ILE
4	A	245	PRO
5	B	1042	GLY
4	A	89	PRO
4	A	99	ILE
5	B	292	ILE
5	B	482	VAL
4	A	916	GLY
4	A	1388	GLY
5	B	824	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 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	1225/1520 (81%)	1026 (84%)	199 (16%)	2	8
5	B	967/1061 (91%)	829 (86%)	138 (14%)	3	11
6	C	234/274 (85%)	205 (88%)	29 (12%)	4	15
7	E	196/197 (100%)	167 (85%)	29 (15%)	3	10
8	F	75/137 (55%)	69 (92%)	6 (8%)	11	34
9	H	117/128 (91%)	91 (78%)	26 (22%)	1	3
10	I	113/116 (97%)	96 (85%)	17 (15%)	3	10
11	J	60/65 (92%)	49 (82%)	11 (18%)	2	6
12	K	99/102 (97%)	88 (89%)	11 (11%)	6	20
13	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
All	All	3126/3657 (86%)	2648 (85%)	478 (15%)	3	9

All (478) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	21	LEU
4	A	30	ILE
4	A	34	LYS
4	A	41	MET
4	A	43	GLU
4	A	47	ARG
4	A	50	ILE
4	A	54	ASN
4	A	57	ARG
4	A	58	LEU
4	A	64	ASN
4	A	65	LEU
4	A	68	GLN
4	A	69	THR
4	A	70	CYS
4	A	71	GLN
4	A	86	LEU
4	A	93	VAL
4	A	118	HIS
4	A	121	LEU
4	A	130	ASP
4	A	132	LYS
4	A	143	LYS

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Mol	Chain	Res	Type
4	A	147	VAL
4	A	163	SER
4	A	171	GLN
4	A	179	LEU
4	A	186	LYS
4	A	206	GLU
4	A	208	LEU
4	A	209	ASN
4	A	225	ASN
4	A	227	VAL
4	A	235	ILE
4	A	237	THR
4	A	250	ILE
4	A	252	PHE
4	A	253	ASN
4	A	256	GLN
4	A	271	LYS
4	A	274	ILE
4	A	289	ILE
4	A	298	PHE
4	A	303	TYR
4	A	313	GLN
4	A	315	LEU
4	A	316	GLN
4	A	323	LYS
4	A	325	ILE
4	A	330	LYS
4	A	333	GLU
4	A	335	ARG
4	A	337	ARG
4	A	351	THR
4	A	353	ILE
4	A	359	LEU
4	A	370	ILE
4	A	379	VAL
4	A	392	VAL
4	A	403	LYS
4	A	424	ILE
4	A	427	GLN
4	A	433	GLU
4	A	436	ILE
4	A	440	ASP

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Mol	Chain	Res	Type
4	A	443	LEU
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	455	MET
4	A	463	ILE
4	A	466	SER
4	A	469	ARG
4	A	470	LEU
4	A	472	LEU
4	A	475	THR
4	A	481	ASP
4	A	496	GLU
4	A	501	LEU
4	A	509	LEU
4	A	533	LYS
4	A	535	THR
4	A	541	ILE
4	A	560	ILE
4	A	566	ILE
4	A	571	LEU
4	A	590	ARG
4	A	595	THR
4	A	598	LEU
4	A	612	ILE
4	A	618	GLU
4	A	629	LEU
4	A	635	ARG
4	A	658	LEU
4	A	670	ILE
4	A	672	ASP
4	A	678	GLU
4	A	682	THR
4	A	688	LYS
4	A	691	LEU
4	A	695	LYS
4	A	702	LEU
4	A	703	THR
4	A	710	LEU
4	A	722	LEU
4	A	768	GLN
4	A	771	GLU

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Mol	Chain	Res	Type
4	A	801	GLU
4	A	821	ARG
4	A	830	LYS
4	A	833	GLU
4	A	855	THR
4	A	865	GLN
4	A	867	ILE
4	A	878	ILE
4	A	879	GLU
4	A	886	ILE
4	A	896	ARG
4	A	902	LEU
4	A	907	THR
4	A	908	LEU
4	A	920	LEU
4	A	932	GLU
4	A	934	LYS
4	A	938	LYS
4	A	960	ILE
4	A	961	ARG
4	A	969	GLN
4	A	973	ILE
4	A	974	ASP
4	A	976	THR
4	A	977	LYS
4	A	982	THR
4	A	992	ASP
4	A	994	GLN
4	A	999	VAL
4	A	1001	ARG
4	A	1005	GLU
4	A	1029	ARG
4	A	1034	GLU
4	A	1037	LEU
4	A	1058	VAL
4	A	1077	THR
4	A	1082	ASN
4	A	1084	PHE
4	A	1085	HIS
4	A	1086	PHE
4	A	1094	VAL
4	A	1095	THR

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Mol	Chain	Res	Type
4	A	1109	LYS
4	A	1110	ASN
4	A	1112	LYS
4	A	1130	GLN
4	A	1138	ILE
4	A	1142	THR
4	A	1146	VAL
4	A	1162	VAL
4	A	1171	GLN
4	A	1172	LEU
4	A	1173	HIS
4	A	1174	PHE
4	A	1176	LEU
4	A	1215	ARG
4	A	1221	LYS
4	A	1234	GLU
4	A	1237	ILE
4	A	1243	VAL
4	A	1256	GLU
4	A	1261	LYS
4	A	1264	GLU
4	A	1269	GLU
4	A	1270	ASN
4	A	1280	GLU
4	A	1283	VAL
4	A	1291	VAL
4	A	1293	SER
4	A	1297	GLU
4	A	1299	VAL
4	A	1307	GLU
4	A	1308	THR
4	A	1322	ILE
4	A	1325	THR
4	A	1329	THR
4	A	1333	ILE
4	A	1354	ASN
4	A	1372	VAL
4	A	1376	THR
4	A	1382	THR
4	A	1391	ARG
4	A	1393	ASN
4	A	1394	THR

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Mol	Chain	Res	Type
4	A	1398	MET
4	A	1403	GLU
4	A	1422	ARG
4	A	1425	SER
4	A	1426	GLU
4	A	1436	ILE
4	A	1438	THR
5	B	62	ILE
5	B	63	ILE
5	B	65	GLU
5	B	68	THR
5	B	70	ILE
5	B	94	LYS
5	B	133	LYS
5	B	137	TYR
5	B	164	LYS
5	B	183	GLU
5	B	194	GLU
5	B	217	ARG
5	B	234	ILE
5	B	244	LEU
5	B	245	GLU
5	B	246	LYS
5	B	267	ARG
5	B	268	THR
5	B	273	LEU
5	B	276	ILE
5	B	277	LYS
5	B	299	GLU
5	B	323	VAL
5	B	324	ILE
5	B	346	GLU
5	B	361	LEU
5	B	366	GLN
5	B	391	ASP
5	B	393	LYS
5	B	396	ASP
5	B	398	ARG
5	B	404	LYS
5	B	408	LEU
5	B	416	LEU
5	B	425	THR

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Mol	Chain	Res	Type
5	B	426	LYS
5	B	432	MET
5	B	437	GLU
5	B	453	ILE
5	B	468	GLU
5	B	469	GLN
5	B	471	LYS
5	B	475	SER
5	B	479	VAL
5	B	482	VAL
5	B	485	ARG
5	B	495	LEU
5	B	498	THR
5	B	537	LYS
5	B	541	LEU
5	B	542	MET
5	B	547	VAL
5	B	554	ILE
5	B	555	ILE
5	B	567	GLU
5	B	574	SER
5	B	579	ARG
5	B	619	ILE
5	B	623	GLU
5	B	624	LEU
5	B	628	THR
5	B	637	LEU
5	B	642	ASP
5	B	646	LEU
5	B	650	GLU
5	B	655	LYS
5	B	658	ILE
5	B	666	TYR
5	B	690	VAL
5	B	708	GLU
5	B	710	LEU
5	B	731	VAL
5	B	734	HIS
5	B	739	THR
5	B	742	GLU
5	B	751	VAL
5	B	763	GLN

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Mol	Chain	Res	Type
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	807	ARG
5	B	825	VAL
5	B	827	ILE
5	B	831	SER
5	B	841	MET
5	B	864	LYS
5	B	866	TYR
5	B	869	SER
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	882	THR
5	B	886	LYS
5	B	899	ILE
5	B	916	THR
5	B	933	SER
5	B	944	THR
5	B	959	ASP
5	B	963	PHE
5	B	964	VAL
5	B	967	ARG
5	B	969	ARG
5	B	983	ARG
5	B	987	LYS
5	B	996	ARG
5	B	997	GLU
5	B	999	MET
5	B	1007	VAL
5	B	1010	LEU
5	B	1022	THR
5	B	1028	GLU
5	B	1041	GLU
5	B	1050	ILE
5	B	1057	LYS
5	B	1065	GLN
5	B	1085	ILE
5	B	1092	TYR
5	B	1094	ARG
5	B	1096	ARG

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Mol	Chain	Res	Type
5	B	1099	VAL
5	B	1101	ASP
5	B	1103	ILE
5	B	1111	MET
5	B	1138	MET
5	B	1147	LEU
5	B	1148	LYS
5	B	1160	VAL
5	B	1166	CYS
5	B	1176	ASN
5	B	1178	ASN
5	B	1181	GLU
5	B	1182	CYS
5	B	1186	ASP
5	B	1190	ASP
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1222	ARG
6	C	18	VAL
6	C	25	VAL
6	C	27	LEU
6	C	32	SER
6	C	36	VAL
6	C	57	VAL
6	C	75	MET
6	C	77	ILE
6	C	89	GLU
6	C	93	ASP
6	C	99	LEU
6	C	106	GLU
6	C	120	ILE
6	C	121	VAL
6	C	129	ILE
6	C	137	LYS
6	C	140	ASN
6	C	143	LEU
6	C	145	CYS
6	C	156	THR
6	C	196	ASP
6	C	210	GLU
6	C	214	ASN

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Mol	Chain	Res	Type
6	C	215	GLU
6	C	231	ASN
6	C	235	VAL
6	C	240	VAL
6	C	244	VAL
6	C	254	LYS
7	E	30	ILE
7	E	31	THR
7	E	37	LEU
7	E	43	LYS
7	E	46	TYR
7	E	52	ARG
7	E	61	GLN
7	E	65	THR
7	E	66	GLU
7	E	67	GLU
7	E	87	SER
7	E	92	THR
7	E	95	THR
7	E	107	THR
7	E	109	ILE
7	E	122	LYS
7	E	127	ILE
7	E	132	ILE
7	E	150	VAL
7	E	152	LYS
7	E	162	ARG
7	E	165	LEU
7	E	169	ARG
7	E	171	LYS
7	E	172	GLU
7	E	175	LEU
7	E	204	THR
7	E	207	ARG
7	E	213	ILE
8	F	82	THR
8	F	90	ARG
8	F	93	ILE
8	F	111	LEU
8	F	133	VAL
8	F	155	LEU
9	H	2	SER

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Mol	Chain	Res	Type
9	H	4	THR
9	H	11	GLN
9	H	15	VAL
9	H	19	ARG
9	H	22	LYS
9	H	31	THR
9	H	33	GLN
9	H	35	GLN
9	H	36	CYS
9	H	49	VAL
9	H	53	ASP
9	H	58	THR
9	H	59	ILE
9	H	76	THR
9	H	89	LEU
9	H	92	ASP
9	H	94	ASP
9	H	110	ASP
9	H	112	ILE
9	H	121	LEU
9	H	123	MET
9	H	130	ARG
9	H	132	LEU
9	H	136	LYS
9	H	145	ARG
10	I	29	CYS
10	I	33	SER
10	I	40	SER
10	I	50	THR
10	I	52	ILE
10	I	55	THR
10	I	59	VAL
10	I	61	ASP
10	I	70	ARG
10	I	74	GLU
10	I	78	CYS
10	I	83	ASN
10	I	84	VAL
10	I	90	GLN
10	I	92	ARG
10	I	94	ASP
10	I	104	LEU

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Mol	Chain	Res	Type
11	J	2	ILE
11	J	3	VAL
11	J	5	VAL
11	J	7	CYS
11	J	13	VAL
11	J	19	GLU
11	J	23	ASN
11	J	27	GLU
11	J	28	ASP
11	J	48	ARG
11	J	55	ASP
12	K	1	MET
12	K	11	LEU
12	K	18	LYS
12	K	20	LYS
12	K	31	VAL
12	K	42	LEU
12	K	50	LEU
12	K	51	LEU
12	K	78	THR
12	K	101	LEU
12	K	103	THR
13	L	27	LEU
13	L	31	CYS
13	L	34	CYS
13	L	38	LEU
13	L	42	ARG
13	L	47	ARG
13	L	48	CYS
13	L	55	ILE
13	L	61	THR
13	L	63	ARG
13	L	65	VAL
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	18	GLN
4	A	54	ASN
4	A	83	HIS

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Mol	Chain	Res	Type
4	A	92	HIS
4	A	119	ASN
4	A	225	ASN
4	A	253	ASN
4	A	282	ASN
4	A	299	HIS
4	A	313	GLN
4	A	339	ASN
4	A	394	ASN
4	A	397	ASN
4	A	503	GLN
4	A	517	ASN
4	A	584	ASN
4	A	589	GLN
4	A	611	GLN
4	A	631	HIS
4	A	741	ASN
4	A	757	ASN
4	A	768	GLN
4	A	786	HIS
4	A	926	GLN
4	A	935	GLN
4	A	965	GLN
4	A	968	GLN
4	A	969	GLN
4	A	996	ASN
4	A	1009	ASN
4	A	1033	GLN
4	A	1052	GLN
4	A	1082	ASN
4	A	1110	ASN
4	A	1130	GLN
4	A	1140	HIS
4	A	1222	ASN
4	A	1364	ASN
4	A	1387	HIS
4	A	1393	ASN
4	A	1427	ASN
4	A	1432	GLN
5	B	121	ASN
5	B	206	ASN
5	B	215	GLN

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Mol	Chain	Res	Type
5	B	255	GLN
5	B	325	GLN
5	B	366	GLN
5	B	383	ASN
5	B	395	GLN
5	B	415	GLN
5	B	433	GLN
5	B	484	ASN
5	B	499	ASN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	657	HIS
5	B	733	HIS
5	B	740	HIS
5	B	744	HIS
5	B	762	ASN
5	B	770	GLN
5	B	794	ASN
5	B	822	ASN
5	B	887	HIS
5	B	957	ASN
5	B	984	HIS
5	B	1015	HIS
5	B	1062	HIS
5	B	1076	HIS
5	B	1093	GLN
5	B	1141	HIS
5	B	1161	HIS
5	B	1195	HIS
6	C	65	HIS
6	C	73	GLN
6	C	79	GLN
6	C	112	ASN
6	C	123	ASN
6	C	140	ASN
6	C	167	HIS
6	C	203	GLN
6	C	214	ASN
6	C	231	ASN
6	C	242	GLN

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Mol	Chain	Res	Type
6	C	264	GLN
7	E	63	ASN
7	E	104	ASN
7	E	146	HIS
9	H	3	ASN
9	H	11	GLN
9	H	33	GLN
9	H	133	ASN
10	I	12	ASN
10	I	89	GLN
10	I	116	ASN
11	J	64	ASN
12	K	29	ASN
12	K	40	HIS
12	K	52	ASN
12	K	65	HIS
12	K	76	GLN
12	K	89	ASN
13	L	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U

There are no RNA pucker outliers to report.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	DUT	T	29[A]	16	28,29,29	1.22	1 (3%)	41,45,45	1.69	5 (12%)
14	DUT	T	29[B]	16	28,29,29	1.24	1 (3%)	41,45,45	3.02	16 (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
14	DUT	T	29[A]	16	-	4/22/34/34	0/2/2/2
14	DUT	T	29[B]	16	-	4/22/34/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	29[B]	DUT	C2-N1	-2.56	1.34	1.38
14	T	29[A]	DUT	C2-N1	-2.56	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	29[B]	DUT	O4'-C4'-C5'	11.81	147.16	109.33
14	T	29[B]	DUT	O5'-C5'-C4'	7.83	135.64	108.99
14	T	29[B]	DUT	O2G-PG-O3B	-5.77	85.27	104.64
14	T	29[A]	DUT	C4-N3-C2	-5.62	119.63	126.61
14	T	29[A]	DUT	N3-C2-N1	4.58	120.86	114.89
14	T	29[B]	DUT	O2G-PG-O1G	4.22	127.28	110.83
14	T	29[B]	DUT	C2'-C1'-N1	-4.14	103.46	113.81
14	T	29[A]	DUT	O4'-C1'-N1	3.75	114.52	107.86
14	T	29[A]	DUT	C5-C4-N3	3.50	119.71	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	29[B]	DUT	O3B-PG-O1G	-3.28	93.80	111.04
14	T	29[B]	DUT	C1'-N1-C2	3.24	124.00	117.66
14	T	29[B]	DUT	N3-C2-N1	3.05	118.86	114.89
14	T	29[B]	DUT	C5'-C4'-C3'	-2.97	98.02	114.64
14	T	29[A]	DUT	O4-C4-C5	-2.82	120.31	125.16
14	T	29[B]	DUT	O3G-PG-O2G	2.63	117.64	107.80
14	T	29[B]	DUT	O3'-C3'-C2'	-2.61	101.81	110.88
14	T	29[B]	DUT	O2B-PB-O3B	2.37	113.67	107.27
14	T	29[B]	DUT	C6-N1-C2	-2.15	118.38	121.00
14	T	29[B]	DUT	O4'-C1'-N1	2.11	111.61	107.86
14	T	29[B]	DUT	C4-N3-C2	-2.05	124.07	126.61
14	T	29[B]	DUT	C1'-N1-C6	-2.04	117.52	121.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	29[B]	DUT	C4'-C5'-O5'-PA
14	T	29[B]	DUT	C5'-O5'-PA-O2A
14	T	29[B]	DUT	C5'-O5'-PA-O3A
14	T	29[A]	DUT	C3'-C4'-C5'-O5'
14	T	29[A]	DUT	O4'-C4'-C5'-O5'
14	T	29[B]	DUT	O4'-C4'-C5'-O5'
14	T	29[A]	DUT	C4'-C5'-O5'-PA
14	T	29[A]	DUT	PA-O3A-PB-O2B

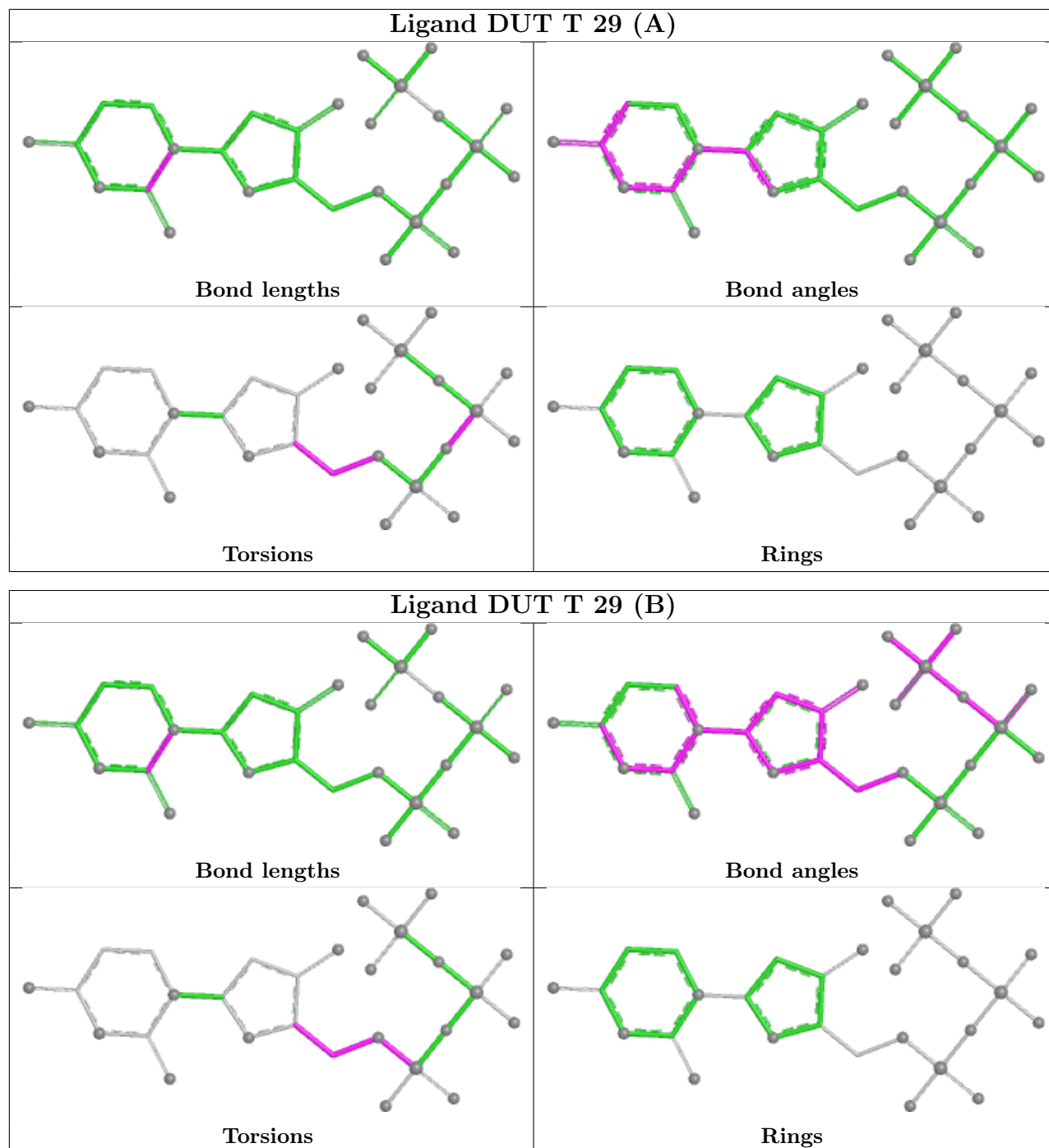
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	29[A]	DUT	3	0
14	T	29[B]	DUT	13	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 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	10/10 (100%)	-0.23	0 100 100	30, 50, 93, 109	0
2	T	28/28 (100%)	0.90	4 (14%) 6 5	40, 108, 139, 145	0
3	N	14/14 (100%)	1.98	4 (28%) 1 1	73, 119, 144, 149	0
4	A	1405/1733 (81%)	0.62	112 (7%) 18 15	24, 56, 77, 131	0
5	B	1114/1224 (91%)	0.62	82 (7%) 20 17	28, 55, 84, 104	0
6	C	266/318 (83%)	0.33	1 (0%) 88 85	40, 54, 73, 99	0
7	E	214/215 (99%)	0.98	37 (17%) 4 3	43, 64, 88, 91	0
8	F	85/155 (54%)	0.28	1 (1%) 76 69	44, 59, 81, 90	0
9	H	133/146 (91%)	1.14	19 (14%) 6 5	52, 66, 88, 94	0
10	I	119/122 (97%)	0.59	6 (5%) 34 27	37, 51, 84, 96	0
11	J	65/70 (92%)	0.32	1 (1%) 72 64	44, 56, 72, 81	0
12	K	114/120 (95%)	0.35	2 (1%) 67 59	45, 57, 73, 82	0
13	L	46/70 (65%)	1.43	11 (23%) 2 2	57, 87, 98, 101	0
All	All	3613/4225 (85%)	0.63	280 (7%) 19 16	24, 57, 85, 149	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	65	LEU	7.2
5	B	882	THR	6.5
13	L	27	LEU	6.4
5	B	883	LEU	6.2
5	B	250	PHE	6.1
4	A	1089	VAL	5.9
5	B	869	SER	5.9
4	A	1086	PHE	5.8
4	A	1090	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
4	A	1087	ALA	5.8
4	A	69	THR	5.7
4	A	311	GLN	5.5
4	A	1082	ASN	5.4
5	B	647	GLY	5.3
3	N	1	DC	5.1
9	H	132	LEU	5.0
5	B	870	ILE	4.9
4	A	1083	THR	4.9
5	B	731	VAL	4.7
4	A	252	PHE	4.7
5	B	246	LYS	4.7
4	A	1085	HIS	4.5
4	A	250	ILE	4.5
4	A	1173	HIS	4.5
7	E	123	LEU	4.5
5	B	474	SER	4.5
4	A	1176	LEU	4.4
5	B	509	ALA	4.4
7	E	124	VAL	4.4
4	A	1081	LEU	4.3
5	B	1184	GLY	4.2
5	B	866	TYR	4.2
5	B	709	ASP	4.2
4	A	51	GLY	4.1
5	B	1224	PHE	4.1
10	I	2	THR	3.9
5	B	715	ALA	3.9
4	A	316	GLN	3.8
5	B	251	ILE	3.8
5	B	502	ILE	3.8
5	B	880	THR	3.8
8	F	155	LEU	3.8
4	A	315	LEU	3.8
9	H	63	LEU	3.8
5	B	475	SER	3.7
5	B	708	GLU	3.7
5	B	252	SER	3.6
13	L	55	ILE	3.6
4	A	1254	ALA	3.6
13	L	25	ALA	3.6
4	A	44	THR	3.5

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Mol	Chain	Res	Type	RSRZ
7	E	93	MET	3.5
5	B	1222	ARG	3.5
4	A	318	SER	3.5
5	B	429	PHE	3.4
9	H	85	GLY	3.4
4	A	152	VAL	3.4
7	E	97	VAL	3.4
4	A	1084	PHE	3.4
5	B	477	ALA	3.3
4	A	141	LEU	3.3
5	B	244	LEU	3.3
3	N	14	DG	3.3
4	A	146	MET	3.3
4	A	348	SER	3.3
4	A	168	GLY	3.3
2	T	1	DC	3.3
4	A	149	GLU	3.3
4	A	1234	GLU	3.2
4	A	64	ASN	3.2
7	E	90	VAL	3.2
12	K	114	LEU	3.2
5	B	711	GLU	3.2
4	A	41	MET	3.2
7	E	46	TYR	3.2
5	B	249	ARG	3.1
7	E	95	THR	3.1
4	A	199	LEU	3.1
5	B	646	LEU	3.1
5	B	230	ALA	3.1
4	A	121	LEU	3.1
5	B	710	LEU	3.1
4	A	103	CYS	3.1
5	B	865	LYS	3.1
7	E	96	PHE	3.0
7	E	121	MET	3.0
4	A	1175	SER	3.0
4	A	165	GLY	3.0
4	A	183	GLY	3.0
4	A	171	GLN	3.0
5	B	730	ARG	3.0
7	E	119	SER	3.0
4	A	56	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
4	A	1315	GLU	3.0
5	B	243	ALA	3.0
4	A	182	VAL	3.0
9	H	136	LYS	3.0
4	A	161	LEU	2.9
5	B	446	LEU	2.9
9	H	90	ALA	2.9
5	B	733	HIS	2.9
7	E	120	ALA	2.9
9	H	135	LEU	2.9
3	N	13	DA	2.9
5	B	881	ASN	2.9
4	A	314	ALA	2.9
4	A	1174	PHE	2.9
5	B	976	ILE	2.9
10	I	120	GLN	2.8
4	A	1257	ASP	2.8
5	B	645	SER	2.8
13	L	53	HIS	2.8
4	A	181	LEU	2.8
4	A	308	ILE	2.8
5	B	245	GLU	2.8
7	E	130	ALA	2.8
13	L	45	ALA	2.8
4	A	153	PRO	2.8
5	B	229	ALA	2.8
5	B	447	ALA	2.8
7	E	127	ILE	2.8
4	A	150	THR	2.8
4	A	177	ASP	2.8
5	B	248	SER	2.8
5	B	436	VAL	2.7
5	B	918	ILE	2.7
2	T	2	DT	2.7
4	A	253	ASN	2.7
5	B	1223	ASP	2.7
5	B	480	SER	2.7
9	H	82	PRO	2.7
4	A	57	ARG	2.7
4	A	147	VAL	2.7
5	B	140	ILE	2.7
10	I	52	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
5	B	137	TYR	2.7
13	L	40	LEU	2.7
4	A	286	HIS	2.7
9	H	86	ASP	2.7
4	A	251	SER	2.7
5	B	139	ALA	2.7
5	B	473	MET	2.7
5	B	734	HIS	2.7
5	B	478	GLY	2.7
7	E	88	VAL	2.7
4	A	210	ILE	2.6
4	A	1091	SER	2.7
4	A	91	PHE	2.6
5	B	987	LYS	2.6
7	E	57	MET	2.6
4	A	105	CYS	2.6
4	A	307	ASP	2.6
5	B	884	ARG	2.6
4	A	672	ASP	2.6
5	B	1190	ASP	2.6
4	A	154	SER	2.6
7	E	103	LYS	2.6
12	K	1	MET	2.6
5	B	713	ALA	2.6
4	A	1088	GLY	2.5
9	H	92	ASP	2.5
5	B	712	PRO	2.5
7	E	132	ILE	2.5
7	E	16	PHE	2.5
4	A	114	LEU	2.5
5	B	479	VAL	2.5
5	B	944	THR	2.5
9	H	35	GLN	2.5
5	B	476	ARG	2.5
5	B	1220	ARG	2.5
4	A	1256	GLU	2.5
5	B	665	GLU	2.5
5	B	666	TYR	2.5
10	I	4	PHE	2.5
7	E	83	CYS	2.5
5	B	895	ASP	2.4
4	A	115	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	1206	ASP	2.4
4	A	109	HIS	2.4
7	E	73	PRO	2.4
4	A	59	GLY	2.4
4	A	567	LYS	2.4
5	B	879	ARG	2.4
5	B	370	PHE	2.4
4	A	254	GLU	2.4
4	A	108	MET	2.4
7	E	128	PRO	2.4
4	A	130	ASP	2.3
13	L	59	ALA	2.3
4	A	113	LEU	2.3
7	E	98	ILE	2.3
4	A	317	LYS	2.3
4	A	162	VAL	2.3
7	E	82	PHE	2.3
4	A	122	MET	2.3
4	A	1188	GLN	2.3
7	E	54	GLN	2.3
4	A	975	HIS	2.3
4	A	128	ILE	2.3
11	J	52	THR	2.3
7	E	53	PRO	2.3
9	H	104	PHE	2.3
4	A	72	GLU	2.3
13	L	64	LEU	2.3
4	A	255	SER	2.3
4	A	1092	LYS	2.3
7	E	79	TRP	2.3
9	H	79	TRP	2.3
10	I	118	ARG	2.3
5	B	1013	ASN	2.3
4	A	451	HIS	2.3
7	E	69	ILE	2.3
7	E	80	VAL	2.3
7	E	105	PHE	2.2
9	H	84	ALA	2.2
4	A	399	HIS	2.2
5	B	265	SER	2.2
4	A	52	GLY	2.2
4	A	753	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
5	B	988	GLY	2.2
4	A	211	PHE	2.2
4	A	176	LYS	2.2
5	B	483	LEU	2.2
6	C	233	GLU	2.2
9	H	139	ASN	2.2
13	L	65	VAL	2.2
9	H	108	SER	2.2
4	A	205	GLU	2.2
9	H	29	ALA	2.2
13	L	28	LYS	2.2
4	A	164	ARG	2.2
5	B	1046	PRO	2.2
9	H	114	VAL	2.2
5	B	732	SER	2.2
9	H	109	LYS	2.2
4	A	86	LEU	2.2
4	A	658	LEU	2.2
4	A	257	ARG	2.2
4	A	201	VAL	2.2
7	E	86	PRO	2.2
9	H	107	VAL	2.2
7	E	50	MET	2.2
4	A	167	CYS	2.2
4	A	120	GLU	2.2
4	A	280	GLU	2.2
4	A	1187	GLN	2.1
7	E	65	THR	2.1
13	L	43	THR	2.1
4	A	200	ARG	2.1
2	T	4	DC	2.1
5	B	66	ASP	2.1
4	A	319	GLY	2.1
5	B	1022	THR	2.1
7	E	87	SER	2.1
5	B	531	GLN	2.1
4	A	1258	HIS	2.1
4	A	1156	PRO	2.1
7	E	2	ASP	2.1
4	A	136	ALA	2.1
5	B	981	ALA	2.1
5	B	242	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	T	7	DA	2.1
4	A	455	MET	2.1
7	E	104	ASN	2.1
10	I	116	ASN	2.1
5	B	112	LEU	2.1
4	A	1391	ARG	2.1
5	B	529	GLU	2.1
3	N	12	DT	2.0
4	A	1094	VAL	2.0
7	E	129	PRO	2.0
4	A	166	GLY	2.0
5	B	247	GLY	2.0
5	B	335	GLY	2.0
4	A	71	GLN	2.0
4	A	249	SER	2.0
7	E	49	SER	2.0
4	A	173	THR	2.0
5	B	136	THR	2.0
4	A	345	VAL	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 oligosaccharides 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(Å ²)	Q<0.9
14	DUT	T	29[A]	28/28	0.69	0.29	76,80,97,98	28
14	DUT	T	29[B]	28/28	0.69	0.29	70,73,79,80	28
16	MG	A	2002[A]	1/1	0.80	0.47	43,43,43,43	1
16	MG	A	2002[B]	1/1	0.80	0.47	33,33,33,33	1

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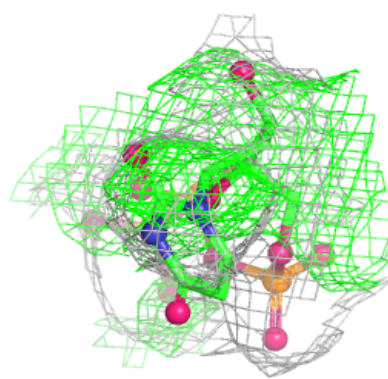
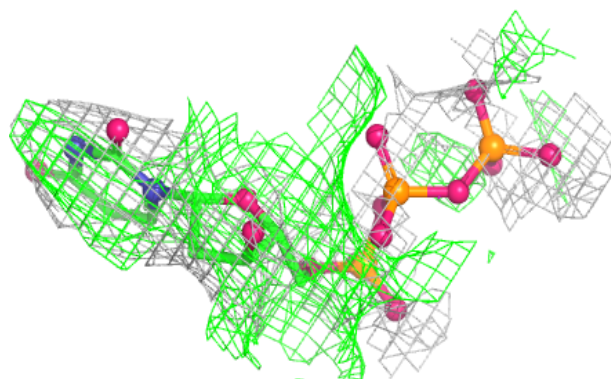
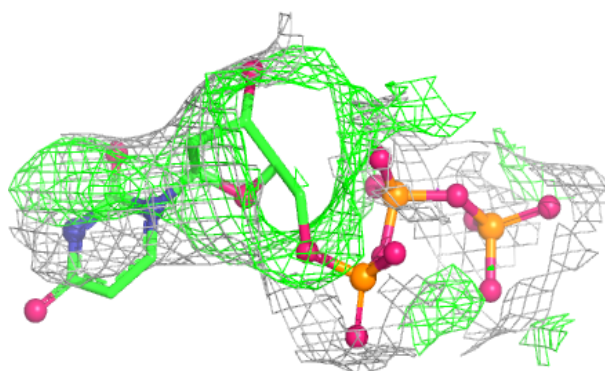
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	A	2001	1/1	0.85	0.13	46,46,46,46	0
15	ZN	A	1734	1/1	0.92	0.14	84,84,84,84	0
15	ZN	L	105	1/1	0.95	0.08	91,91,91,91	0
15	ZN	B	1307	1/1	0.96	0.12	80,80,80,80	0
15	ZN	I	204	1/1	0.97	0.08	57,57,57,57	0
15	ZN	A	1735	1/1	0.98	0.04	78,78,78,78	0
15	ZN	C	319	1/1	0.99	0.03	48,48,48,48	0
15	ZN	J	101	1/1	0.99	0.04	50,50,50,50	0
15	ZN	I	203	1/1	0.99	0.07	83,83,83,83	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.

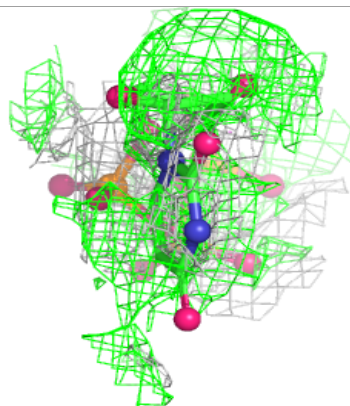
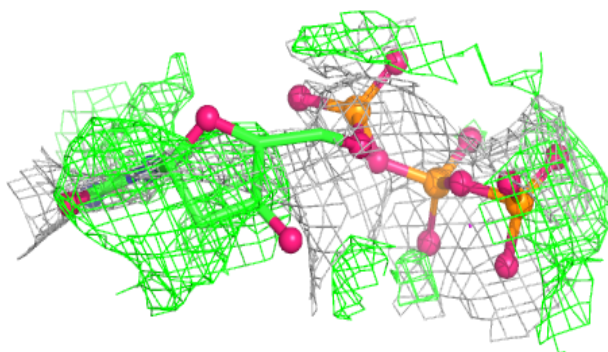
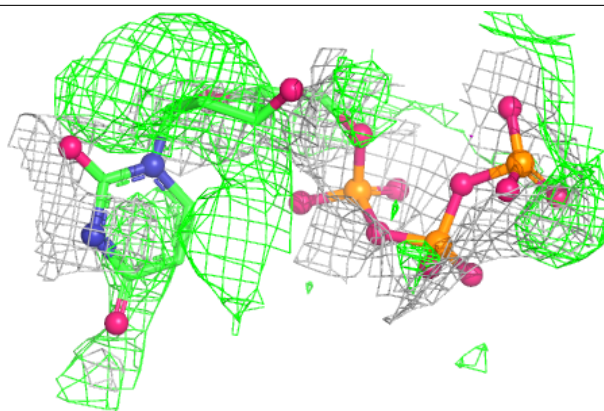
Electron density around DUT T 29 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DUT T 29 (B):

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.