



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:07 PM EDT

PDB ID : 3M3Y / pdb_00003m3y
Title : RNA polymerase II elongation complex C
Authors : Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.
Deposited on : 2010-03-10
Resolution : 3.18 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
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

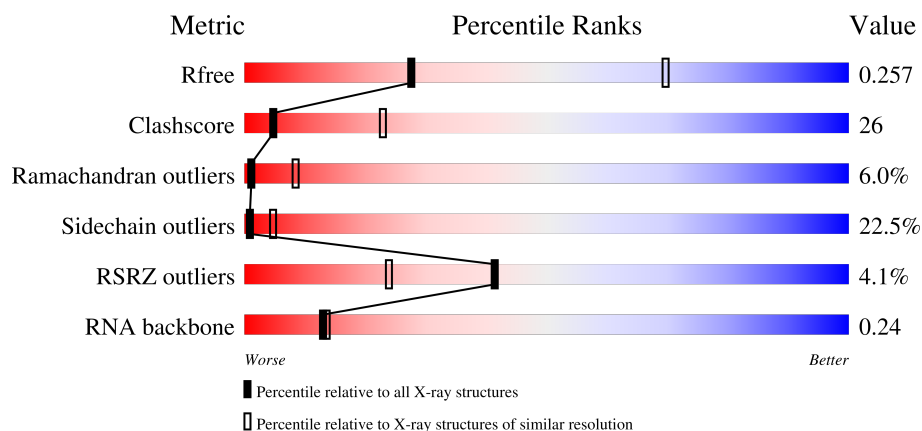
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)
RNA backbone	3983	1138 (3.46-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	1733	 3% 38% 30% 11% • 20%
2	B	1224	 3% 43% 33% 11% • 10%
3	C	318	 38% 32% 12% • 16%
4	E	215	 2% 52% 38% 9% •

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Mol	Chain	Length	Quality of chain
5	F	155	%27%21%5%•46%
6	H	146	10%42%33%14%•9%
7	I	122	4%50%34%11%••
8	J	70	36%36%17%•7%
9	K	120	%57%33%5%5%
10	L	70	9%26%27%11%•34%
11	R	11	100%45%36%18%
12	T	28	50%29%68%•
13	N	14	14%100%

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29241 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	11	Total	C	N	O	P	0	0	0
			240	108	50	72	10			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			550	265	92	166	27			

- Molecule 13 is a DNA chain called DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			293	140	55	85	13			

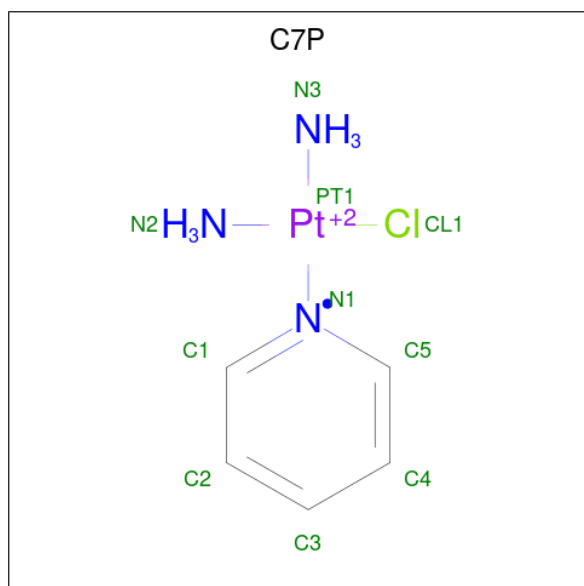
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (CCD ID: C7P) (formula: C₅H₁₁ClN₃Pt).

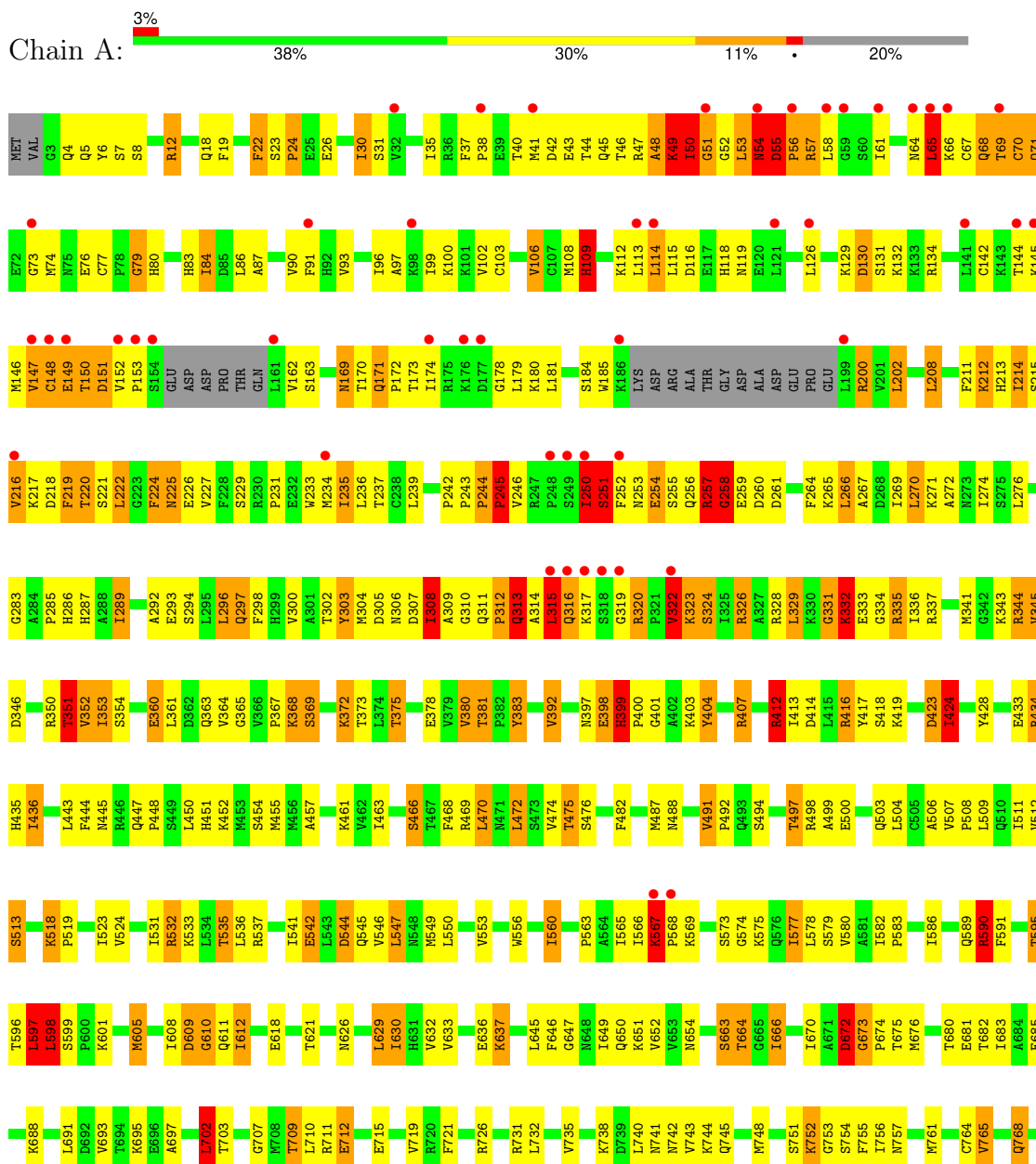


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	T	1	Total	C	N	Pt	0	0
			9	5	3	1		

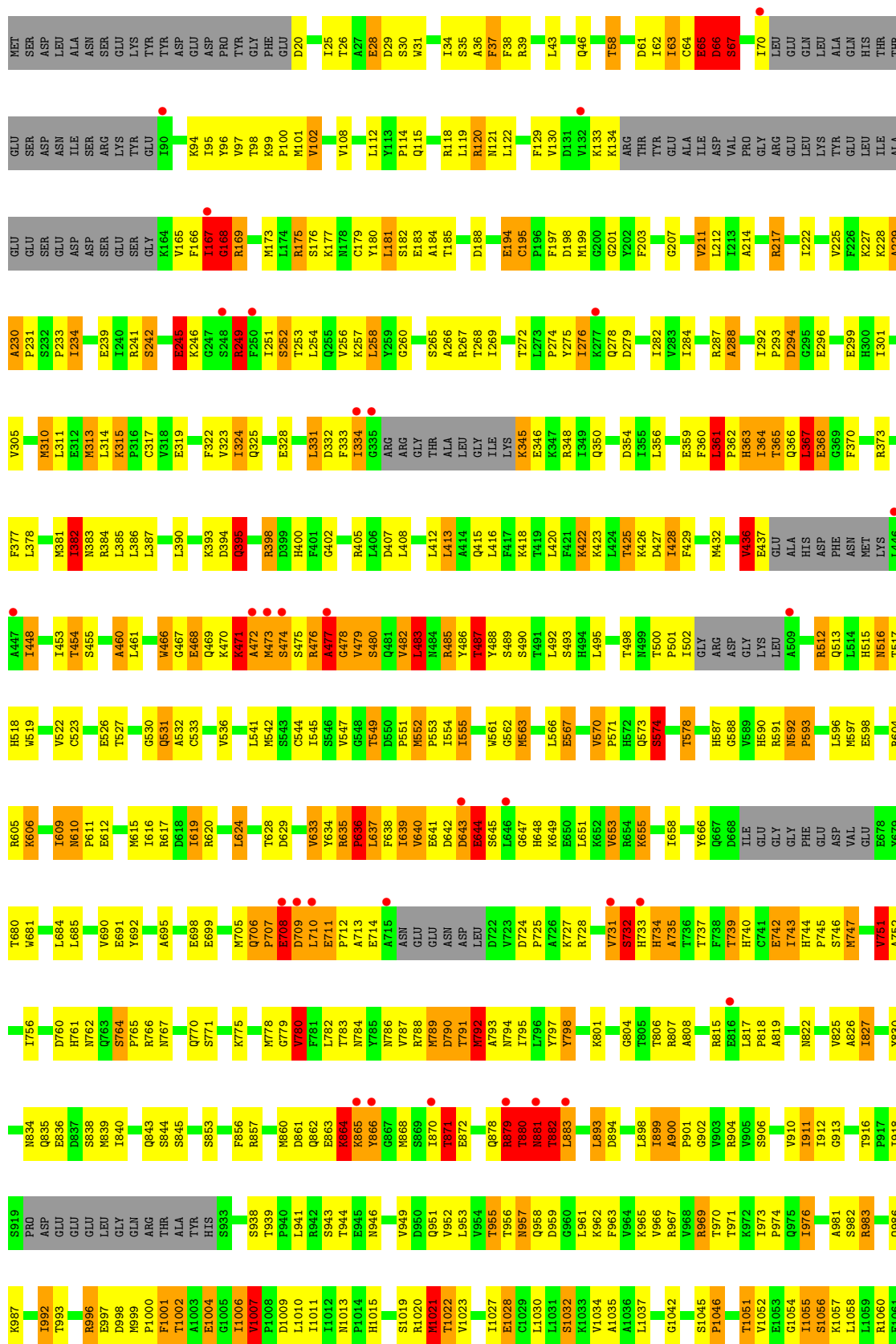
3 Residue-property plots

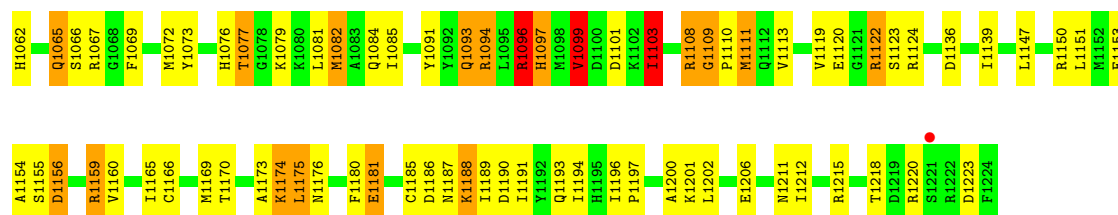
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

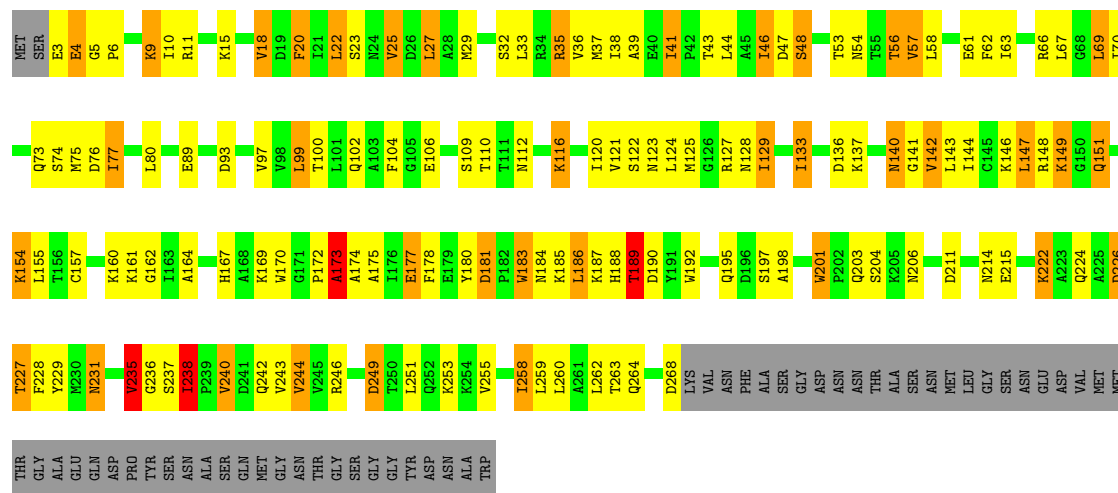




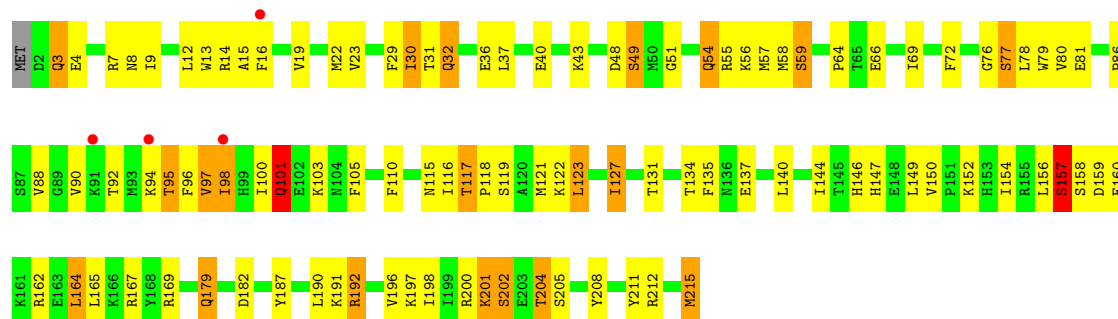




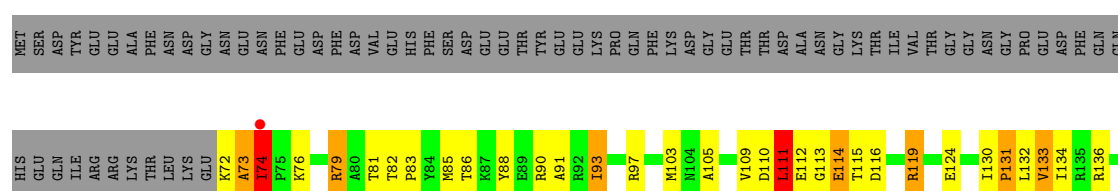
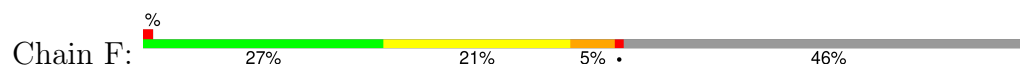
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

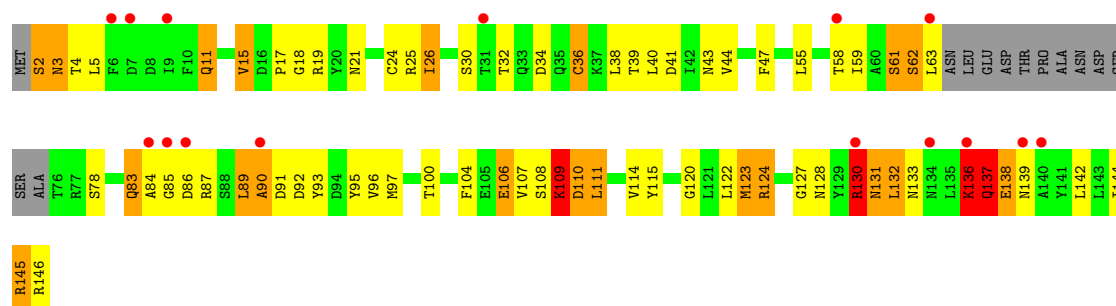


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

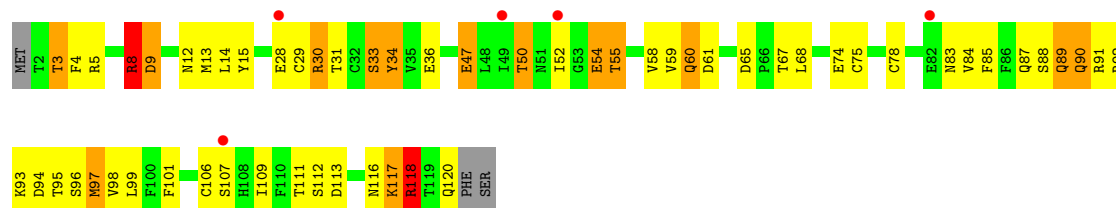




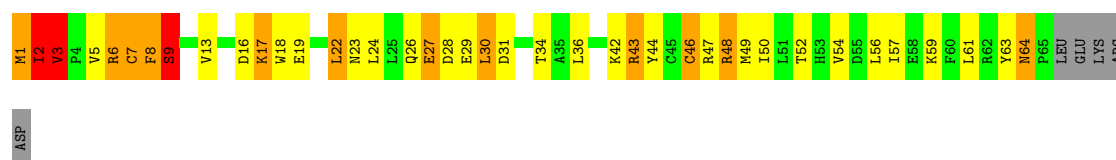
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



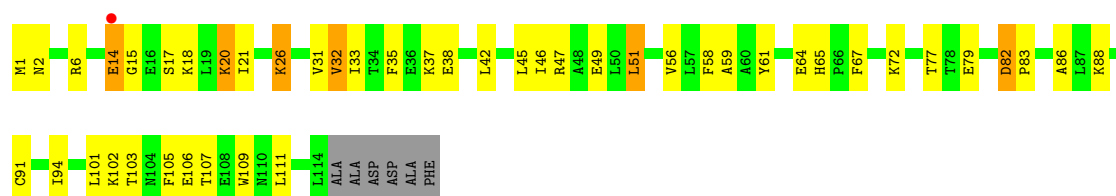
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



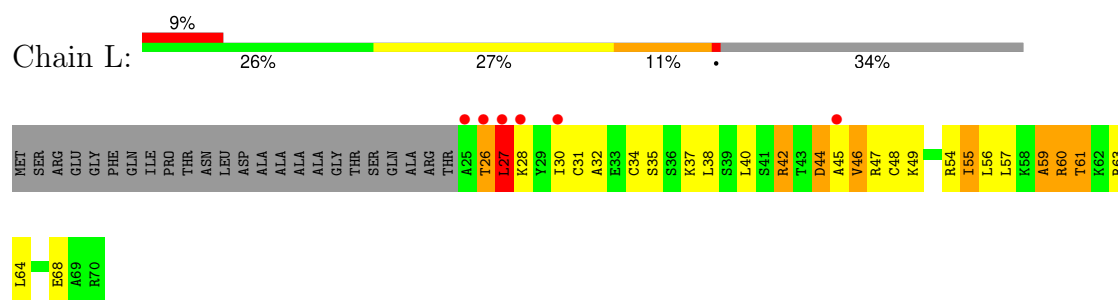
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



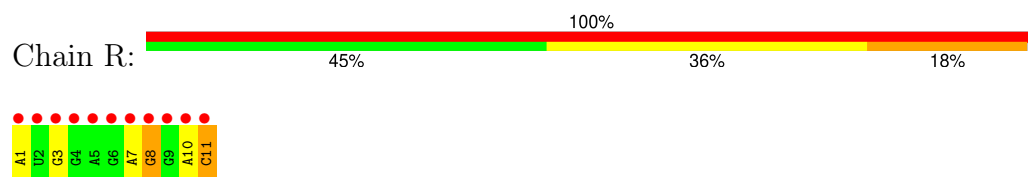
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



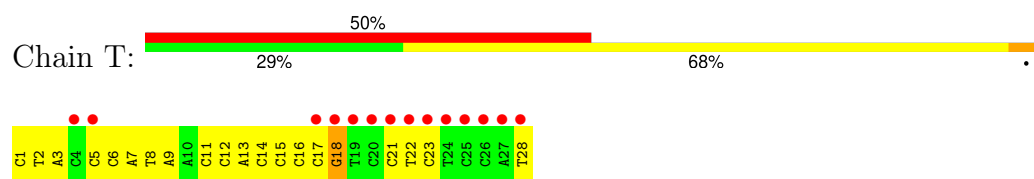
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



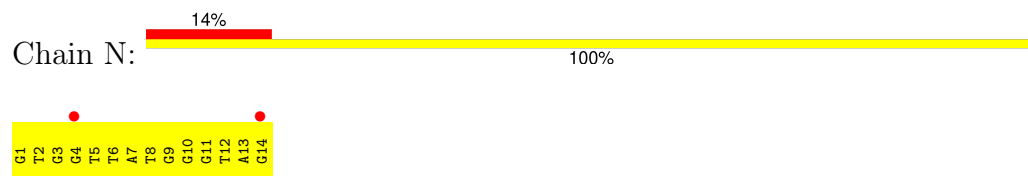
- Molecule 11: RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP*C)-3')



- Molecule 12: DNA (28-MER)



- Molecule 13: DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.48Å 223.12Å 193.81Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	40.00 – 3.18 40.00 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-3.18) 98.5 (40.00-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.207 , 0.255 0.222 , 0.257	Depositor DCC
R_{free} test set	5827 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29241	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, C7P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.94	4/11163 (0.0%)	1.21	66/15091 (0.4%)
2	B	1.07	9/8963 (0.1%)	1.30	66/12086 (0.5%)
3	C	1.03	2/2133 (0.1%)	1.26	11/2891 (0.4%)
4	E	0.76	0/1788	1.09	4/2406 (0.2%)
5	F	0.88	0/691	1.13	3/933 (0.3%)
6	H	0.86	0/1086	1.15	7/1470 (0.5%)
7	I	1.05	0/989	1.20	6/1331 (0.5%)
8	J	1.04	0/541	1.36	4/727 (0.6%)
9	K	0.96	1/937 (0.1%)	1.10	3/1265 (0.2%)
10	L	1.24	1/365 (0.3%)	1.52	8/485 (1.6%)
11	R	0.94	0/270	1.48	4/421 (1.0%)
12	T	0.65	0/612	1.13	2/937 (0.2%)
13	N	0.15	0/329	0.34	0/509
All	All	0.97	17/29867 (0.1%)	1.23	184/40552 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	5
4	E	0	1
6	H	0	3
8	J	0	1
10	L	0	1
All	All	0	14

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	436	VAL	CA-CB	6.80	1.63	1.54
1	A	352	VAL	CA-CB	-6.41	1.47	1.54
2	B	477	ALA	CA-CB	5.99	1.63	1.53
9	K	32	VAL	CA-CB	5.95	1.60	1.53
2	B	1165	ILE	CA-CB	5.71	1.62	1.54
2	B	65	GLU	N-CA	5.58	1.53	1.46
1	A	315	LEU	CA-C	5.40	1.60	1.52
2	B	1099	VAL	CA-CB	-5.29	1.47	1.54
3	C	181	ASP	C-O	-5.22	1.21	1.23
10	L	26	THR	CA-CB	5.18	1.62	1.53
2	B	1007	VAL	C-O	-5.15	1.20	1.24
1	A	150	THR	CA-C	5.13	1.55	1.52
2	B	487	THR	CA-C	-5.10	1.46	1.52
1	A	250	ILE	N-CA	5.10	1.52	1.46
2	B	976	ILE	CA-C	-5.06	1.46	1.53
2	B	460	ALA	CA-CB	-5.05	1.45	1.53
3	C	235	VAL	CA-CB	-5.04	1.48	1.54

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1109	GLY	CA-C-N	10.99	131.08	119.76
2	B	1109	GLY	C-N-CA	10.99	131.08	119.76
2	B	37	PHE	N-CA-C	-10.77	96.44	110.33
2	B	1007	VAL	N-CA-C	-10.63	100.47	109.19
2	B	167	ILE	CB-CA-C	-10.62	96.51	111.38
2	B	211	VAL	CB-CA-C	-10.20	96.07	110.96
1	A	598	LEU	N-CA-C	-9.53	100.15	114.64
1	A	513	SER	CA-C-N	9.52	129.27	119.56
1	A	513	SER	C-N-CA	9.52	129.27	119.56
2	B	711	GLU	CA-C-N	-9.42	110.68	120.85
2	B	711	GLU	C-N-CA	-9.42	110.68	120.85
5	F	74	ILE	CA-C-N	9.39	131.57	119.84
5	F	74	ILE	C-N-CA	9.39	131.57	119.84
1	A	399	HIS	CA-C-N	-8.99	108.60	119.84
1	A	399	HIS	C-N-CA	-8.99	108.60	119.84
11	R	8	G	C4'-C3'-C2'	-8.88	93.72	102.60
2	B	363	HIS	N-CA-C	-8.62	99.80	110.41
1	A	331	GLY	N-CA-C	8.56	123.50	112.54
2	B	361	LEU	CA-C-N	8.45	128.14	119.19
2	B	361	LEU	C-N-CA	8.45	128.14	119.19
2	B	780	VAL	CB-CA-C	-8.16	102.46	111.35
2	B	1099	VAL	CB-CA-C	-7.96	101.39	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	714	GLU	N-CA-C	7.89	122.07	108.02
2	B	1156	ASP	N-CA-C	7.71	122.44	112.26
1	A	149	GLU	N-CA-C	7.60	119.25	108.00
9	K	64	GLU	N-CA-C	7.42	119.37	111.28
4	E	117	THR	CA-C-N	7.36	129.04	119.84
4	E	117	THR	C-N-CA	7.36	129.04	119.84
2	B	739	THR	N-CA-C	-7.34	105.50	114.75
6	H	36	CYS	N-CA-C	7.33	120.36	107.61
12	T	18	DG	N9-C1'-C2'	-7.30	102.54	113.50
8	J	3	VAL	CA-C-N	7.28	127.71	119.93
8	J	3	VAL	C-N-CA	7.28	127.71	119.93
1	A	973	ILE	N-CA-C	7.26	118.28	108.11
7	I	84	VAL	N-CA-C	-7.25	98.05	108.42
1	A	1444	MET	N-CA-C	7.25	117.59	108.45
6	H	84	ALA	N-CA-C	7.25	120.61	111.69
1	A	566	ILE	CB-CA-C	-7.20	105.59	111.71
2	B	780	VAL	N-CA-C	7.19	117.75	108.12
10	L	64	LEU	N-CA-C	7.17	122.00	109.96
1	A	1392	SER	N-CA-C	7.09	119.58	110.65
8	J	3	VAL	CB-CA-C	-7.07	98.50	111.36
1	A	626	ASN	N-CA-C	7.04	118.85	111.03
2	B	866	TYR	N-CA-C	6.89	125.47	110.80
4	E	115	ASN	N-CA-C	6.89	118.66	108.60
1	A	1207	LEU	N-CA-C	6.86	119.69	108.52
10	L	63	ARG	CA-C-N	-6.84	111.96	122.09
10	L	63	ARG	C-N-CA	-6.84	111.96	122.09
2	B	478	GLY	N-CA-C	-6.83	96.98	113.18
2	B	636	PRO	CA-C-N	6.83	134.00	121.70
2	B	636	PRO	C-N-CA	6.83	134.00	121.70
1	A	229	SER	N-CA-C	6.71	118.44	107.23
1	A	582	ILE	CA-C-N	6.70	128.21	119.84
1	A	582	ILE	C-N-CA	6.70	128.21	119.84
2	B	1096	ARG	N-CA-C	-6.65	101.72	110.43
1	A	921	GLY	N-CA-C	-6.64	105.56	111.67
1	A	595	THR	N-CA-C	6.60	120.06	110.42
2	B	382	ILE	CB-CA-C	-6.59	103.40	112.04
1	A	450	LEU	N-CA-C	6.52	120.44	112.23
1	A	999	VAL	N-CA-C	-6.51	106.47	111.62
2	B	610	ASN	CA-C-N	6.50	127.96	119.84
2	B	610	ASN	C-N-CA	6.50	127.96	119.84
2	B	798	TYR	CA-C-N	6.46	127.92	119.84
2	B	798	TYR	C-N-CA	6.46	127.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ARG	N-CA-C	6.45	117.64	108.54
2	B	711	GLU	N-CA-C	6.44	124.05	109.81
10	L	27	LEU	N-CA-C	6.43	120.13	109.46
1	A	200	ARG	N-CA-C	6.42	118.94	109.69
1	A	597	LEU	CB-CA-C	-6.42	97.65	110.42
2	B	1007	VAL	CB-CA-C	6.38	115.58	109.33
2	B	698	GLU	N-CA-C	-6.37	104.39	111.71
7	I	8	ARG	N-CA-C	-6.35	101.08	110.48
1	A	345	VAL	N-CA-C	6.34	119.41	108.95
1	A	360	GLU	N-CA-C	-6.34	102.61	110.41
2	B	982	SER	N-CA-C	-6.31	99.94	109.79
1	A	491	VAL	CA-C-N	6.30	126.06	119.76
1	A	491	VAL	C-N-CA	6.30	126.06	119.76
1	A	673	GLY	CA-C-N	6.29	127.71	119.84
1	A	673	GLY	C-N-CA	6.29	127.71	119.84
2	B	195	CYS	CA-C-N	-6.26	114.44	120.83
2	B	195	CYS	C-N-CA	-6.26	114.44	120.83
1	A	1332	PHE	N-CA-C	-6.25	105.69	113.38
1	A	1319	VAL	CA-C-N	6.21	126.18	120.03
1	A	1319	VAL	C-N-CA	6.21	126.18	120.03
1	A	524	VAL	N-CA-C	6.19	118.84	108.81
10	L	63	ARG	N-CA-C	-6.17	101.05	110.30
1	A	821	ARG	N-CA-C	-6.13	104.71	111.82
6	H	145	ARG	N-CA-C	6.12	118.65	108.13
1	A	313	GLN	N-CA-C	6.06	123.70	110.80
2	B	751	VAL	N-CA-C	6.06	121.94	109.34
7	I	31	THR	N-CA-C	-6.04	105.93	113.55
1	A	598	LEU	N-CA-CB	6.03	120.65	111.06
1	A	993	LEU	N-CA-C	-5.97	103.54	111.24
3	C	238	ILE	CA-C-N	-5.96	113.82	120.14
3	C	238	ILE	C-N-CA	-5.96	113.82	120.14
1	A	351	THR	CB-CA-C	-5.92	99.71	111.91
10	L	68	GLU	N-CA-C	-5.92	101.52	110.28
1	A	151	ASP	N-CA-C	5.91	116.04	108.24
3	C	198	ALA	N-CA-C	5.91	117.72	111.28
1	A	886	ILE	N-CA-C	5.88	119.31	111.44
1	A	672	ASP	N-CA-C	5.87	117.90	110.33
2	B	184	ALA	N-CA-C	5.86	119.45	110.20
6	H	137	GLN	N-CA-C	5.85	119.21	110.14
11	R	10	A	O4'-C1'-C2'	-5.82	101.78	107.60
2	B	616	ILE	CB-CA-C	-5.75	104.71	111.09
2	B	165	VAL	N-CA-C	5.73	115.91	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	883	LEU	CA-CB-CG	5.70	136.23	116.30
2	B	1056	SER	N-CA-C	5.67	118.20	111.33
11	R	10	A	C4'-C3'-C2'	-5.67	96.93	102.60
1	A	885	THR	N-CA-C	-5.65	105.88	112.89
2	B	911	ILE	CB-CA-C	-5.64	104.68	112.24
9	K	82	ASP	CA-C-N	5.63	126.88	119.84
9	K	82	ASP	C-N-CA	5.63	126.88	119.84
2	B	99	LYS	N-CA-C	-5.59	102.00	110.39
1	A	74	MET	N-CA-C	-5.56	105.11	113.89
1	A	1237	ILE	N-CA-C	5.55	116.12	108.12
1	A	590	ARG	N-CA-C	5.53	122.57	110.80
2	B	66	ASP	N-CA-C	-5.53	105.26	111.28
2	B	606	LYS	N-CA-C	-5.49	106.30	114.64
1	A	250	ILE	N-CA-C	5.48	120.74	109.34
1	A	827	THR	N-CA-C	-5.47	106.28	113.12
2	B	871	THR	CB-CA-C	-5.46	104.66	111.43
1	A	239	LEU	CA-C-N	5.45	125.37	119.76
1	A	239	LEU	C-N-CA	5.45	125.37	119.76
3	C	104	PHE	N-CA-C	-5.45	100.14	109.24
1	A	916	GLY	N-CA-C	5.44	119.26	112.73
10	L	32	ALA	N-CA-C	5.42	117.00	111.14
3	C	173	ALA	N-CA-C	5.42	122.33	110.80
3	C	20	PHE	N-CA-C	5.42	118.09	109.81
11	R	11	C	C4'-C3'-C2'	-5.39	97.21	102.60
6	H	109	LYS	CA-C-N	5.39	131.40	121.70
6	H	109	LYS	C-N-CA	5.39	131.40	121.70
7	I	78	CYS	CB-CA-C	-5.39	100.84	110.70
3	C	201	TRP	CA-C-N	-5.36	113.14	119.84
3	C	201	TRP	C-N-CA	-5.36	113.14	119.84
2	B	1055	ILE	N-CA-C	-5.36	105.39	110.42
12	T	18	DG	N3-C4-C5	-5.36	120.37	128.40
1	A	332	LYS	N-CA-C	-5.33	99.45	110.80
3	C	155	LEU	N-CA-C	5.32	115.30	108.34
8	J	50	ILE	CB-CA-C	-5.32	105.44	111.55
2	B	779	GLY	N-CA-C	-5.31	103.63	110.69
1	A	407	ARG	N-CA-C	5.30	118.58	110.36
1	A	919	ILE	CB-CA-C	5.29	116.38	111.30
2	B	593	PRO	N-CA-C	-5.28	106.84	114.18
1	A	56	PRO	N-CA-C	-5.26	101.62	112.47
1	A	251	SER	N-CA-C	5.25	121.98	110.80
2	B	276	ILE	N-CA-C	5.23	115.38	107.80
2	B	767	ASN	N-CA-C	-5.23	105.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1412	ALA	N-CA-C	-5.22	106.41	112.89
2	B	422	LYS	N-CA-C	-5.22	105.27	111.69
1	A	1406	VAL	N-CA-C	5.21	116.68	111.00
1	A	1403	GLU	N-CA-C	5.20	121.88	110.80
2	B	1009	ASP	N-CA-C	-5.20	106.44	112.89
7	I	85	PHE	N-CA-C	5.19	116.69	108.96
7	I	118	ARG	N-CA-C	5.18	116.67	108.96
1	A	171	GLN	CA-C-N	5.14	125.12	120.03
1	A	171	GLN	C-N-CA	5.14	125.12	120.03
2	B	609	ILE	N-CA-C	-5.14	101.08	108.48
3	C	189	THR	CB-CA-C	-5.13	101.23	110.36
3	C	243	VAL	N-CA-CB	5.11	115.98	110.62
2	B	168	GLY	N-CA-C	5.09	125.25	113.18
10	L	40	LEU	N-CA-C	5.09	117.72	110.24
2	B	1096	ARG	CA-C-O	-5.09	116.27	121.87
6	H	85	GLY	N-CA-C	-5.08	107.65	115.73
2	B	472	ALA	N-CA-C	-5.08	105.02	111.11
1	A	315	LEU	CA-C-N	5.08	130.84	121.70
1	A	315	LEU	C-N-CA	5.08	130.84	121.70
2	B	640	VAL	CB-CA-C	-5.07	106.11	111.23
5	F	105	ALA	N-CA-C	-5.07	102.89	110.20
2	B	902	GLY	N-CA-C	5.07	118.81	112.73
1	A	702	LEU	CA-CB-CG	5.06	134.02	116.30
4	E	157	SER	N-CA-C	5.06	117.59	108.48
1	A	399	HIS	N-CA-CB	5.06	119.37	110.37
2	B	574	SER	CA-C-N	5.06	125.13	119.87
2	B	574	SER	C-N-CA	5.06	125.13	119.87
2	B	900	ALA	CA-C-N	5.05	126.15	119.84
2	B	900	ALA	C-N-CA	5.05	126.15	119.84
2	B	918	ILE	N-CA-C	5.04	115.11	107.75
1	A	743	VAL	N-CA-C	-5.04	105.48	110.62
2	B	791	THR	N-CA-C	-5.03	102.61	110.10
2	B	971	THR	N-CA-C	-5.03	101.52	109.76
2	B	1001	PHE	N-CA-C	5.02	117.63	109.24
1	A	258	GLY	N-CA-C	5.02	125.07	113.18
2	B	1022	THR	CB-CA-C	5.02	119.12	111.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1391	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	252	PHE	Peptide
1	A	71	GLN	Peptide
2	B	1076	HIS	Peptide
2	B	245	GLU	Peptide
2	B	265	SER	Peptide
2	B	644	GLU	Peptide
2	B	882	THR	Peptide
4	E	157	SER	Peptide
6	H	136	LYS	Peptide
6	H	138	GLU	Peptide
6	H	61	SER	Peptide
8	J	64	ASN	Peptide
10	L	42	ARG	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	A	10969	0	11071	613	0
2	B	8792	0	8824	479	0
3	C	2095	0	2051	119	0
4	E	1752	0	1776	67	0
5	F	679	0	701	27	0
6	H	1068	0	1040	74	0
7	I	971	0	927	42	0
8	J	532	0	543	43	0
9	K	919	0	929	25	0
10	L	363	0	387	13	0
11	R	240	0	122	2	0
12	T	550	0	316	66	0
13	N	293	0	161	75	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	1	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	T	9	0	5	0	0
All	All	29241	0	28853	1478	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 26.

All (1478) 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)
12:T:2:DT:H2''	12:T:3:DA:C5'	1.47	1.44
12:T:2:DT:C2'	12:T:3:DA:H5'	1.42	1.43
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.60	1.30
13:N:1:DG:H2''	13:N:2:DT:C7	1.71	1.19
12:T:8:DT:H2''	12:T:9:DA:C8	1.79	1.18
2:B:747:MET:HE3	2:B:747:MET:HA	1.23	1.18
1:A:567:LYS:HB3	6:H:96:VAL:H	1.03	1.17
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.78	1.13
13:N:1:DG:H2''	13:N:2:DT:C5	1.84	1.12
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.12	1.11
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.28	1.10
1:A:423:ASP:O	1:A:424:ILE:HB	1.50	1.09
12:T:1:DC:H2''	12:T:2:DT:OP2	1.45	1.08
12:T:7:DA:C2	12:T:8:DT:C4	2.41	1.07
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.29	1.06
1:A:630:ILE:HD12	1:A:630:ILE:H	1.21	1.06
1:A:567:LYS:HB3	6:H:96:VAL:N	1.72	1.05
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.39	1.04
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.33	1.04
1:A:214:ILE:HG22	1:A:215:SER:H	1.21	1.04
1:A:53:LEU:HD23	1:A:54:ASN:H	1.19	1.02
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.38	1.01
1:A:412:ARG:HG3	1:A:412:ARG:HH11	1.22	1.01
13:N:4:DG:H1'	13:N:5:DT:H5''	1.44	1.00
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.43	0.99
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.23	0.99
2:B:485:ARG:HG2	2:B:485:ARG:HH11	1.27	0.99
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.58	0.99
1:A:853:ASP:OD1	1:A:855:THR:HB	1.63	0.98
1:A:855:THR:HG21	1:A:857:ARG:HE	1.27	0.98
13:N:4:DG:C2	13:N:5:DT:C2	2.51	0.98
4:E:90:VAL:HG23	4:E:123:LEU:HD21	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:2:DT:H2'	12:T:3:DA:C8	2.00	0.96
3:C:73:GLN:HE21	3:C:75:MET:H	0.99	0.95
13:N:4:DG:N2	13:N:5:DT:C2	2.33	0.95
2:B:744:HIS:CD2	2:B:746:SER:H	1.85	0.95
2:B:744:HIS:HD2	2:B:746:SER:H	1.02	0.95
4:E:15:ALA:O	4:E:19:VAL:HG23	1.67	0.94
7:I:111:THR:HG22	7:I:113:ASP:H	1.32	0.94
1:A:961:ARG:HH11	1:A:961:ARG:HB3	1.30	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.82	0.94
13:N:3:DG:H2''	13:N:4:DG:OP2	1.67	0.94
13:N:1:DG:C2'	13:N:2:DT:C7	2.46	0.93
3:C:222:LYS:HA	3:C:222:LYS:HE3	1.47	0.93
1:A:1116:LEU:HD13	1:A:1329:THR:CG2	1.98	0.93
1:A:780:VAL:HG22	2:B:699:GLU:OE2	1.70	0.92
2:B:423:LYS:O	2:B:427:ASP:HB2	1.70	0.91
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.35	0.91
2:B:801:LYS:O	8:J:52:THR:HG23	1.69	0.91
2:B:363:HIS:O	2:B:364:ILE:HB	1.69	0.91
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	1.83	0.90
13:N:4:DG:C6	13:N:5:DT:C4	2.59	0.90
13:N:13:DA:H8	13:N:13:DA:OP2	1.54	0.90
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.18	0.90
12:T:8:DT:C2'	12:T:9:DA:C8	2.54	0.90
12:T:6:DC:C2	12:T:7:DA:N7	2.40	0.89
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.54	0.89
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.54	0.89
2:B:175:ARG:HH11	2:B:175:ARG:CG	1.86	0.88
1:A:313:GLN:HB2	1:A:322:VAL:HG22	1.54	0.88
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.53	0.88
2:B:260:GLY:O	2:B:267:ARG:HD3	1.72	0.88
12:T:7:DA:C2	12:T:8:DT:N3	2.42	0.88
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.55	0.88
10:L:47:ARG:NH1	10:L:54:ARG:HE	1.70	0.87
1:A:783:THR:HG21	1:A:796:SER:O	1.75	0.87
8:J:44:TYR:HA	8:J:47:ARG:HB3	1.55	0.87
1:A:567:LYS:HG3	1:A:568:PRO:HD2	0.89	0.87
1:A:412:ARG:HH11	1:A:412:ARG:CG	1.87	0.87
2:B:986:GLN:NE2	2:B:1022:THR:HG21	1.90	0.87
12:T:8:DT:H2''	12:T:9:DA:H8	1.39	0.87
1:A:532:ARG:HH11	1:A:532:ARG:CG	1.88	0.86
1:A:171:GLN:HG2	1:A:172:PRO:HD2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:DT:C2	13:N:7:DA:C5	2.63	0.86
2:B:175:ARG:HG3	2:B:175:ARG:NH1	1.90	0.86
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.38	0.86
13:N:5:DT:H2''	13:N:6:DT:C6	2.11	0.86
6:H:89:LEU:HD23	6:H:92:ASP:H	1.40	0.85
2:B:635:ARG:HG2	2:B:635:ARG:O	1.76	0.85
2:B:63:ILE:O	2:B:67:SER:HB2	1.77	0.85
1:A:901:LEU:H	1:A:926:GLN:HE21	1.20	0.85
13:N:5:DT:H2'	13:N:6:DT:H71	1.57	0.85
1:A:630:ILE:HD12	1:A:630:ILE:N	1.92	0.85
1:A:567:LYS:CB	1:A:568:PRO:CD	2.55	0.84
12:T:6:DC:C2	12:T:7:DA:C8	2.66	0.84
13:N:13:DA:OP2	13:N:13:DA:C8	2.30	0.84
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.57	0.84
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.06	0.84
1:A:412:ARG:HG3	1:A:412:ARG:NH1	1.88	0.84
2:B:1051:THR:HG22	2:B:1054:GLY:H	1.42	0.84
13:N:12:DT:H2''	13:N:13:DA:OP2	1.75	0.84
1:A:567:LYS:CG	1:A:568:PRO:CD	2.47	0.83
12:T:6:DC:H2''	12:T:7:DA:OP2	1.77	0.83
3:C:54:ASN:OD1	3:C:56:THR:HB	1.79	0.83
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.43	0.83
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.09	0.82
1:A:821:ARG:O	1:A:825:ILE:HG12	1.79	0.82
1:A:902:LEU:HD11	1:A:926:GLN:HG3	1.60	0.82
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.44	0.82
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.62	0.82
1:A:50:ILE:HG22	1:A:52:GLY:H	1.44	0.82
1:A:1116:LEU:CD1	1:A:1329:THR:HG23	2.08	0.82
2:B:732:SER:HB2	2:B:734:HIS:NE2	1.94	0.82
1:A:472:LEU:O	1:A:475:THR:HB	1.79	0.81
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.91	0.81
8:J:23:ASN:HB3	8:J:27:GLU:OE2	1.80	0.81
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.28	0.81
3:C:73:GLN:NE2	3:C:75:MET:H	1.76	0.81
3:C:37:MET:HA	3:C:41:ILE:HD11	1.61	0.81
3:C:73:GLN:HE21	3:C:75:MET:N	1.76	0.81
13:N:1:DG:H2''	13:N:2:DT:H71	1.58	0.81
1:A:265:LYS:C	1:A:267:ALA:H	1.86	0.80
1:A:55:ASP:O	1:A:56:PRO:C	2.22	0.80
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:H	2:B:231:PRO:CD	1.95	0.80
2:B:747:MET:HA	2:B:747:MET:CE	2.08	0.80
1:A:261:ASP:OD2	1:A:323:LYS:HD2	1.82	0.80
12:T:6:DC:H1'	12:T:7:DA:C8	2.18	0.79
1:A:902:LEU:CD1	1:A:926:GLN:HG3	2.12	0.79
2:B:378:LEU:O	2:B:382:ILE:HG12	1.82	0.79
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.65	0.79
1:A:315:LEU:CB	1:A:316:GLN:HA	2.11	0.79
2:B:778:MET:HE1	2:B:853:SER:HB3	1.62	0.79
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.12	0.79
1:A:320:ARG:HG3	1:A:320:ARG:NH1	1.91	0.79
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.12	0.79
13:N:5:DT:C2'	13:N:6:DT:H71	2.12	0.79
1:A:115:LEU:HD22	1:A:119:ASN:HB2	1.65	0.79
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.17	0.79
13:N:6:DT:O2	13:N:7:DA:C5	2.36	0.79
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.19	0.78
6:H:89:LEU:CD2	6:H:92:ASP:H	1.96	0.78
7:I:92:ARG:HG2	7:I:93:LYS:H	1.47	0.78
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.63	0.78
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.63	0.78
1:A:53:LEU:HD23	1:A:54:ASN:N	1.98	0.78
1:A:567:LYS:CB	6:H:96:VAL:H	1.92	0.78
1:A:630:ILE:H	1:A:630:ILE:CD1	1.97	0.78
13:N:5:DT:H2'	13:N:6:DT:C7	2.14	0.78
13:N:6:DT:C2	13:N:7:DA:C6	2.71	0.78
4:E:116:ILE:CG2	4:E:121:MET:HG3	2.15	0.77
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.46	0.77
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.67	0.77
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.30	0.77
1:A:215:SER:C	1:A:217:LYS:H	1.92	0.77
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.67	0.76
1:A:296:LEU:HG	1:A:296:LEU:O	1.83	0.76
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.67	0.76
1:A:855:THR:CG2	1:A:857:ARG:HE	1.97	0.76
1:A:1322:ILE:HG12	1:A:1323:ASP:N	2.00	0.76
2:B:644:GLU:HA	2:B:644:GLU:OE1	1.84	0.76
2:B:778:MET:CE	2:B:853:SER:HB3	2.14	0.76
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.50	0.76
1:A:315:LEU:HB3	1:A:316:GLN:CA	2.14	0.76
8:J:7:CYS:HA	8:J:49:MET:HG2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:4:DG:C2	13:N:5:DT:N1	2.54	0.76
1:A:741:ASN:HD22	1:A:744:LYS:H	1.31	0.76
4:E:19:VAL:O	4:E:23:VAL:HG23	1.86	0.76
1:A:114:LEU:O	1:A:115:LEU:HG	1.86	0.76
2:B:590:HIS:HD2	2:B:596:LEU:HD22	1.50	0.75
7:I:8:ARG:O	7:I:9:ASP:HB2	1.85	0.75
13:N:13:DA:H2"	13:N:14:DG:C8	2.20	0.75
2:B:515:HIS:HD2	2:B:517:THR:H	1.34	0.75
1:A:67:CYS:O	1:A:68:GLN:HG3	1.87	0.75
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.26	0.75
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.17	0.75
9:K:65:HIS:HD2	9:K:67:PHE:H	1.30	0.75
5:F:85:MET:HE1	5:F:148:VAL:HG13	1.69	0.75
1:A:1383:SER:O	1:A:1388:GLY:HA3	1.86	0.75
2:B:100:PRO:O	2:B:101:MET:HG3	1.86	0.74
2:B:641:GLU:HB3	2:B:643:ASP:OD1	1.87	0.74
3:C:123:ASN:HD21	3:C:125:MET:HB3	1.52	0.74
7:I:92:ARG:HG2	7:I:93:LYS:N	2.00	0.74
1:A:882:SER:HB3	1:A:953:ASN:OD1	1.88	0.74
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.70	0.74
2:B:241:ARG:HA	2:B:253:THR:HG22	1.69	0.74
12:T:6:DC:N1	12:T:7:DA:N7	2.35	0.74
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.52	0.74
2:B:313:MET:HE2	2:B:390:LEU:HG	1.69	0.74
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.17	0.74
6:H:63:LEU:C	6:H:90:ALA:HB3	2.12	0.74
1:A:961:ARG:HB3	1:A:961:ARG:NH1	2.01	0.74
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.21	0.74
1:A:108:MET:O	1:A:109:HIS:HB2	1.87	0.74
1:A:1206:ASP:H	1:A:1274:ARG:HH12	1.34	0.74
4:E:147:HIS:HD2	4:E:149:LEU:H	1.35	0.73
1:A:961:ARG:HH11	1:A:961:ARG:CB	1.99	0.73
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.23	0.73
2:B:1103:ILE:O	2:B:1103:ILE:HG22	1.86	0.73
3:C:148:ARG:HG2	3:C:149:LYS:N	2.02	0.73
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.70	0.73
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.68	0.73
1:A:596:THR:O	1:A:598:LEU:N	2.22	0.73
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.23	0.73
1:A:1435:PRO:O	1:A:1436:ILE:HD12	1.89	0.73
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.69	0.73
8:J:8:PHE:H	8:J:49:MET:HE3	1.53	0.73
1:A:1129:GLU:HA	1:A:1132:LYS:HE2	1.71	0.73
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.17	0.73
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.71	0.73
2:B:29:ASP:OD2	2:B:655:LYS:HE2	1.89	0.73
6:H:2:SER:O	6:H:3:ASN:HB2	1.88	0.73
1:A:68:GLN:HE21	1:A:70:CYS:HB3	1.54	0.72
1:A:317:LYS:O	12:T:28:DT:H4'	1.89	0.72
1:A:1430:LEU:O	2:B:1196:ILE:HG22	1.88	0.72
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.23	0.72
1:A:869:GLY:O	4:E:204:THR:HG21	1.90	0.72
1:A:709:THR:HB	1:A:712:GLU:H	1.54	0.72
2:B:516:ASN:H	2:B:516:ASN:HD22	1.36	0.72
6:H:63:LEU:C	6:H:90:ALA:CB	2.62	0.72
12:T:6:DC:C1'	12:T:7:DA:C8	2.72	0.72
1:A:553:VAL:HG23	1:A:652:VAL:CG2	2.20	0.72
2:B:485:ARG:HH11	2:B:485:ARG:CG	2.02	0.72
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.71	0.72
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.70	0.72
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.52	0.72
2:B:881:ASN:HA	2:B:883:LEU:HD23	1.72	0.72
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.72
2:B:345:LYS:O	2:B:348:ARG:HG2	1.89	0.72
2:B:428:ILE:HG13	2:B:448:ILE:HD13	1.71	0.72
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.71	0.71
12:T:8:DT:O4	13:N:7:DA:N1	2.23	0.71
1:A:423:ASP:O	1:A:424:ILE:CB	2.32	0.71
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.69	0.71
13:N:1:DG:C2'	13:N:2:DT:H73	2.19	0.71
13:N:4:DG:C1'	13:N:5:DT:H5''	2.20	0.71
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.73	0.71
7:I:5:ARG:HD3	7:I:36:GLU:OE2	1.90	0.71
12:T:9:DA:C2	13:N:7:DA:C2	2.78	0.71
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.71
3:C:148:ARG:HG2	3:C:149:LYS:H	1.55	0.71
12:T:7:DA:N1	12:T:8:DT:C4	2.59	0.71
1:A:214:ILE:HG22	1:A:215:SER:N	1.99	0.71
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.72	0.71
1:A:567:LYS:HE2	6:H:97:MET:HG2	1.72	0.71
2:B:1187:ASN:HD21	2:B:1190:ASP:H	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:6:DT:N3	13:N:7:DA:N6	2.38	0.71
1:A:1029:ARG:HH11	1:A:1029:ARG:HG2	1.55	0.70
2:B:25:ILE:CG2	2:B:29:ASP:HB2	2.20	0.70
13:N:4:DG:N1	13:N:5:DT:C4	2.60	0.70
1:A:922:ASP:O	1:A:923:LEU:HG	1.92	0.70
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.72	0.70
1:A:532:ARG:HH11	1:A:532:ARG:HG2	1.56	0.70
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.73	0.70
12:T:1:DC:C2'	12:T:2:DT:OP2	2.30	0.70
2:B:789:MET:HE2	2:B:965:LYS:HB2	1.73	0.70
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.55	0.70
1:A:726:ARG:HG2	1:A:726:ARG:O	1.90	0.70
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.25	0.70
3:C:69:LEU:HB2	8:J:5:VAL:CG1	2.21	0.70
3:C:32:SER:O	3:C:36:VAL:HG23	1.91	0.69
3:C:56:THR:CG2	3:C:58:LEU:H	2.05	0.69
1:A:86:LEU:HD12	1:A:236:LEU:O	1.91	0.69
2:B:744:HIS:HD2	2:B:746:SER:N	1.84	0.69
1:A:650:GLN:O	1:A:654:ASN:HB2	1.92	0.69
1:A:1029:ARG:HG2	1:A:1029:ARG:NH1	2.06	0.69
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.74	0.69
4:E:116:ILE:HG21	4:E:121:MET:HG3	1.75	0.69
2:B:167:ILE:HD13	2:B:167:ILE:N	2.07	0.69
12:T:6:DC:N1	12:T:7:DA:C8	2.60	0.69
1:A:134:ARG:HD3	1:A:221:SER:O	1.92	0.69
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.73	0.69
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.56	0.69
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.56	0.68
3:C:142:VAL:H	8:J:16:ASP:HB3	1.58	0.68
3:C:66:ARG:NH2	8:J:3:VAL:O	2.26	0.68
4:E:72:PHE:CE2	4:E:157:SER:HB3	2.28	0.68
1:A:64:ASN:O	1:A:66:LYS:N	2.27	0.68
1:A:711:ARG:HG2	7:I:97:MET:HE3	1.74	0.68
1:A:1206:ASP:H	1:A:1274:ARG:NH1	1.90	0.68
1:A:55:ASP:O	1:A:57:ARG:N	2.25	0.68
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.59	0.68
4:E:55:ARG:C	4:E:57:MET:H	2.00	0.68
6:H:131:ASN:C	6:H:133:ASN:H	2.02	0.68
1:A:91:PHE:HB2	1:A:297:GLN:OE1	1.94	0.68
1:A:260:ASP:OD1	1:A:261:ASP:N	2.25	0.68
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:H	1:A:926:GLN:NE2	1.92	0.68
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.94	0.68
6:H:89:LEU:C	6:H:91:ASP:H	2.02	0.68
13:N:9:DG:H2"	13:N:10:DG:C8	2.29	0.68
1:A:399:HIS:O	1:A:401:GLY:N	2.27	0.68
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.76	0.68
1:A:1437:GLY:O	1:A:1439:GLY:N	2.27	0.68
13:N:2:DT:H2"	13:N:3:DG:C8	2.28	0.68
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.76	0.68
2:B:476:ARG:O	2:B:478:GLY:N	2.26	0.68
1:A:50:ILE:HG22	1:A:52:GLY:N	2.09	0.67
13:N:4:DG:N1	13:N:5:DT:N3	2.41	0.67
1:A:90:VAL:HB	1:A:297:GLN:NE2	2.09	0.67
3:C:99:LEU:HD23	3:C:99:LEU:N	2.08	0.67
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.74	0.67
1:A:1189:SER:OG	1:A:1190:PRO:HD2	1.94	0.67
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.59	0.67
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.28	0.67
1:A:532:ARG:HH11	1:A:532:ARG:HG3	1.58	0.67
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.24	0.67
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.77	0.67
1:A:70:CYS:HA	2:B:1174:LYS:HD3	1.77	0.67
1:A:256:GLN:HB3	1:A:257:ARG:HD2	1.77	0.67
2:B:640:VAL:HG12	2:B:640:VAL:O	1.93	0.67
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.95	0.67
2:B:211:VAL:O	2:B:480:SER:HA	1.93	0.67
13:N:4:DG:C5	13:N:5:DT:C5	2.83	0.67
13:N:9:DG:H2"	13:N:10:DG:N7	2.09	0.67
1:A:53:LEU:CD2	1:A:54:ASN:H	2.03	0.67
1:A:1397:LEU:HB2	1:A:1426:GLU:OE2	1.94	0.67
2:B:473:MET:C	2:B:475:SER:H	2.02	0.67
4:E:147:HIS:CD2	4:E:149:LEU:H	2.12	0.67
2:B:843:GLN:HB2	2:B:993:THR:HB	1.77	0.66
2:B:880:THR:CG2	2:B:880:THR:O	2.43	0.66
1:A:542:GLU:OE1	1:A:569:LYS:NZ	2.28	0.66
1:A:609:ASP:O	1:A:611:GLN:N	2.28	0.66
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.28	0.66
7:I:111:THR:CG2	7:I:113:ASP:HB3	2.25	0.66
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.25	0.66
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.77	0.66
1:A:1206:ASP:N	1:A:1274:ARG:HH12	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.21	0.66
13:N:6:DT:N3	13:N:7:DA:C6	2.64	0.66
1:A:1029:ARG:O	1:A:1033:GLN:HB2	1.96	0.66
2:B:470:LYS:O	2:B:471:LYS:HG3	1.96	0.66
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.94	0.66
12:T:6:DC:H1'	12:T:7:DA:H8	1.59	0.66
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.27	0.65
2:B:1028:GLU:O	2:B:1032:SER:HB2	1.95	0.65
3:C:56:THR:HG22	3:C:58:LEU:H	1.59	0.65
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.77	0.65
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.78	0.65
2:B:230:ALA:H	2:B:231:PRO:HD3	1.60	0.65
1:A:1116:LEU:H	1:A:1308:THR:HB	1.61	0.65
2:B:365:THR:HG23	2:B:367:LEU:H	1.61	0.65
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.16	0.65
1:A:6:TYR:HD2	1:A:7:SER:N	1.94	0.65
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.77	0.65
1:A:470:LEU:HD21	1:A:487:MET:CE	2.25	0.65
1:A:1438:THR:H	5:F:88:TYR:HB3	1.60	0.65
2:B:482:VAL:C	2:B:483:LEU:O	2.36	0.65
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.78	0.65
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.97	0.65
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.79	0.65
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.79	0.65
1:A:1341:ILE:HG22	4:E:182:ASP:OD2	1.95	0.65
2:B:299:GLU:OE2	2:B:571:PRO:HD2	1.97	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.79	0.65
1:A:1036:ARG:HG3	1:A:1036:ARG:HH11	1.62	0.65
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.31	0.64
2:B:282:ILE:HD12	2:B:382:ILE:HD12	1.79	0.64
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.79	0.64
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.26	0.64
6:H:89:LEU:O	6:H:91:ASP:N	2.30	0.64
3:C:222:LYS:HA	3:C:222:LYS:CE	2.21	0.64
1:A:537:ARG:HD3	6:H:120:GLY:O	1.96	0.64
1:A:809:THR:HB	1:A:810:PRO:HD2	1.78	0.64
2:B:770:GLN:CG	2:B:770:GLN:O	2.45	0.64
2:B:955:THR:HG23	10:L:54:ARG:O	1.96	0.64
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.62	0.64
2:B:25:ILE:HG22	2:B:26:THR:N	2.12	0.64
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.61	0.64
7:I:8:ARG:O	7:I:9:ASP:CB	2.45	0.64
13:N:4:DG:C4	13:N:5:DT:C6	2.85	0.64
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.64
1:A:567:LYS:NZ	6:H:95:TYR:CZ	2.59	0.64
1:A:1156:PRO:O	1:A:1158:PRO:HD3	1.98	0.64
1:A:351:THR:HG22	1:A:352:VAL:H	1.63	0.64
1:A:928:LEU:O	1:A:931:GLU:HB3	1.98	0.64
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.80	0.64
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	1.98	0.64
2:B:167:ILE:O	2:B:168:GLY:O	2.15	0.64
12:T:6:DC:C2	12:T:7:DA:C5	2.86	0.64
1:A:353:ILE:HD13	1:A:487:MET:CE	2.28	0.63
3:C:123:ASN:ND2	3:C:125:MET:HB3	2.13	0.63
2:B:647:GLY:C	2:B:648:HIS:ND1	2.57	0.63
2:B:822:ASN:O	8:J:48:ARG:NH1	2.31	0.63
4:E:96:PHE:C	4:E:98:ILE:H	2.07	0.63
1:A:265:LYS:C	1:A:267:ALA:N	2.55	0.63
2:B:864:LYS:HD2	2:B:865:LYS:N	2.13	0.63
1:A:870:GLU:OE1	4:E:202:SER:HB2	1.98	0.63
2:B:482:VAL:O	2:B:483:LEU:O	2.16	0.63
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.80	0.63
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.80	0.63
1:A:532:ARG:CG	1:A:532:ARG:NH1	2.55	0.63
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.79	0.63
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.80	0.63
2:B:770:GLN:O	2:B:770:GLN:HG3	1.98	0.63
1:A:114:LEU:HD12	1:A:145:LYS:HB3	1.80	0.63
1:A:874:ASP:HB2	1:A:1058:VAL:HG23	1.81	0.63
1:A:1173:HIS:O	1:A:1174:PHE:HB3	1.99	0.63
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.80	0.63
8:J:46:CYS:SG	14:J:101:ZN:ZN	1.85	0.63
1:A:1140:HIS:HB2	1:A:1276:VAL:O	1.99	0.63
1:A:215:SER:C	1:A:217:LYS:N	2.57	0.62
2:B:732:SER:CB	2:B:734:HIS:CD2	2.82	0.62
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.80	0.62
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.81	0.62
2:B:363:HIS:O	2:B:364:ILE:CB	2.45	0.62
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.98	0.62
1:A:261:ASP:HB3	1:A:323:LYS:HG3	1.82	0.62
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ASN:H	2:B:516:ASN:ND2	1.97	0.62
1:A:567:LYS:CE	6:H:97:MET:HG2	2.29	0.62
1:A:768:GLN:CG	1:A:816:HIS:HA	2.29	0.62
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.64	0.62
6:H:89:LEU:CD2	6:H:92:ASP:N	2.62	0.62
13:N:4:DG:N3	13:N:5:DT:C6	2.67	0.62
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.30	0.62
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.25	0.62
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.64	0.62
6:H:83:GLN:HB3	6:H:86:ASP:OD1	2.00	0.62
12:T:6:DC:C2'	12:T:7:DA:OP2	2.48	0.62
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.15	0.61
1:A:795:GLU:HG3	2:B:731:VAL:HG11	1.82	0.61
13:N:4:DG:N2	13:N:5:DT:O2	2.33	0.61
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.00	0.61
1:A:320:ARG:HH11	1:A:320:ARG:CG	2.02	0.61
1:A:369:SER:HB3	9:K:2:ASN:OD1	1.99	0.61
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.36	0.61
2:B:708:GLU:O	2:B:710:LEU:N	2.33	0.61
2:B:880:THR:O	2:B:880:THR:HG23	1.99	0.61
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.66	0.61
1:A:57:ARG:CA	1:A:68:GLN:HB3	2.30	0.61
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.49	0.61
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.35	0.61
2:B:879:ARG:HG2	2:B:880:THR:N	2.15	0.61
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.65	0.61
12:T:2:DT:OP2	12:T:2:DT:H71	2.00	0.61
6:H:26:ILE:O	6:H:39:THR:HA	2.00	0.61
1:A:508:PRO:O	1:A:511:ILE:HG13	2.00	0.61
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	2.16	0.61
2:B:708:GLU:O	2:B:709:ASP:C	2.44	0.61
2:B:751:VAL:CG1	2:B:752:ALA:N	2.63	0.61
2:B:789:MET:HE2	2:B:965:LYS:CB	2.30	0.61
3:C:74:SER:O	3:C:77:ILE:HB	2.01	0.61
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.82	0.61
2:B:422:LYS:O	2:B:425:THR:HG22	2.01	0.61
12:T:7:DA:H2''	12:T:8:DT:H5''	1.82	0.61
1:A:106:VAL:HG21	1:A:214:ILE:HD12	1.81	0.60
1:A:331:GLY:O	1:A:332:LYS:HB3	1.99	0.60
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.60
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:145:ARG:HD2	6:H:146:ARG:HD2	1.83	0.60
1:A:901:LEU:N	1:A:926:GLN:HE21	1.95	0.60
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.83	0.60
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.50	0.60
1:A:283:GLY:O	1:A:285:PRO:HD3	2.02	0.60
1:A:399:HIS:O	1:A:400:PRO:C	2.41	0.60
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.83	0.60
7:I:111:THR:CG2	7:I:113:ASP:H	2.12	0.60
13:N:1:DG:H2'	13:N:2:DT:H73	1.82	0.60
2:B:864:LYS:HD3	2:B:870:ILE:O	2.02	0.60
1:A:53:LEU:HD11	1:A:266:LEU:O	2.01	0.60
2:B:173:MET:O	2:B:176:SER:HB3	2.02	0.60
2:B:797:TYR:O	8:J:1:MET:HG3	2.01	0.60
2:B:570:VAL:HG21	2:B:573:GLN:HE21	1.67	0.60
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.66	0.60
4:E:179:GLN:O	4:E:182:ASP:HB2	2.01	0.60
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.83	0.59
1:A:715:GLU:O	1:A:719:VAL:HG23	2.02	0.59
2:B:234:ILE:HG21	2:B:257:LYS:HD3	1.85	0.59
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.83	0.59
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.83	0.59
1:A:1256:GLU:HA	1:A:1259:MET:HB2	1.85	0.59
1:A:809:THR:HB	1:A:810:PRO:CD	2.32	0.59
1:A:858:ASN:HD22	1:A:860:LEU:H	1.50	0.59
2:B:185:THR:O	2:B:188:ASP:HB2	2.01	0.59
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.84	0.59
3:C:3:GLU:HG3	3:C:4:GLU:N	2.17	0.59
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.67	0.59
12:T:8:DT:H3	13:N:7:DA:H2	1.46	0.59
13:N:4:DG:C2	13:N:5:DT:C6	2.91	0.59
2:B:313:MET:CE	2:B:390:LEU:HG	2.33	0.59
4:E:100:ILE:O	4:E:101:GLN:C	2.45	0.59
5:F:110:ASP:O	5:F:111:LEU:C	2.46	0.59
2:B:373:ARG:HD2	2:B:566:LEU:HD23	1.85	0.59
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.36	0.59
8:J:57:ILE:O	8:J:61:LEU:HG	2.01	0.59
1:A:503:GLN:HE22	5:F:90:ARG:NH2	1.99	0.59
2:B:953:LEU:HD11	10:L:55:ILE:HG22	1.85	0.59
3:C:260:LEU:HG	3:C:264:GLN:HE21	1.67	0.59
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.17	0.59
13:N:1:DG:C2'	13:N:2:DT:H71	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:HB	1:A:184:SER:HB3	1.84	0.58
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.84	0.58
1:A:995:GLU:OE2	1:A:995:GLU:HA	2.01	0.58
2:B:322:PHE:CZ	7:I:30:ARG:HG2	2.37	0.58
2:B:1081:LEU:O	3:C:189:THR:HG23	2.03	0.58
4:E:13:TRP:O	4:E:16:PHE:HB3	2.03	0.58
4:E:135:PHE:CD2	4:E:140:LEU:HD21	2.38	0.58
5:F:109:VAL:HG22	5:F:124:GLU:HG3	1.85	0.58
12:T:12:DC:H2''	12:T:13:DA:C8	2.37	0.58
2:B:747:MET:HE3	2:B:747:MET:CA	2.14	0.58
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.34	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.29	0.58
8:J:16:ASP:OD1	8:J:17:LYS:HG2	2.04	0.58
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.86	0.58
6:H:83:GLN:O	6:H:87:ARG:HG3	2.03	0.58
7:I:47:GLU:OE1	7:I:50:THR:HG22	2.02	0.58
13:N:1:DG:C2'	13:N:2:DT:C5	2.76	0.58
1:A:261:ASP:HB3	1:A:323:LYS:CG	2.33	0.58
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.19	0.58
1:A:215:SER:O	1:A:217:LYS:N	2.37	0.58
2:B:882:THR:H	2:B:883:LEU:HB3	1.67	0.58
2:B:1166:CYS:O	2:B:1215:ARG:HD3	2.04	0.58
12:T:8:DT:C4	13:N:7:DA:N1	2.72	0.58
13:N:6:DT:H1'	13:N:7:DA:C8	2.38	0.58
1:A:317:LYS:HB3	12:T:28:DT:O3'	2.04	0.58
1:A:532:ARG:HG3	1:A:532:ARG:NH1	2.14	0.58
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.04	0.58
4:E:127:ILE:O	4:E:127:ILE:HG12	2.04	0.58
1:A:563:PRO:HB2	1:A:565:ILE:O	2.04	0.57
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.37	0.57
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.87	0.57
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.39	0.57
7:I:111:THR:HG21	7:I:113:ASP:HB3	1.86	0.57
12:T:3:DA:H8	12:T:3:DA:OP2	1.87	0.57
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.33	0.57
2:B:778:MET:CE	2:B:853:SER:CB	2.83	0.57
3:C:184:ASN:OD1	3:C:187:LYS:HA	2.04	0.57
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.33	0.57
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.39	0.57
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.04	0.57
2:B:249:ARG:HG3	2:B:251:ILE:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.37	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.18	0.57
2:B:899:ILE:HG22	2:B:900:ALA:N	2.20	0.57
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.40	0.57
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.39	0.57
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.87	0.57
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.87	0.57
6:H:131:ASN:O	6:H:133:ASN:N	2.36	0.57
1:A:307:ASP:O	1:A:308:ILE:C	2.48	0.57
1:A:332:LYS:H	1:A:337:ARG:HB2	1.69	0.57
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.57
1:A:304:MET:O	1:A:324:SER:HB2	2.05	0.57
1:A:365:GLY:O	1:A:468:PHE:HA	2.05	0.57
2:B:122:LEU:CD2	2:B:958:GLN:HB2	2.35	0.57
2:B:332:ASP:C	2:B:334:ILE:H	2.12	0.57
2:B:1082:MET:O	3:C:189:THR:HG22	2.05	0.57
1:A:211:PHE:O	1:A:214:ILE:HG12	2.05	0.56
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.87	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.87	0.56
2:B:996:ARG:HH22	3:C:173:ALA:HB1	1.71	0.56
8:J:24:LEU:HB3	8:J:30:LEU:HD12	1.86	0.56
1:A:780:VAL:CG2	2:B:699:GLU:OE2	2.48	0.56
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.05	0.56
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.69	0.56
3:C:185:LYS:NZ	3:C:211:ASP:O	2.31	0.56
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.87	0.56
7:I:120:GLN:OE1	7:I:120:GLN:HA	2.05	0.56
12:T:7:DA:OP2	12:T:7:DA:H8	1.89	0.56
1:A:1338:VAL:HG12	1:A:1339:LEU:HD23	1.88	0.56
1:A:40:THR:HG21	1:A:259:GLU:CD	2.31	0.56
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.88	0.56
2:B:37:PHE:O	2:B:38:PHE:HB2	2.06	0.56
2:B:1096:ARG:O	2:B:1097:HIS:CD2	2.59	0.56
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.88	0.56
2:B:65:GLU:N	2:B:67:SER:HB3	2.21	0.56
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.56
2:B:1065:GLN:NE2	2:B:1069:PHE:HD1	2.03	0.56
1:A:541:ILE:N	1:A:541:ILE:HD12	2.20	0.56
6:H:44:VAL:O	6:H:44:VAL:CG1	2.53	0.56
7:I:111:THR:HG22	7:I:113:ASP:N	2.11	0.56
12:T:11:DC:C5	12:T:12:DC:N4	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:O	2:B:691:GLU:O	2.24	0.56
4:E:117:THR:O	4:E:119:SER:N	2.39	0.56
6:H:17:PRO:O	6:H:19:ARG:N	2.38	0.56
1:A:424:ILE:HG22	1:A:424:ILE:O	2.05	0.56
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.40	0.56
2:B:58:THR:O	2:B:62:ILE:HG12	2.04	0.56
2:B:278:GLN:HG2	2:B:279:ASP:H	1.70	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.04	0.56
6:H:89:LEU:C	6:H:91:ASP:N	2.63	0.56
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.41	0.56
1:A:401:GLY:C	1:A:435:HIS:CD2	2.84	0.56
1:A:596:THR:C	1:A:598:LEU:H	2.14	0.56
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.40	0.56
4:E:64:PRO:CD	4:E:76:GLY:HA2	2.36	0.55
12:T:6:DC:C6	12:T:7:DA:N7	2.74	0.55
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.36	0.55
13:N:4:DG:C4	13:N:5:DT:C5	2.94	0.55
1:A:345:VAL:HB	2:B:1154:ALA:HB1	1.87	0.55
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.06	0.55
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.71	0.55
1:A:709:THR:HG23	7:I:94:ASP:HA	1.88	0.55
1:A:907:THR:HG22	1:A:908:LEU:N	2.21	0.55
5:F:132:LEU:O	5:F:148:VAL:HG23	2.07	0.55
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.40	0.55
1:A:381:THR:HG23	1:A:383:TYR:H	1.72	0.55
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.88	0.55
2:B:642:ASP:HA	2:B:649:LYS:HA	1.89	0.55
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.42	0.55
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.70	0.55
1:A:754:SER:N	1:A:757:ASN:HD22	2.04	0.55
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.89	0.55
5:F:73:ALA:O	5:F:74:ILE:HG12	2.06	0.55
6:H:109:LYS:NZ	6:H:111:LEU:HD12	2.20	0.55
2:B:203:PHE:CE1	2:B:212:LEU:HD12	2.41	0.55
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.88	0.55
4:E:116:ILE:HG22	4:E:121:MET:HG3	1.85	0.55
7:I:15:TYR:CE1	7:I:30:ARG:HD3	2.41	0.55
7:I:47:GLU:OE1	7:I:50:THR:CG2	2.54	0.55
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.87	0.55
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:C	2:B:30:SER:H	2.14	0.55
3:C:251:LEU:O	3:C:255:VAL:HG23	2.07	0.55
13:N:4:DG:C6	13:N:5:DT:C5	2.95	0.55
2:B:541:LEU:HD12	2:B:747:MET:CE	2.26	0.55
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.41	0.55
4:E:54:GLN:HA	4:E:54:GLN:OE1	2.05	0.55
1:A:244:PRO:O	1:A:246:VAL:N	2.39	0.54
6:H:106:GLU:C	6:H:108:SER:H	2.14	0.54
1:A:50:ILE:C	1:A:52:GLY:H	2.15	0.54
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.37	0.54
12:T:6:DC:C4	12:T:7:DA:N6	2.75	0.54
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.89	0.54
2:B:315:LYS:CG	7:I:13:MET:HE1	2.38	0.54
1:A:265:LYS:O	1:A:267:ALA:N	2.40	0.54
1:A:574:GLY:O	1:A:577:ILE:HD12	2.06	0.54
1:A:786:HIS:HE1	2:B:742:GLU:OE1	1.91	0.54
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.88	0.54
6:H:108:SER:O	6:H:109:LYS:HB2	2.07	0.54
13:N:6:DT:O2	13:N:7:DA:C4	2.60	0.54
1:A:86:LEU:HD13	1:A:90:VAL:HG22	1.89	0.54
1:A:361:LEU:HD22	1:A:646:PHE:CD1	2.43	0.54
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.90	0.54
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.07	0.54
12:T:2:DT:O2	13:N:13:DA:N1	2.40	0.54
1:A:424:ILE:O	1:A:424:ILE:CG2	2.54	0.54
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.72	0.54
1:A:56:PRO:O	1:A:58:LEU:N	2.41	0.54
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.90	0.54
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.23	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.20	0.54
7:I:92:ARG:CG	7:I:93:LYS:H	2.20	0.54
12:T:7:DA:N1	12:T:8:DT:O4	2.40	0.54
2:B:322:PHE:HZ	7:I:30:ARG:HG2	1.72	0.54
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.37	0.54
1:A:364:VAL:O	1:A:364:VAL:HG13	2.06	0.54
1:A:984:LYS:O	1:A:988:LEU:HB3	2.08	0.54
2:B:473:MET:O	2:B:475:SER:N	2.41	0.54
12:T:6:DC:C1'	12:T:7:DA:H8	2.17	0.54
1:A:67:CYS:C	1:A:68:GLN:HG3	2.33	0.53
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.23	0.53
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLY:O	3:C:142:VAL:HB	2.07	0.53
1:A:315:LEU:HD12	1:A:319:GLY:O	2.07	0.53
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.38	0.53
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.92	0.53
1:A:608:ILE:O	1:A:609:ASP:O	2.26	0.53
1:A:1230:GLU:O	1:A:1233:ASP:HB2	2.08	0.53
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.43	0.53
3:C:56:THR:HG22	3:C:58:LEU:N	2.22	0.53
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.53
1:A:151:ASP:CG	1:A:163:SER:HA	2.34	0.53
1:A:305:ASP:HA	1:A:326:ARG:HB2	1.90	0.53
1:A:44:THR:HG22	1:A:44:THR:O	2.08	0.53
1:A:335:ARG:O	1:A:335:ARG:HG3	2.09	0.53
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.23	0.53
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.61	0.53
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.39	0.53
13:N:6:DT:H2''	13:N:7:DA:OP2	2.09	0.53
1:A:218:ASP:O	1:A:222:LEU:HG	2.09	0.53
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.90	0.53
2:B:36:ALA:C	2:B:37:PHE:O	2.42	0.53
9:K:21:ILE:HG12	9:K:33:ILE:HG12	1.91	0.53
13:N:6:DT:C4	13:N:7:DA:N6	2.77	0.53
2:B:65:GLU:H	2:B:67:SER:HB3	1.73	0.53
2:B:1109:GLY:O	2:B:1111:MET:HE2	2.09	0.53
13:N:5:DT:C2'	13:N:6:DT:C7	2.81	0.53
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.90	0.53
4:E:55:ARG:O	4:E:57:MET:N	2.42	0.53
12:T:3:DA:N1	13:N:12:DT:C4	2.77	0.53
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.38	0.52
2:B:637:LEU:HD13	2:B:740:HIS:HB3	1.91	0.52
2:B:751:VAL:HG13	2:B:752:ALA:N	2.23	0.52
4:E:32:GLN:HE21	4:E:32:GLN:HA	1.74	0.52
12:T:2:DT:H2'	12:T:3:DA:H8	1.65	0.52
1:A:550:LEU:HD11	1:A:580:VAL:HG21	1.90	0.52
6:H:83:GLN:O	6:H:86:ASP:HB3	2.10	0.52
12:T:21:DC:H2''	12:T:22:DT:H5'	1.90	0.52
1:A:577:ILE:HD12	1:A:578:LEU:H	1.73	0.52
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.92	0.52
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.91	0.52
8:J:1:MET:N	8:J:57:ILE:H	2.07	0.52
1:A:77:CYS:C	1:A:79:GLY:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:7:A:H2'	11:R:8:G:O4'	2.10	0.52
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.92	0.52
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.91	0.52
2:B:487:THR:HG23	2:B:488:TYR:N	2.25	0.52
2:B:635:ARG:O	2:B:636:PRO:O	2.26	0.52
2:B:778:MET:HE1	2:B:853:SER:CB	2.35	0.52
4:E:156:LEU:HD23	4:E:197:LYS:HB2	1.92	0.52
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.24	0.52
2:B:325:GLN:NE2	7:I:12:ASN:OD1	2.43	0.52
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.32	0.52
12:T:7:DA:OP2	12:T:7:DA:H2'	2.10	0.52
13:N:3:DG:C2'	13:N:4:DG:OP2	2.50	0.52
1:A:225:ASN:C	1:A:225:ASN:HD22	2.18	0.52
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.10	0.52
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.44	0.52
12:T:8:DT:N3	13:N:7:DA:C2	2.74	0.52
1:A:65:LEU:C	1:A:66:LYS:HG3	2.34	0.52
1:A:511:ILE:O	1:A:519:PRO:HA	2.10	0.52
1:A:855:THR:HG21	1:A:857:ARG:NE	2.11	0.52
2:B:25:ILE:HG22	2:B:26:THR:O	2.10	0.52
2:B:986:GLN:HE21	2:B:1022:THR:CG2	2.23	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.52
3:C:69:LEU:CB	8:J:5:VAL:CG1	2.88	0.52
1:A:276:LEU:HD11	1:A:293:GLU:HG2	1.92	0.51
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.25	0.51
2:B:64:CYS:O	2:B:65:GLU:CD	2.53	0.51
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.92	0.51
1:A:289:ILE:O	1:A:293:GLU:HG3	2.10	0.51
1:A:404:TYR:HA	1:A:413:ILE:O	2.11	0.51
1:A:969:GLN:C	1:A:971:PHE:H	2.18	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.91	0.51
2:B:169:ARG:HG3	2:B:454:THR:HG23	1.91	0.51
2:B:475:SER:O	2:B:476:ARG:C	2.52	0.51
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.57	0.51
2:B:487:THR:CG2	2:B:488:TYR:N	2.73	0.51
2:B:605:ARG:HH21	2:B:639:ILE:HG12	1.76	0.51
2:B:681:TRP:O	2:B:684:LEU:HB2	2.10	0.51
9:K:83:PRO:O	9:K:86:ALA:HB3	2.10	0.51
1:A:23:SER:O	1:A:26:GLU:N	2.43	0.51
1:A:1067:LEU:HD12	1:A:1067:LEU:O	2.10	0.51
1:A:1355:VAL:HG12	1:A:1356:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:LEU:HD23	2:B:381:MET:CE	2.23	0.51
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.92	0.51
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.46	0.51
9:K:37:LYS:O	9:K:38:GLU:HG2	2.11	0.51
10:L:44:ASP:O	10:L:46:VAL:N	2.43	0.51
2:B:489:SER:HA	2:B:492:LEU:HB2	1.93	0.51
1:A:24:PRO:HB3	1:A:237:THR:HB	1.92	0.51
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.92	0.51
1:A:596:THR:O	1:A:597:LEU:C	2.52	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
1:A:1423:GLY:O	1:A:1424:VAL:C	2.53	0.51
6:H:5:LEU:HD11	6:H:61:SER:HB3	1.93	0.51
7:I:60:GLN:HE21	7:I:60:GLN:HA	1.75	0.51
12:T:7:DA:C2	12:T:8:DT:C5	2.97	0.51
1:A:244:PRO:C	1:A:246:VAL:H	2.19	0.51
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.93	0.51
2:B:1072:MET:HE2	2:B:1085:ILE:CB	2.41	0.51
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.93	0.51
12:T:3:DA:C2	13:N:12:DT:N3	2.73	0.51
1:A:68:GLN:C	1:A:70:CYS:H	2.19	0.51
1:A:225:ASN:C	1:A:225:ASN:ND2	2.69	0.51
1:A:858:ASN:ND2	1:A:860:LEU:H	2.08	0.51
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.46	0.51
2:B:487:THR:H	2:B:490:SER:HB3	1.76	0.51
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.91	0.51
3:C:133:ILE:CD1	3:C:237:SER:HA	2.41	0.51
6:H:131:ASN:C	6:H:133:ASN:N	2.69	0.51
2:B:485:ARG:HG2	2:B:485:ARG:NH1	2.08	0.51
6:H:137:GLN:C	6:H:139:ASN:H	2.18	0.51
12:T:7:DA:N3	12:T:8:DT:C5	2.78	0.51
1:A:507:VAL:N	1:A:508:PRO:CD	2.73	0.51
1:A:1121:GLU:O	1:A:1124:HIS:O	2.29	0.51
6:H:2:SER:HA	6:H:62:SER:HB3	1.93	0.51
6:H:109:LYS:HB2	6:H:110:ASP:O	2.11	0.51
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.93	0.50
6:H:41:ASP:OD2	6:H:122:LEU:N	2.39	0.50
7:I:111:THR:HG22	7:I:113:ASP:HB3	1.93	0.50
13:N:12:DT:H1'	13:N:13:DA:C8	2.46	0.50
13:N:13:DA:H8	13:N:13:DA:P	2.35	0.50
1:A:276:LEU:HD13	1:A:292:ALA:O	2.11	0.50
2:B:120:ARG:CD	2:B:955:THR:HG21	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:97:VAL:HG12	4:E:97:VAL:O	2.11	0.50
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.50
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.75	0.50
2:B:398:ARG:HB3	2:B:398:ARG:NH1	2.27	0.50
6:H:131:ASN:OD1	6:H:132:LEU:N	2.42	0.50
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.92	0.50
1:A:920:LEU:HD23	1:A:921:GLY:N	2.27	0.50
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.41	0.50
1:A:256:GLN:CA	1:A:257:ARG:HB3	2.41	0.50
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.27	0.50
1:A:553:VAL:CG2	1:A:652:VAL:CG2	2.88	0.50
1:A:647:GLY:O	1:A:651:LYS:HG3	2.11	0.50
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.46	0.50
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.94	0.50
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.92	0.50
12:T:7:DA:C2	12:T:8:DT:C2	3.00	0.50
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.50
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.46	0.50
2:B:176:SER:O	2:B:182:SER:HB3	2.12	0.50
2:B:878:GLN:O	2:B:879:ARG:C	2.55	0.50
13:N:5:DT:H2"	13:N:6:DT:C5	2.46	0.50
1:A:114:LEU:HD11	1:A:171:GLN:HE21	1.77	0.50
1:A:219:PHE:O	1:A:222:LEU:N	2.43	0.50
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50
2:B:981:ALA:O	2:B:1093:GLN:HG2	2.11	0.50
5:F:79:ARG:HG2	5:F:144:GLU:HB3	1.93	0.50
12:T:14:DC:H2"	12:T:15:DC:OP2	2.12	0.50
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.93	0.50
4:E:179:GLN:HA	4:E:179:GLN:NE2	2.27	0.50
4:E:179:GLN:HE22	4:E:215:MET:HE2	1.76	0.50
1:A:65:LEU:O	1:A:66:LYS:HG3	2.11	0.50
2:B:63:ILE:O	2:B:67:SER:CB	2.55	0.50
2:B:680:THR:O	2:B:681:TRP:C	2.53	0.50
2:B:797:TYR:CE2	3:C:62:PHE:CD2	3.00	0.50
4:E:72:PHE:HE2	4:E:157:SER:HB3	1.77	0.50
8:J:48:ARG:HE	8:J:49:MET:HE2	1.77	0.50
12:T:5:DC:C4	12:T:6:DC:C4	2.99	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.36	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.20	0.49
7:I:59:VAL:HG12	7:I:61:ASP:H	1.76	0.49
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.36	0.49
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.93	0.49
1:A:560:ILE:N	6:H:78:SER:HB2	2.28	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.12	0.49
2:B:471:LYS:HD2	2:B:471:LYS:O	2.11	0.49
2:B:563:MET:HG3	2:B:563:MET:O	2.13	0.49
2:B:574:SER:HB3	2:B:591:ARG:HH22	1.78	0.49
2:B:863:GLU:OE1	2:B:962:LYS:HB3	2.12	0.49
12:T:6:DC:N3	12:T:7:DA:C5	2.79	0.49
1:A:567:LYS:HD2	6:H:95:TYR:CD1	2.48	0.49
1:A:907:THR:HG22	1:A:908:LEU:H	1.78	0.49
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.45	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.59	0.49
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.12	0.49
7:I:99:LEU:HB2	7:I:112:SER:HB3	1.93	0.49
1:A:303:TYR:O	1:A:303:TYR:CG	2.66	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.93	0.49
1:A:697:ALA:HB2	1:A:702:LEU:HD23	1.93	0.49
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.76	0.49
2:B:361:LEU:N	2:B:362:PRO:HD3	2.27	0.49
7:I:47:GLU:HG2	7:I:50:THR:HG23	1.94	0.49
13:N:4:DG:C2'	13:N:5:DT:H5''	2.42	0.49
1:A:322:VAL:C	1:A:323:LYS:HD3	2.37	0.49
1:A:350:ARG:HG3	1:A:488:ASN:OD1	2.13	0.49
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.95	0.49
2:B:487:THR:HG22	2:B:489:SER:N	2.28	0.49
7:I:33:SER:O	7:I:34:TYR:O	2.30	0.49
2:B:764:SER:O	2:B:765:PRO:C	2.55	0.49
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.95	0.49
4:E:59:SER:HB3	4:E:81:GLU:HA	1.95	0.49
1:A:103:CYS:O	1:A:174:ILE:HD12	2.13	0.49
1:A:550:LEU:HG	1:A:556:TRP:CE2	2.47	0.49
1:A:560:ILE:H	6:H:78:SER:HB2	1.78	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.76	0.49
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.94	0.49
2:B:906:SER:HA	2:B:946:ASN:HB2	1.93	0.49
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.40	0.49
2:B:487:THR:O	2:B:490:SER:HB3	2.12	0.49
6:H:109:LYS:HB3	6:H:110:ASP:CB	2.43	0.49
12:T:2:DT:C3'	12:T:3:DA:H5'	2.32	0.49
1:A:401:GLY:N	1:A:435:HIS:HD2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:SER:OG	2:B:775:LYS:HE2	2.13	0.49
8:J:1:MET:HB2	8:J:56:LEU:HD12	1.94	0.49
1:A:494:SER:O	1:A:498:ARG:HG2	2.12	0.48
1:A:605:MET:HA	1:A:605:MET:CE	2.43	0.48
1:A:977:LYS:HE3	1:A:977:LYS:HA	1.94	0.48
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.28	0.48
1:A:1386:ARG:HE	1:A:1403:GLU:HG2	1.78	0.48
2:B:197:PHE:CE1	2:B:817:LEU:HD11	2.48	0.48
2:B:254:LEU:CD2	2:B:381:MET:CE	2.87	0.48
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.48
1:A:1392:SER:O	1:A:1394:THR:N	2.46	0.48
2:B:25:ILE:CG2	2:B:26:THR:N	2.76	0.48
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.48	0.48
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.95	0.48
1:A:55:ASP:N	1:A:56:PRO:HD2	2.28	0.48
1:A:218:ASP:O	1:A:222:LEU:CD1	2.61	0.48
1:A:574:GLY:HA2	1:A:577:ILE:HD11	1.95	0.48
1:A:663:SER:HB2	2:B:827:ILE:O	2.13	0.48
1:A:836:TYR:O	1:A:837:ILE:C	2.56	0.48
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.48
2:B:519:TRP:CH2	2:B:705:MET:HE1	2.48	0.48
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.49	0.48
2:B:635:ARG:C	2:B:636:PRO:O	2.56	0.48
2:B:760:ASP:OD1	2:B:760:ASP:N	2.36	0.48
2:B:879:ARG:O	2:B:880:THR:C	2.56	0.48
6:H:91:ASP:O	6:H:92:ASP:OD2	2.31	0.48
12:T:7:DA:C4	12:T:8:DT:C5	3.01	0.48
13:N:2:DT:H2''	13:N:3:DG:O5'	2.13	0.48
1:A:260:ASP:CG	1:A:261:ASP:H	2.21	0.48
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.96	0.48
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.43	0.48
1:A:1438:THR:N	5:F:88:TYR:HB3	2.27	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.26	0.48
2:B:834:ASN:ND2	2:B:1011:ILE:HG22	2.29	0.48
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.94	0.48
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.51	0.48
2:B:1072:MET:HE2	2:B:1085:ILE:HB	1.94	0.48
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.76	0.48
1:A:546:VAL:O	1:A:550:LEU:HB2	2.12	0.48
1:A:1356:ILE:HD13	1:A:1356:ILE:N	2.28	0.48
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CZ	1:A:1064:VAL:CG2	2.97	0.48
2:B:100:PRO:C	2:B:101:MET:HG3	2.38	0.48
2:B:532:ALA:HB1	2:B:536:VAL:HG23	1.95	0.48
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.13	0.48
1:A:1110:ASN:ND2	1:A:1110:ASN:H	2.11	0.48
2:B:287:ARG:NH1	2:B:324:ILE:O	2.44	0.48
2:B:470:LYS:C	2:B:472:ALA:H	2.22	0.48
2:B:591:ARG:O	2:B:592:ASN:CB	2.61	0.48
2:B:806:THR:HG22	2:B:808:ALA:H	1.78	0.48
3:C:231:ASN:C	3:C:231:ASN:ND2	2.71	0.48
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.49	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.48
1:A:752:LYS:HD3	2:B:1019:SER:HB3	1.95	0.48
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.22	0.48
1:A:1386:ARG:NE	1:A:1403:GLU:HG2	2.28	0.48
2:B:211:VAL:CG2	2:B:483:LEU:HD23	2.43	0.48
2:B:315:LYS:HG2	7:I:13:MET:HE1	1.94	0.48
2:B:734:HIS:O	2:B:735:ALA:HB3	2.12	0.48
1:A:1159:ARG:NH1	1:A:1159:ARG:HB3	2.28	0.48
2:B:706:GLN:O	2:B:710:LEU:HB2	2.14	0.48
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.79	0.48
3:C:99:LEU:HD23	3:C:99:LEU:H	1.77	0.48
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.95	0.48
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.95	0.48
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.29	0.48
2:B:778:MET:HE3	2:B:853:SER:HB3	1.92	0.48
3:C:73:GLN:NE2	3:C:75:MET:N	2.49	0.48
3:C:262:LEU:CD1	9:K:88:LYS:HG2	2.44	0.48
1:A:567:LYS:HD2	6:H:95:TYR:CE1	2.49	0.47
1:A:629:LEU:HD22	1:A:633:VAL:HG23	1.94	0.47
1:A:871:ASP:HB3	4:E:205:SER:HB3	1.95	0.47
2:B:770:GLN:O	2:B:770:GLN:CD	2.57	0.47
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	1.95	0.47
13:N:2:DT:C2'	13:N:3:DG:C8	2.95	0.47
1:A:8:SER:HB3	2:B:1180:PHE:HE1	1.79	0.47
1:A:664:THR:HG23	1:A:742:ASN:HB2	1.95	0.47
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.28	0.47
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.96	0.47
2:B:957:ASN:CG	2:B:958:GLN:N	2.73	0.47
12:T:5:DC:C5	12:T:6:DC:C4	3.03	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:O	1:A:983:ILE:C	2.57	0.47
1:A:1312:ASN:ND2	1:A:1314:SER:OG	2.47	0.47
2:B:227:LYS:H	2:B:395:GLN:HG3	1.79	0.47
2:B:334:ILE:HG22	2:B:334:ILE:O	2.14	0.47
2:B:365:THR:HG23	2:B:367:LEU:N	2.28	0.47
1:A:96:ILE:O	1:A:97:ALA:C	2.58	0.47
1:A:108:MET:HE2	1:A:202:LEU:HD21	1.96	0.47
1:A:974:ASP:OD1	1:A:977:LYS:HB2	2.14	0.47
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.13	0.47
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.47
2:B:826:ALA:O	2:B:1011:ILE:HA	2.14	0.47
2:B:951:GLN:HG2	10:L:57:LEU:HD22	1.95	0.47
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.14	0.47
3:C:9:LYS:HB2	3:C:9:LYS:HE2	1.62	0.47
3:C:167:HIS:HD2	3:C:169:LYS:H	1.62	0.47
4:E:192:ARG:O	4:E:192:ARG:HG3	2.14	0.47
13:N:3:DG:OP2	13:N:3:DG:H2'	2.14	0.47
13:N:10:DG:H2''	13:N:11:DG:OP2	2.14	0.47
1:A:43:GLU:O	1:A:43:GLU:HG2	2.14	0.47
1:A:553:VAL:HG23	1:A:652:VAL:HG23	1.96	0.47
1:A:672:ASP:HB3	1:A:675:THR:H	1.79	0.47
3:C:172:PRO:O	3:C:235:VAL:HG23	2.14	0.47
1:A:100:LYS:HG3	1:A:181:LEU:HD22	1.95	0.47
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.96	0.47
1:A:550:LEU:HD12	1:A:550:LEU:HA	1.58	0.47
2:B:862:GLN:HE21	2:B:961:LEU:CD1	2.28	0.47
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.50	0.47
1:A:328:ARG:HD3	2:B:1206:GLU:OE1	2.14	0.47
1:A:445:ASN:CG	1:A:455:MET:HE3	2.40	0.47
1:A:492:PRO:CB	1:A:497:THR:HG23	2.44	0.47
1:A:535:THR:O	1:A:536:LEU:C	2.58	0.47
1:A:754:SER:H	1:A:757:ASN:HD22	1.61	0.47
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.15	0.47
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.47
3:C:29:MET:HA	9:K:45:LEU:CD1	2.45	0.47
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.59	0.47
8:J:36:LEU:HD13	8:J:47:ARG:HG3	1.96	0.47
12:T:6:DC:N4	12:T:7:DA:N6	2.62	0.47
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.14	0.47
1:A:567:LYS:CB	6:H:95:TYR:HA	2.45	0.47
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ARG:CZ	7:I:68:LEU:HD21	2.44	0.47
1:A:208:LEU:HD21	1:A:212:LYS:NZ	2.30	0.47
1:A:243:PRO:O	1:A:244:PRO:C	2.57	0.47
1:A:499:ALA:O	1:A:503:GLN:HG2	2.14	0.47
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.50	0.47
2:B:473:MET:C	2:B:475:SER:N	2.72	0.47
2:B:512:ARG:HB3	2:B:533:CYS:O	2.15	0.47
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.47
2:B:797:TYR:CE2	3:C:62:PHE:HD2	2.32	0.47
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.14	0.47
3:C:76:ASP:OD2	3:C:128:ASN:N	2.46	0.47
13:N:4:DG:N1	13:N:5:DT:C2	2.81	0.47
1:A:1128:GLN:HB2	1:A:1304:TRP:NE1	2.30	0.47
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.97	0.47
2:B:115:GLN:HE21	2:B:119:LEU:HD11	1.81	0.47
3:C:47:ASP:O	3:C:48:SER:HB2	2.15	0.47
4:E:76:GLY:O	4:E:77:SER:C	2.58	0.47
10:L:47:ARG:NH1	10:L:54:ARG:NE	2.52	0.47
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.13	0.46
2:B:957:ASN:ND2	2:B:959:ASP:HB2	2.30	0.46
3:C:190:ASP:C	3:C:190:ASP:OD1	2.58	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.80	0.46
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.97	0.46
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.45	0.46
1:A:312:PRO:C	1:A:313:GLN:HE21	2.23	0.46
1:A:741:ASN:ND2	1:A:744:LYS:H	2.07	0.46
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.96	0.46
1:A:899:VAL:HB	1:A:929:LEU:HD13	1.98	0.46
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.79	0.46
2:B:258:LEU:HD12	2:B:269:ILE:HG12	1.98	0.46
2:B:331:LEU:O	2:B:334:ILE:HB	2.15	0.46
2:B:744:HIS:O	2:B:747:MET:HB2	2.15	0.46
2:B:778:MET:O	2:B:819:ALA:HB1	2.16	0.46
5:F:113:GLY:O	5:F:115:THR:HG23	2.15	0.46
1:A:68:GLN:NE2	1:A:70:CYS:HB3	2.27	0.46
1:A:253:ASN:O	1:A:254:GLU:HB2	2.15	0.46
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.97	0.46
1:A:1166:ASP:HA	1:A:1169:ILE:HD13	1.98	0.46
6:H:93:TYR:HB3	6:H:144:ILE:O	2.16	0.46
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.40	0.46
1:A:372:LYS:HD3	1:A:397:ASN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:ILE:HG13	2:B:633:VAL:HG13	1.96	0.46
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.97	0.46
2:B:1079:LYS:HE2	3:C:188:HIS:CE1	2.51	0.46
3:C:236:GLY:C	3:C:238:ILE:H	2.23	0.46
1:A:573:SER:O	1:A:574:GLY:C	2.59	0.46
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.55	0.46
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.97	0.46
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.48	0.46
2:B:485:ARG:CG	2:B:485:ARG:NH1	2.68	0.46
2:B:592:ASN:H	2:B:593:PRO:HD3	1.80	0.46
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.27	0.46
9:K:20:LYS:O	9:K:33:ILE:HA	2.15	0.46
1:A:134:ARG:CD	1:A:221:SER:O	2.63	0.46
1:A:351:THR:HG21	1:A:466:SER:O	2.16	0.46
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.81	0.46
1:A:1308:THR:HG22	1:A:1310:GLY:O	2.14	0.46
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.46	0.46
2:B:1077:THR:HG23	2:B:1079:LYS:HB2	1.98	0.46
1:A:965:GLN:HA	1:A:968:GLN:HG2	1.98	0.46
1:A:1392:SER:C	1:A:1394:THR:H	2.24	0.46
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.46	0.46
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.50	0.46
13:N:4:DG:C5	13:N:5:DT:C7	2.98	0.46
1:A:351:THR:HG22	1:A:352:VAL:N	2.29	0.46
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.46
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	1.97	0.46
1:A:1443:VAL:O	1:A:1444:MET:HG3	2.16	0.46
2:B:176:SER:OG	2:B:177:LYS:N	2.48	0.46
2:B:1065:GLN:HE21	2:B:1069:PHE:HD1	1.63	0.46
2:B:1072:MET:HE2	2:B:1085:ILE:HG21	1.98	0.46
1:A:579:SER:HB3	1:A:611:GLN:HA	1.97	0.46
1:A:856:THR:O	1:A:856:THR:HG22	2.15	0.46
1:A:856:THR:HG22	1:A:864:ILE:HB	1.97	0.46
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.97	0.46
1:A:1035:TYR:O	1:A:1037:LEU:N	2.49	0.46
2:B:28:GLU:C	2:B:30:SER:N	2.74	0.46
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.94	0.46
2:B:635:ARG:O	2:B:636:PRO:C	2.59	0.46
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.42	0.46
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.74	0.46
2:B:864:LYS:HD2	2:B:865:LYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.98	0.46
2:B:1187:ASN:HD22	2:B:1188:LYS:N	2.14	0.46
3:C:69:LEU:O	8:J:6:ARG:NH1	2.49	0.46
4:E:119:SER:HB2	13:N:12:DT:H5''	1.98	0.46
12:T:1:DC:N4	13:N:13:DA:N6	2.63	0.46
1:A:31:SER:CB	1:A:83:HIS:HD2	2.28	0.45
1:A:180:LYS:HE3	1:A:294:SER:HB3	1.97	0.45
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.16	0.45
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.51	0.45
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.15	0.45
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.87	0.45
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.98	0.45
1:A:23:SER:O	1:A:24:PRO:C	2.59	0.45
1:A:214:ILE:CG2	1:A:215:SER:N	2.70	0.45
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.98	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.98	0.45
1:A:1107:VAL:HG23	1:A:1383:SER:HB3	1.97	0.45
2:B:230:ALA:N	2:B:231:PRO:CD	2.73	0.45
1:A:53:LEU:CD1	1:A:266:LEU:O	2.65	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:CG2	2.98	0.45
2:B:486:TYR:CE2	2:B:1096:ARG:HG2	2.52	0.45
3:C:180:TYR:O	3:C:181:ASP:C	2.59	0.45
12:T:7:DA:C2'	12:T:8:DT:H5''	2.45	0.45
13:N:4:DG:H2''	13:N:5:DT:C5'	2.46	0.45
1:A:709:THR:CG2	7:I:94:ASP:HA	2.46	0.45
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.31	0.45
1:A:1297:GLU:CD	1:A:1297:GLU:H	2.24	0.45
2:B:551:PRO:C	2:B:553:PRO:HD2	2.41	0.45
3:C:33:LEU:HG	3:C:37:MET:HE2	1.98	0.45
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.50	0.45
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.29	0.45
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.96	0.45
1:A:852:TYR:O	5:F:81:THR:HG22	2.17	0.45
1:A:1372:VAL:O	1:A:1376:THR:HB	2.16	0.45
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.97	0.45
2:B:957:ASN:HD21	2:B:959:ASP:HB2	1.80	0.45
3:C:67:LEU:HD23	3:C:144:ILE:HD11	1.98	0.45
1:A:43:GLU:OE1	1:A:43:GLU:N	2.48	0.45
1:A:265:LYS:HZ1	1:A:303:TYR:N	2.14	0.45
1:A:962:ARG:O	1:A:966:ASN:HB2	2.16	0.45
2:B:65:GLU:HG2	2:B:66:ASP:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.78	0.45
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.98	0.45
2:B:872:GLU:HG2	2:B:916:THR:HB	1.99	0.45
2:B:999:MET:HE3	2:B:1011:ILE:CD1	2.46	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.99	0.45
4:E:29:PHE:C	4:E:30:ILE:HD12	2.42	0.45
12:T:2:DT:H3'	12:T:2:DT:H6	1.82	0.45
1:A:272:ALA:O	1:A:296:LEU:HB2	2.17	0.45
1:A:375:THR:HG21	1:A:433:GLU:OE1	2.16	0.45
1:A:472:LEU:HD11	2:B:835:GLN:HE22	1.80	0.45
2:B:706:GLN:O	2:B:707:PRO:C	2.58	0.45
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.97	0.45
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.32	0.45
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.51	0.45
1:A:151:ASP:OD2	1:A:163:SER:HA	2.17	0.45
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.47	0.45
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.94	0.45
3:C:142:VAL:HG13	8:J:5:VAL:HG23	1.98	0.45
5:F:114:GLU:OE1	5:F:119:ARG:HG3	2.17	0.45
6:H:11:GLN:HE21	6:H:11:GLN:HB2	1.60	0.45
12:T:2:DT:O2	13:N:13:DA:C2	2.69	0.45
13:N:14:DG:OP2	13:N:14:DG:H2'	2.17	0.45
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.81	0.45
2:B:647:GLY:O	2:B:648:HIS:ND1	2.50	0.45
2:B:708:GLU:O	2:B:712:PRO:HD3	2.16	0.45
12:T:16:DC:H2''	12:T:17:DC:C5	2.52	0.45
1:A:313:GLN:HB3	1:A:314:ALA:H	1.42	0.45
1:A:1258:HIS:O	1:A:1262:LYS:NZ	2.47	0.45
2:B:167:ILE:HG21	2:B:453:ILE:HD12	1.99	0.45
6:H:110:ASP:O	6:H:111:LEU:HG	2.16	0.45
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.47	0.45
13:N:5:DT:C2'	13:N:6:DT:C5	2.99	0.45
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.99	0.44
1:A:1349:TYR:O	1:A:1350:LYS:C	2.58	0.44
2:B:1093:GLN:HG2	2:B:1093:GLN:H	1.70	0.44
3:C:99:LEU:N	3:C:99:LEU:CD2	2.76	0.44
5:F:136:ARG:O	5:F:143:PHE:HA	2.17	0.44
6:H:109:LYS:HZ3	6:H:111:LEU:HD12	1.81	0.44
8:J:8:PHE:H	8:J:49:MET:CE	2.26	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.81	0.44
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:ASP:C	1:A:1325:THR:H	2.24	0.44
2:B:228:LYS:HB3	2:B:228:LYS:HE2	1.73	0.44
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.98	0.44
1:A:783:THR:CG2	1:A:784:LEU:N	2.80	0.44
1:A:1194:ARG:NH2	1:A:1237:ILE:CD1	2.80	0.44
1:A:1206:ASP:N	1:A:1206:ASP:OD2	2.51	0.44
1:A:251:SER:HB2	11:R:1:A:N3	2.32	0.44
1:A:960:ILE:O	1:A:961:ARG:C	2.61	0.44
2:B:764:SER:O	2:B:766:ARG:N	2.51	0.44
2:B:382:ILE:HG12	2:B:382:ILE:H	1.65	0.44
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.83	0.44
3:C:127:ARG:HE	3:C:127:ARG:HB2	1.54	0.44
8:J:22:LEU:HA	8:J:22:LEU:HD12	1.59	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.50	0.44
1:A:417:TYR:O	1:A:418:SER:HB3	2.18	0.44
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.52	0.44
1:A:858:ASN:C	1:A:858:ASN:ND2	2.70	0.44
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.53	0.44
2:B:1181:GLU:H	2:B:1181:GLU:HG2	1.55	0.44
12:T:5:DC:C4	12:T:6:DC:N3	2.85	0.44
13:N:1:DG:H2''	13:N:2:DT:C6	2.46	0.44
2:B:475:SER:C	2:B:477:ALA:N	2.75	0.44
2:B:857:ARG:O	2:B:967:ARG:HA	2.18	0.44
8:J:52:THR:HG22	8:J:52:THR:O	2.17	0.44
12:T:22:DT:C2'	12:T:23:DC:O5'	2.65	0.44
2:B:43:LEU:HD23	2:B:43:LEU:HA	1.76	0.44
2:B:217:ARG:NH2	2:B:405:ARG:HG3	2.33	0.44
2:B:792:MET:HE3	2:B:792:MET:HB2	1.91	0.44
2:B:1169:MET:HE3	2:B:1169:MET:HB2	1.79	0.44
4:E:190:LEU:HD11	4:E:196:VAL:HG13	2.00	0.44
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.53	0.44
9:K:109:TRP:C	9:K:111:LEU:H	2.25	0.44
1:A:472:LEU:HD21	2:B:835:GLN:CB	2.48	0.44
2:B:1109:GLY:HA3	2:B:1110:PRO:HD2	1.67	0.44
1:A:114:LEU:HD11	1:A:171:GLN:NE2	2.33	0.43
1:A:302:THR:HG21	1:A:313:GLN:OE1	2.18	0.43
1:A:328:ARG:C	1:A:329:LEU:HD23	2.42	0.43
1:A:835:GLY:HA3	12:T:18:DG:H1'	1.98	0.43
1:A:1312:ASN:OD1	1:A:1315:GLU:HG3	2.18	0.43
2:B:493:SER:HA	2:B:751:VAL:HG11	1.99	0.43
2:B:547:VAL:N	2:B:612:GLU:OE2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:CB	2:B:637:LEU:HA	2.48	0.43
3:C:69:LEU:HB3	8:J:6:ARG:HD3	2.00	0.43
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.65	0.43
1:A:91:PHE:N	1:A:297:GLN:HE22	2.15	0.43
1:A:577:ILE:H	1:A:577:ILE:HG13	1.57	0.43
2:B:242:SER:HB2	2:B:252:SER:O	2.17	0.43
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.48	0.43
2:B:913:GLY:HA2	2:B:938:SER:OG	2.18	0.43
3:C:44:LEU:HD12	3:C:160:LYS:C	2.43	0.43
3:C:112:ASN:HD21	3:C:146:LYS:HD3	1.83	0.43
3:C:129:ILE:HA	3:C:129:ILE:HD12	1.74	0.43
1:A:610:GLY:O	1:A:611:GLN:NE2	2.51	0.43
1:A:973:ILE:HD12	1:A:974:ASP:H	1.83	0.43
1:A:1155:ASP:HA	1:A:1156:PRO:HD3	1.75	0.43
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.01	0.43
2:B:453:ILE:O	2:B:454:THR:C	2.61	0.43
2:B:518:HIS:O	2:B:519:TRP:C	2.60	0.43
2:B:724:ASP:HA	2:B:725:PRO:HD3	1.90	0.43
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.60	0.43
1:A:269:ILE:HD13	1:A:300:VAL:HG22	2.00	0.43
1:A:533:LYS:HD3	1:A:745:GLN:NE2	2.33	0.43
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.74	0.43
1:A:825:ILE:HD12	2:B:512:ARG:HB2	2.00	0.43
1:A:913:LEU:HD11	1:A:981:LEU:O	2.18	0.43
2:B:597:MET:HE1	2:B:615:MET:HB2	2.00	0.43
4:E:88:VAL:HG11	4:E:110:PHE:CE2	2.53	0.43
13:N:7:DA:H2"	13:N:8:DT:C6	2.54	0.43
1:A:112:LYS:HG2	1:A:113:LEU:N	2.34	0.43
1:A:352:VAL:CG2	2:B:1099:VAL:HG13	2.48	0.43
1:A:1156:PRO:HD2	1:A:1157:ASP:H	1.83	0.43
2:B:549:THR:O	2:B:628:THR:CG2	2.67	0.43
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.32	0.43
2:B:1058:LEU:HD23	2:B:1058:LEU:HA	1.87	0.43
3:C:56:THR:HG23	3:C:58:LEU:H	1.83	0.43
3:C:142:VAL:N	8:J:16:ASP:HB3	2.31	0.43
7:I:111:THR:CG2	7:I:113:ASP:CB	2.93	0.43
1:A:99:ILE:HD13	1:A:235:ILE:HG23	1.99	0.43
1:A:354:SER:HA	1:A:482:PHE:CD2	2.53	0.43
2:B:121:ASN:HD22	2:B:121:ASN:HA	1.61	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
1:A:754:SER:O	1:A:755:PHE:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.44	0.43
2:B:476:ARG:C	2:B:478:GLY:H	2.27	0.43
3:C:133:ILE:HD13	3:C:236:GLY:C	2.43	0.43
4:E:88:VAL:HG11	4:E:110:PHE:HE2	1.84	0.43
5:F:76:LYS:O	5:F:79:ARG:HD3	2.18	0.43
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.99	0.43
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.43
2:B:483:LEU:HD23	2:B:483:LEU:HA	1.93	0.43
6:H:83:GLN:C	6:H:87:ARG:HG3	2.43	0.43
8:J:3:VAL:HG11	8:J:18:TRP:HB2	2.01	0.43
1:A:211:PHE:O	1:A:213:HIS:N	2.52	0.43
1:A:873:MET:HE1	1:A:1057:VAL:HG22	2.01	0.43
1:A:979:SER:OG	1:A:981:LEU:HD12	2.19	0.43
1:A:1017:LEU:HB2	4:E:205:SER:C	2.43	0.43
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.48	0.43
2:B:1021:MET:HB2	2:B:1021:MET:HE3	1.50	0.43
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.69	0.43
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.87	0.43
3:C:77:ILE:HD12	3:C:161:LYS:HG3	2.01	0.43
6:H:106:GLU:C	6:H:108:SER:N	2.77	0.43
1:A:31:SER:OG	1:A:83:HIS:HD2	2.02	0.43
1:A:129:LYS:O	1:A:130:ASP:HB3	2.19	0.43
1:A:368:LYS:HB2	1:A:368:LYS:HE2	1.75	0.43
2:B:64:CYS:O	2:B:65:GLU:HB3	2.18	0.43
2:B:229:ALA:HB1	2:B:231:PRO:CD	2.44	0.43
2:B:274:PRO:HB2	2:B:359:GLU:HB3	2.01	0.43
2:B:801:LYS:O	8:J:52:THR:CG2	2.54	0.43
2:B:911:ILE:HD13	2:B:911:ILE:HG21	1.60	0.43
2:B:1200:ALA:O	2:B:1201:LYS:C	2.59	0.43
8:J:8:PHE:N	8:J:49:MET:HE3	2.26	0.43
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.84	0.42
1:A:261:ASP:CG	1:A:323:LYS:HD2	2.41	0.42
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.19	0.42
2:B:293:PRO:C	2:B:294:ASP:O	2.59	0.42
2:B:541:LEU:HB2	2:B:747:MET:HE2	1.99	0.42
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.54	0.42
3:C:183:TRP:O	3:C:184:ASN:C	2.61	0.42
13:N:6:DT:C2	13:N:7:DA:N7	2.87	0.42
1:A:398:GLU:O	1:A:399:HIS:C	2.61	0.42
1:A:981:LEU:HD21	1:A:1039:LYS:HA	2.02	0.42
1:A:1019:CYS:O	1:A:1020:CYS:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:GLY:O	1:A:1440:ALA:N	2.43	0.42
4:E:22:MET:HB2	4:E:187:TYR:CE1	2.54	0.42
4:E:157:SER:O	4:E:159:ASP:N	2.52	0.42
1:A:313:GLN:HB2	1:A:322:VAL:CG2	2.37	0.42
1:A:598:LEU:O	1:A:599:SER:C	2.62	0.42
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.42
1:A:992:ASP:O	1:A:995:GLU:HB2	2.19	0.42
1:A:1159:ARG:HB3	1:A:1159:ARG:HH11	1.84	0.42
2:B:642:ASP:O	2:B:644:GLU:N	2.52	0.42
3:C:226:ASP:O	3:C:227:THR:O	2.37	0.42
4:E:122:LYS:HB3	4:E:123:LEU:HD23	2.02	0.42
4:E:157:SER:N	4:E:160:GLU:OE1	2.52	0.42
6:H:43:ASN:OD1	6:H:43:ASN:C	2.62	0.42
7:I:101:PHE:O	7:I:109:ILE:HA	2.20	0.42
1:A:116:ASP:C	1:A:118:HIS:N	2.76	0.42
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.49	0.42
1:A:323:LYS:O	1:A:324:SER:CB	2.66	0.42
3:C:246:ARG:HA	3:C:249:ASP:HB2	2.02	0.42
4:E:48:ASP:O	4:E:49:SER:C	2.61	0.42
7:I:96:SER:C	7:I:98:VAL:H	2.28	0.42
1:A:783:THR:HG23	1:A:815:PHE:HZ	1.84	0.42
1:A:969:GLN:O	1:A:971:PHE:N	2.52	0.42
2:B:212:LEU:HD23	2:B:480:SER:HB3	2.02	0.42
2:B:542:MET:SD	2:B:747:MET:HG3	2.59	0.42
2:B:1034:VAL:O	2:B:1035:ALA:C	2.62	0.42
3:C:63:ILE:HA	3:C:66:ARG:HG3	2.00	0.42
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.52	0.42
6:H:38:LEU:HG	6:H:39:THR:N	2.34	0.42
7:I:117:LYS:C	7:I:118:ARG:HG2	2.45	0.42
1:A:902:LEU:H	1:A:902:LEU:HG	1.37	0.42
1:A:1157:ASP:O	1:A:1158:PRO:C	2.62	0.42
1:A:1433:MET:HE3	1:A:1439:GLY:HA2	2.01	0.42
2:B:382:ILE:O	2:B:383:ASN:C	2.62	0.42
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.85	0.42
2:B:1124:ARG:HE	2:B:1124:ARG:HB2	1.66	0.42
3:C:69:LEU:CB	8:J:5:VAL:HG13	2.50	0.42
3:C:142:VAL:H	8:J:16:ASP:CB	2.28	0.42
4:E:96:PHE:C	4:E:98:ILE:N	2.70	0.42
7:I:58:VAL:HG11	7:I:109:ILE:HD11	2.02	0.42
1:A:380:VAL:CG1	1:A:428:TYR:HA	2.37	0.42
2:B:515:HIS:HD2	2:B:517:THR:N	2.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:THR:O	2:B:881:ASN:C	2.62	0.42
3:C:143:LEU:HG	8:J:2:ILE:HD11	2.00	0.42
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.34	0.42
1:A:1060:PRO:HD2	5:F:86:THR:HG21	2.02	0.42
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.35	0.42
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.55	0.42
2:B:413:LEU:HD23	2:B:413:LEU:HA	1.81	0.42
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.54	0.42
2:B:1027:ILE:HG23	2:B:1052:VAL:HG22	2.02	0.42
3:C:43:THR:HG22	3:C:44:LEU:N	2.35	0.42
6:H:91:ASP:O	6:H:92:ASP:CG	2.63	0.42
8:J:8:PHE:O	8:J:9:SER:C	2.63	0.42
1:A:257:ARG:HG2	1:A:258:GLY:N	2.34	0.42
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.97	0.42
2:B:35:SER:O	2:B:37:PHE:O	2.38	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.01	0.42
2:B:1187:ASN:HD21	2:B:1190:ASP:N	2.12	0.42
4:E:3:GLN:HB2	4:E:4:GLU:H	1.63	0.42
6:H:107:VAL:HG12	6:H:107:VAL:O	2.20	0.42
10:L:27:LEU:HD22	10:L:37:LYS:NZ	2.35	0.42
1:A:401:GLY:C	1:A:435:HIS:HD2	2.25	0.42
1:A:1110:ASN:C	1:A:1110:ASN:HD22	2.28	0.42
2:B:120:ARG:HD2	2:B:955:THR:CG2	2.39	0.42
2:B:314:LEU:O	2:B:317:CYS:HB2	2.19	0.42
2:B:685:LEU:HD21	2:B:692:TYR:CE1	2.54	0.42
2:B:804:GLY:HA2	2:B:1042:GLY:O	2.20	0.42
2:B:839:MET:HE1	2:B:1010:LEU:HD21	2.02	0.42
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.85	0.42
13:N:4:DG:C2	13:N:5:DT:N3	2.80	0.42
1:A:99:ILE:CD1	1:A:235:ILE:HG23	2.50	0.41
1:A:775:ILE:H	1:A:775:ILE:HG12	1.69	0.41
1:A:808:LEU:O	2:B:728:ARG:NH1	2.53	0.41
1:A:821:ARG:HH11	1:A:821:ARG:HD3	1.69	0.41
1:A:943:LEU:O	1:A:946:VAL:N	2.51	0.41
2:B:310:MET:O	2:B:313:MET:HB2	2.21	0.41
10:L:59:ALA:O	10:L:60:ARG:HB3	2.19	0.41
1:A:77:CYS:C	1:A:79:GLY:N	2.78	0.41
1:A:804:TYR:O	2:B:761:HIS:ND1	2.48	0.41
2:B:288:ALA:HB1	2:B:331:LEU:HD13	2.02	0.41
2:B:301:ILE:HG21	2:B:314:LEU:HD11	2.02	0.41
2:B:332:ASP:C	2:B:334:ILE:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:PHE:HA	2:B:432:MET:HE2	2.02	0.41
2:B:1002:THR:HG21	2:B:1006:ILE:CG1	2.50	0.41
2:B:1056:SER:O	2:B:1066:SER:HB2	2.20	0.41
6:H:40:LEU:HD12	6:H:41:ASP:H	1.84	0.41
1:A:322:VAL:HB	1:A:323:LYS:H	1.29	0.41
2:B:35:SER:O	2:B:39:ARG:HB2	2.20	0.41
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.21	0.41
12:T:7:DA:H2	12:T:8:DT:N3	2.07	0.41
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.55	0.41
2:B:122:LEU:HD21	2:B:958:GLN:HB2	2.02	0.41
2:B:195:CYS:SG	2:B:783:THR:HB	2.60	0.41
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.85	0.41
4:E:7:ARG:O	4:E:8:ASN:C	2.63	0.41
10:L:59:ALA:O	10:L:60:ARG:CB	2.68	0.41
1:A:53:LEU:HD23	1:A:54:ASN:HB3	2.01	0.41
1:A:1060:PRO:HD2	5:F:86:THR:CG2	2.49	0.41
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.41
2:B:542:MET:SD	2:B:636:PRO:HG3	2.61	0.41
2:B:778:MET:HE3	2:B:853:SER:CB	2.50	0.41
6:H:62:SER:HB2	6:H:63:LEU:H	1.41	0.41
13:N:12:DT:H2"	13:N:13:DA:C8	2.55	0.41
1:A:848:ILE:HD11	1:A:1374:VAL:CG2	2.49	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.41
2:B:500:THR:HA	2:B:501:PRO:HD3	1.94	0.41
2:B:522:VAL:HG12	2:B:523:CYS:N	2.35	0.41
2:B:798:TYR:CZ	3:C:62:PHE:HE2	2.38	0.41
7:I:87:GLN:O	7:I:88:SER:C	2.63	0.41
1:A:255:SER:O	1:A:256:GLN:HB2	2.21	0.41
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.54	0.41
1:A:444:PHE:O	1:A:455:MET:HA	2.21	0.41
1:A:683:ILE:HD13	1:A:683:ILE:HA	1.72	0.41
1:A:1130:GLN:HE21	1:A:1130:GLN:HB3	1.71	0.41
1:A:1284:MET:HE3	1:A:1284:MET:HB2	1.72	0.41
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.85	0.41
2:B:898:LEU:HD23	2:B:898:LEU:HA	1.82	0.41
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.48	0.41
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.19	0.41
1:A:149:GLU:HB3	1:A:150:THR:H	1.63	0.41
1:A:233:TRP:C	1:A:235:ILE:H	2.28	0.41
1:A:553:VAL:CG2	1:A:652:VAL:HG23	2.51	0.41
1:A:575:LYS:HD3	1:A:612:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG21	7:I:93:LYS:O	2.20	0.41
2:B:398:ARG:HB3	2:B:398:ARG:CZ	2.50	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.51	0.41
2:B:956:THR:HB	10:L:46:VAL:HG21	2.03	0.41
6:H:44:VAL:O	6:H:44:VAL:HG12	2.19	0.41
7:I:54:GLU:O	7:I:89:GLN:HB2	2.20	0.41
8:J:1:MET:H2	8:J:57:ILE:H	1.66	0.41
1:A:322:VAL:HG12	1:A:323:LYS:HE2	2.03	0.41
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.86	0.41
1:A:666:ILE:H	1:A:666:ILE:HG13	1.70	0.41
1:A:782:ARG:NH2	7:I:67:THR:CG2	2.84	0.41
1:A:834:THR:HG21	1:A:1077:THR:HA	2.03	0.41
1:A:1015:VAL:O	1:A:1015:VAL:CG1	2.66	0.41
1:A:1036:ARG:HG3	1:A:1036:ARG:NH1	2.31	0.41
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	2.01	0.41
2:B:173:MET:HE2	2:B:201:GLY:O	2.21	0.41
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.33	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.55	0.41
2:B:367:LEU:HB3	2:B:368:GLU:H	1.58	0.41
2:B:373:ARG:HE	2:B:567:GLU:CD	2.27	0.41
2:B:619:ILE:H	2:B:619:ILE:HG12	1.73	0.41
2:B:744:HIS:HA	2:B:745:PRO:HD2	1.96	0.41
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.21	0.41
2:B:864:LYS:HG2	2:B:871:THR:HG23	2.03	0.41
2:B:893:LEU:HD21	2:B:910:VAL:HG12	2.03	0.41
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.36	0.41
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.21	0.41
3:C:133:ILE:HD13	3:C:237:SER:HA	2.03	0.41
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.80	0.41
3:C:259:LEU:HD13	9:K:91:CYS:HB2	2.02	0.41
7:I:55:THR:O	7:I:55:THR:CG2	2.68	0.41
12:T:7:DA:C6	12:T:8:DT:O4	2.74	0.41
12:T:17:DC:H2'	12:T:17:DC:O2	2.21	0.41
1:A:40:THR:HG22	1:A:41:MET:HG3	2.02	0.41
1:A:260:ASP:CG	1:A:261:ASP:N	2.79	0.41
1:A:851:HIS:CD2	1:A:857:ARG:HB2	2.55	0.41
1:A:1280:GLU:O	1:A:1281:ARG:C	2.64	0.41
2:B:619:ILE:HG13	7:I:65:ASP:HB2	2.03	0.41
2:B:817:LEU:N	2:B:818:PRO:CD	2.84	0.41
2:B:1173:ALA:C	2:B:1175:LEU:H	2.28	0.41
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:O	9:K:26:LYS:HD3	2.21	0.40
1:A:707:GLY:O	1:A:1281:ARG:HD2	2.22	0.40
1:A:1062:GLU:O	1:A:1064:VAL:N	2.53	0.40
1:A:1279:ILE:HD13	1:A:1279:ILE:N	2.36	0.40
1:A:1436:ILE:C	1:A:1437:GLY:O	2.64	0.40
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.83	0.40
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.95	0.40
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.66	0.40
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.03	0.40
3:C:57:VAL:HG11	8:J:57:ILE:HG13	2.02	0.40
6:H:30:SER:HB2	6:H:36:CYS:SG	2.61	0.40
10:L:48:CYS:O	10:L:49:LYS:HG2	2.21	0.40
12:T:7:DA:N3	12:T:8:DT:C6	2.89	0.40
1:A:86:LEU:CD1	1:A:236:LEU:O	2.67	0.40
1:A:332:LYS:C	1:A:334:GLY:H	2.29	0.40
1:A:541:ILE:HG23	1:A:545:GLN:NE2	2.37	0.40
1:A:1279:ILE:N	1:A:1279:ILE:CD1	2.84	0.40
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.54	0.40
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.56	0.40
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.92	0.40
1:A:632:VAL:HG13	1:A:962:ARG:HD3	2.02	0.40
2:B:1072:MET:HE2	2:B:1085:ILE:CG2	2.51	0.40
3:C:80:LEU:O	3:C:161:LYS:HE2	2.21	0.40
3:C:262:LEU:HD13	9:K:88:LYS:HG2	2.02	0.40
9:K:14:GLU:O	9:K:15:GLY:C	2.65	0.40
10:L:55:ILE:O	10:L:56:LEU:HB2	2.20	0.40
1:A:43:GLU:OE1	1:A:46:THR:HB	2.22	0.40
1:A:50:ILE:C	1:A:52:GLY:N	2.80	0.40
1:A:1129:GLU:HA	1:A:1132:LYS:CE	2.46	0.40
1:A:1169:ILE:H	1:A:1169:ILE:HD12	1.86	0.40
2:B:199:MET:SD	2:B:199:MET:N	2.95	0.40
2:B:214:ALA:HB2	2:B:408:LEU:HD13	2.03	0.40
2:B:563:MET:HE1	2:B:588:GLY:CA	2.51	0.40
2:B:578:THR:HB	2:B:593:PRO:HG3	2.04	0.40
2:B:624:LEU:HD12	2:B:624:LEU:C	2.47	0.40
2:B:744:HIS:CD2	2:B:744:HIS:C	3.00	0.40
2:B:801:LYS:O	2:B:801:LYS:HG2	2.21	0.40
3:C:44:LEU:HD12	3:C:160:LYS:O	2.20	0.40
3:C:76:ASP:HB2	3:C:129:ILE:HD13	2.04	0.40
3:C:258:ILE:HG12	9:K:35:PHE:HE2	1.87	0.40
6:H:106:GLU:OE1	6:H:108:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:30:LEU:HD22	8:J:34:THR:HG21	2.04	0.40
1:A:23:SER:HA	1:A:24:PRO:HD2	1.91	0.40
1:A:48:ALA:C	1:A:49:LYS:HE2	2.47	0.40
1:A:102:VAL:HG12	1:A:102:VAL:O	2.21	0.40
1:A:447:GLN:HB3	1:A:448:PRO:HA	2.03	0.40
1:A:664:THR:HA	1:A:742:ASN:HD22	1.86	0.40
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.22	0.40
2:B:492:LEU:HD23	2:B:492:LEU:HA	1.61	0.40
2:B:879:ARG:CG	2:B:880:THR:N	2.84	0.40
3:C:186:LEU:HB2	3:C:188:HIS:HD2	1.85	0.40
4:E:95:THR:O	4:E:98:ILE:HG22	2.21	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	
1	A	1383/1733 (80%)	1094 (79%)	201 (14%)	88 (6%)	1	7
2	B	1088/1224 (89%)	900 (83%)	126 (12%)	62 (6%)	1	9
3	C	264/318 (83%)	226 (86%)	30 (11%)	8 (3%)	3	20
4	E	212/215 (99%)	173 (82%)	28 (13%)	11 (5%)	1	11
5	F	82/155 (53%)	63 (77%)	13 (16%)	6 (7%)	1	5
6	H	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	2
7	I	117/122 (96%)	97 (83%)	13 (11%)	7 (6%)	1	8
8	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	4
9	K	112/120 (93%)	105 (94%)	7 (6%)	0	100	100
10	L	44/70 (63%)	25 (57%)	10 (23%)	9 (20%)	0	0
All	All	3494/4173 (84%)	2829 (81%)	457 (13%)	208 (6%)	1	8

All (208) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	65	LEU
1	A	73	GLY
1	A	109	HIS
1	A	148	CYS
1	A	169	ASN
1	A	216	VAL
1	A	226	GLU
1	A	245	PRO
1	A	250	ILE
1	A	258	GLY
1	A	286	HIS
1	A	308	ILE
1	A	315	LEU
1	A	399	HIS
1	A	424	ILE
1	A	567	LYS
1	A	597	LEU
1	A	609	ASP
1	A	610	GLY
1	A	846	GLU
1	A	923	LEU
1	A	972	HIS
1	A	994	GLN
1	A	1014	ALA
1	A	1036	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1438	THR
2	B	65	GLU
2	B	168	GLY
2	B	229	ALA
2	B	230	ALA
2	B	245	GLU
2	B	266	ALA
2	B	395	GLN
2	B	436	VAL
2	B	469	GLN
2	B	473	MET
2	B	474	SER

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Mol	Chain	Res	Type
2	B	477	ALA
2	B	483	LEU
2	B	531	GLN
2	B	592	ASN
2	B	629	ASP
2	B	636	PRO
2	B	645	SER
2	B	708	GLU
2	B	709	ASP
2	B	713	ALA
2	B	733	HIS
2	B	734	HIS
2	B	751	VAL
2	B	866	TYR
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
2	B	1097	HIS
2	B	1223	ASP
3	C	173	ALA
4	E	49	SER
4	E	59	SER
4	E	118	PRO
5	F	73	ALA
6	H	90	ALA
6	H	109	LYS
6	H	111	LEU
6	H	131	ASN
6	H	132	LEU
6	H	138	GLU
7	I	34	TYR
8	J	2	ILE
10	L	34	CYS
10	L	35	SER
10	L	45	ALA
10	L	59	ALA
10	L	60	ARG
1	A	130	ASP
1	A	224	PHE
1	A	257	ARG
1	A	266	LEU
1	A	298	PHE

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Mol	Chain	Res	Type
1	A	309	ALA
1	A	322	VAL
1	A	324	SER
1	A	837	ILE
1	A	1123	GLY
1	A	1174	PHE
1	A	1234	GLU
1	A	1257	ASP
1	A	1388	GLY
1	A	1420	ASP
2	B	67	SER
2	B	249	ARG
2	B	288	ALA
2	B	466	TRP
2	B	643	ASP
2	B	737	THR
2	B	880	THR
2	B	1021	MET
2	B	1103	ILE
2	B	1185	CYS
3	C	48	SER
3	C	142	VAL
3	C	174	ALA
3	C	227	THR
4	E	56	LYS
4	E	77	SER
5	F	111	LEU
6	H	3	ASN
6	H	62	SER
6	H	136	LYS
7	I	3	THR
7	I	9	ASP
7	I	54	GLU
7	I	97	MET
8	J	8	PHE
8	J	30	LEU
10	L	46	VAL
1	A	35	ILE
1	A	54	ASN
1	A	131	SER
1	A	142	CYS
1	A	214	ILE

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Mol	Chain	Res	Type
1	A	251	SER
1	A	673	GLY
1	A	674	PRO
1	A	852	TYR
1	A	1127	ASP
1	A	1278	ASN
2	B	364	ILE
2	B	468	GLU
2	B	471	LYS
2	B	480	SER
2	B	555	ILE
2	B	732	SER
2	B	735	ALA
2	B	792	MET
2	B	864	LYS
4	E	101	GLN
4	E	158	SER
5	F	114	GLU
6	H	128	ASN
7	I	90	GLN
8	J	9	SER
8	J	19	GLU
10	L	44	ASP
1	A	48	ALA
1	A	49	LYS
1	A	69	THR
1	A	147	VAL
1	A	178	GLY
1	A	219	PHE
1	A	220	THR
1	A	404	TYR
1	A	423	ASP
1	A	583	PRO
1	A	958	VAL
1	A	1093	LYS
2	B	367	LEU
2	B	479	VAL
2	B	561	TRP
2	B	644	GLU
2	B	711	GLU
2	B	1108	ARG
4	E	97	VAL

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Mol	Chain	Res	Type
6	H	130	ARG
7	I	47	GLU
1	A	24	PRO
1	A	51	GLY
1	A	234	MET
1	A	254	GLU
1	A	903	ASN
1	A	970	THR
1	A	1151	GLU
2	B	333	PHE
2	B	413	LEU
2	B	476	ARG
2	B	707	PRO
3	C	214	ASN
3	C	215	GLU
4	E	36	GLU
6	H	18	GLY
10	L	26	THR
1	A	38	PRO
1	A	1062	GLU
2	B	233	PRO
2	B	1175	LEU
3	C	136	ASP
4	E	51	GLY
5	F	74	ILE
5	F	154	ASP
1	A	79	GLY
1	A	244	PRO
1	A	1156	PRO
1	A	1424	VAL
1	A	1437	GLY
2	B	467	GLY
1	A	794	PRO
5	F	131	PRO
1	A	312	PRO
1	A	990	VAL
10	L	30	ILE
1	A	310	GLY
1	A	772	GLY
4	E	86	PRO

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	
1	A	1218/1520 (80%)	937 (77%)	281 (23%)	1	4
2	B	960/1061 (90%)	749 (78%)	211 (22%)	1	5
3	C	234/274 (85%)	177 (76%)	57 (24%)	1	3
4	E	196/197 (100%)	154 (79%)	42 (21%)	1	6
5	F	74/137 (54%)	59 (80%)	15 (20%)	1	6
6	H	117/128 (91%)	94 (80%)	23 (20%)	1	7
7	I	113/116 (97%)	90 (80%)	23 (20%)	1	6
8	J	60/65 (92%)	39 (65%)	21 (35%)	0	0
9	K	99/102 (97%)	78 (79%)	21 (21%)	1	6
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	9
All	All	3111/3657 (85%)	2410 (78%)	701 (22%)	1	5

All (701) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	47	ARG
1	A	49	LYS
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN
1	A	55	ASP
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	80	HIS
1	A	84	ILE
1	A	93	VAL
1	A	106	VAL
1	A	109	HIS
1	A	114	LEU
1	A	126	LEU
1	A	132	LYS
1	A	144	THR
1	A	146	MET
1	A	147	VAL
1	A	148	CYS
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	179	LEU
1	A	202	LEU
1	A	208	LEU
1	A	212	LYS
1	A	216	VAL
1	A	220	THR
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	235	ILE
1	A	245	PRO
1	A	250	ILE
1	A	257	ARG
1	A	264	PHE
1	A	270	LEU
1	A	271	LYS
1	A	274	ILE
1	A	287	HIS
1	A	289	ILE
1	A	296	LEU
1	A	297	GLN
1	A	303	TYR
1	A	306	ASN
1	A	308	ILE
1	A	311	GLN
1	A	313	GLN
1	A	315	LEU

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Mol	Chain	Res	Type
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	326	ARG
1	A	329	LEU
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	336	ILE
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	367	PRO
1	A	368	LYS
1	A	369	SER
1	A	372	LYS
1	A	373	THR
1	A	375	THR
1	A	380	VAL
1	A	381	THR
1	A	383	TYR
1	A	392	VAL
1	A	398	GLU
1	A	403	LYS
1	A	412	ARG
1	A	416	ARG
1	A	419	LYS
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	466	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR

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Mol	Chain	Res	Type
1	A	476	SER
1	A	497	THR
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	518	LYS
1	A	523	ILE
1	A	531	ILE
1	A	532	ARG
1	A	535	THR
1	A	542	GLU
1	A	544	ASP
1	A	547	LEU
1	A	560	ILE
1	A	567	LYS
1	A	577	ILE
1	A	589	GLN
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	601	LYS
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	629	LEU
1	A	630	ILE
1	A	637	LYS
1	A	663	SER
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	676	MET
1	A	680	THR
1	A	681	GLU
1	A	682	THR
1	A	685	GLU
1	A	688	LYS
1	A	691	LEU
1	A	695	LYS
1	A	702	LEU

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Mol	Chain	Res	Type
1	A	703	THR
1	A	709	THR
1	A	710	LEU
1	A	712	GLU
1	A	732	LEU
1	A	735	VAL
1	A	740	LEU
1	A	752	LYS
1	A	756	ILE
1	A	764	CYS
1	A	765	VAL
1	A	768	GLN
1	A	780	VAL
1	A	783	THR
1	A	801	GLU
1	A	803	SER
1	A	805	LEU
1	A	821	ARG
1	A	829	VAL
1	A	830	LYS
1	A	834	THR
1	A	838	GLN
1	A	855	THR
1	A	856	THR
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	884	ASP
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	904	THR
1	A	911	SER
1	A	914	GLU
1	A	919	ILE
1	A	922	ASP
1	A	926	GLN
1	A	932	GLU
1	A	936	LEU
1	A	940	ARG

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Mol	Chain	Res	Type
1	A	941	LYS
1	A	949	ASP
1	A	960	ILE
1	A	961	ARG
1	A	965	GLN
1	A	976	THR
1	A	977	LYS
1	A	982	THR
1	A	994	GLN
1	A	995	GLU
1	A	996	ASN
1	A	999	VAL
1	A	1000	LEU
1	A	1001	ARG
1	A	1015	VAL
1	A	1017	LEU
1	A	1029	ARG
1	A	1033	GLN
1	A	1034	GLU
1	A	1047	SER
1	A	1048	ASN
1	A	1050	GLU
1	A	1058	VAL
1	A	1064	VAL
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1095	THR
1	A	1101	LEU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1128	GLN
1	A	1130	GLN
1	A	1146	VAL
1	A	1159	ARG
1	A	1165	GLU
1	A	1167	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1187	GLN
1	A	1192	LEU

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Mol	Chain	Res	Type
1	A	1193	LEU
1	A	1205	LYS
1	A	1206	ASP
1	A	1208	THR
1	A	1219	THR
1	A	1227	ILE
1	A	1237	ILE
1	A	1238	ILE
1	A	1243	VAL
1	A	1257	ASP
1	A	1259	MET
1	A	1261	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1273	LEU
1	A	1274	ARG
1	A	1277	GLU
1	A	1279	ILE
1	A	1280	GLU
1	A	1285	MET
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1300	LYS
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1336	MET
1	A	1345	ARG
1	A	1350	LYS
1	A	1354	ASN
1	A	1355	VAL
1	A	1356	ILE
1	A	1359	ASP
1	A	1374	VAL
1	A	1376	THR

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Mol	Chain	Res	Type
1	A	1384	VAL
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1411	GLU
1	A	1422	ARG
1	A	1426	GLU
1	A	1445	ILE
2	B	20	ASP
2	B	28	GLU
2	B	46	GLN
2	B	58	THR
2	B	61	ASP
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	67	SER
2	B	70	ILE
2	B	94	LYS
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	108	VAL
2	B	120	ARG
2	B	133	LYS
2	B	134	LYS
2	B	167	ILE
2	B	169	ARG
2	B	175	ARG
2	B	179	CYS
2	B	181	LEU
2	B	183	GLU
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	234	ILE

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Mol	Chain	Res	Type
2	B	239	GLU
2	B	242	SER
2	B	245	GLU
2	B	246	LYS
2	B	249	ARG
2	B	252	SER
2	B	258	LEU
2	B	268	THR
2	B	272	THR
2	B	275	TYR
2	B	276	ILE
2	B	284	ILE
2	B	292	ILE
2	B	294	ASP
2	B	305	VAL
2	B	310	MET
2	B	313	MET
2	B	315	LYS
2	B	319	GLU
2	B	323	VAL
2	B	324	ILE
2	B	328	GLU
2	B	331	LEU
2	B	334	ILE
2	B	345	LYS
2	B	346	GLU
2	B	350	GLN
2	B	354	ASP
2	B	361	LEU
2	B	365	THR
2	B	366	GLN
2	B	367	LEU
2	B	368	GLU
2	B	382	ILE
2	B	384	ARG
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	395	GLN
2	B	398	ARG
2	B	415	GLN
2	B	425	THR

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Mol	Chain	Res	Type
2	B	426	LYS
2	B	428	ILE
2	B	436	VAL
2	B	437	GLU
2	B	448	ILE
2	B	454	THR
2	B	455	SER
2	B	461	LEU
2	B	468	GLU
2	B	471	LYS
2	B	474	SER
2	B	479	VAL
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	502	ILE
2	B	512	ARG
2	B	513	GLN
2	B	516	ASN
2	B	527	THR
2	B	531	GLN
2	B	544	CYS
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	574	SER
2	B	578	THR
2	B	598	GLU
2	B	604	ARG
2	B	606	LYS
2	B	609	ILE
2	B	617	ARG
2	B	619	ILE
2	B	624	LEU
2	B	633	VAL
2	B	635	ARG
2	B	637	LEU

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Mol	Chain	Res	Type
2	B	639	ILE
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	655	LYS
2	B	666	TYR
2	B	690	VAL
2	B	706	GLN
2	B	708	GLU
2	B	710	LEU
2	B	731	VAL
2	B	732	SER
2	B	739	THR
2	B	742	GLU
2	B	743	ILE
2	B	747	MET
2	B	751	VAL
2	B	764	SER
2	B	780	VAL
2	B	786	ASN
2	B	787	VAL
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	815	ARG
2	B	825	VAL
2	B	827	ILE
2	B	844	SER
2	B	864	LYS
2	B	865	LYS
2	B	868	MET
2	B	871	THR
2	B	879	ARG
2	B	880	THR
2	B	881	ASN
2	B	882	THR
2	B	893	LEU
2	B	894	ASP
2	B	899	ILE
2	B	901	PRO

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Mol	Chain	Res	Type
2	B	904	ARG
2	B	939	THR
2	B	943	SER
2	B	944	THR
2	B	955	THR
2	B	957	ASN
2	B	963	PHE
2	B	969	ARG
2	B	970	THR
2	B	976	ILE
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	1002	THR
2	B	1004	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1021	MET
2	B	1028	GLU
2	B	1032	SER
2	B	1046	PRO
2	B	1051	THR
2	B	1055	ILE
2	B	1057	LYS
2	B	1065	GLN
2	B	1077	THR
2	B	1082	MET
2	B	1093	GLN
2	B	1094	ARG
2	B	1096	ARG
2	B	1099	VAL
2	B	1101	ASP
2	B	1103	ILE
2	B	1111	MET
2	B	1113	VAL
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1147	LEU
2	B	1150	ARG

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Mol	Chain	Res	Type
2	B	1151	LEU
2	B	1155	SER
2	B	1159	ARG
2	B	1160	VAL
2	B	1174	LYS
2	B	1176	ASN
2	B	1181	GLU
2	B	1186	ASP
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1202	LEU
2	B	1220	ARG
3	C	4	GLU
3	C	9	LYS
3	C	10	ILE
3	C	11	ARG
3	C	15	LYS
3	C	18	VAL
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	27	LEU
3	C	35	ARG
3	C	38	ILE
3	C	41	ILE
3	C	46	ILE
3	C	53	THR
3	C	56	THR
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	89	GLU
3	C	99	LEU
3	C	100	THR
3	C	106	GLU
3	C	109	SER
3	C	110	THR
3	C	116	LYS
3	C	120	ILE
3	C	121	VAL

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Mol	Chain	Res	Type
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	140	ASN
3	C	147	LEU
3	C	149	LYS
3	C	151	GLN
3	C	154	LYS
3	C	177	GLU
3	C	183	TRP
3	C	186	LEU
3	C	189	THR
3	C	195	GLN
3	C	197	SER
3	C	203	GLN
3	C	204	SER
3	C	222	LYS
3	C	224	GLN
3	C	226	ASP
3	C	231	ASN
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	253	LYS
3	C	258	ILE
3	C	263	THR
3	C	268	ASP
4	E	3	GLN
4	E	9	ILE
4	E	14	ARG
4	E	30	ILE
4	E	31	THR
4	E	32	GLN
4	E	37	LEU
4	E	40	GLU
4	E	43	LYS
4	E	54	GLN
4	E	66	GLU
4	E	69	ILE
4	E	78	LEU

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Mol	Chain	Res	Type
4	E	80	VAL
4	E	92	THR
4	E	94	LYS
4	E	95	THR
4	E	98	ILE
4	E	101	GLN
4	E	103	LYS
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	137	GLU
4	E	144	ILE
4	E	146	HIS
4	E	150	VAL
4	E	152	LYS
4	E	154	ILE
4	E	162	ARG
4	E	164	LEU
4	E	165	LEU
4	E	169	ARG
4	E	179	GLN
4	E	191	LYS
4	E	192	ARG
4	E	200	ARG
4	E	201	LYS
4	E	202	SER
4	E	204	THR
4	E	215	MET
5	F	72	LYS
5	F	74	ILE
5	F	79	ARG
5	F	82	THR
5	F	93	ILE
5	F	97	ARG
5	F	103	MET
5	F	111	LEU
5	F	112	GLU
5	F	119	ARG
5	F	133	VAL
5	F	140	ASP
5	F	149	GLU

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Mol	Chain	Res	Type
5	F	150	GLU
5	F	155	LEU
6	H	2	SER
6	H	4	THR
6	H	11	GLN
6	H	15	VAL
6	H	21	ASN
6	H	24	CYS
6	H	26	ILE
6	H	32	THR
6	H	34	ASP
6	H	55	LEU
6	H	58	THR
6	H	59	ILE
6	H	83	GLN
6	H	89	LEU
6	H	100	THR
6	H	106	GLU
6	H	110	ASP
6	H	123	MET
6	H	124	ARG
6	H	130	ARG
6	H	136	LYS
6	H	137	GLN
6	H	142	LEU
7	I	3	THR
7	I	8	ARG
7	I	14	LEU
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	33	SER
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	60	GLN
7	I	74	GLU
7	I	75	CYS
7	I	83	ASN
7	I	89	GLN
7	I	90	GLN
7	I	91	ARG

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Mol	Chain	Res	Type
7	I	95	THR
7	I	106	CYS
7	I	107	SER
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	6	ARG
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	17	LYS
8	J	22	LEU
8	J	26	GLN
8	J	27	GLU
8	J	28	ASP
8	J	29	GLU
8	J	31	ASP
8	J	42	LYS
8	J	43	ARG
8	J	46	CYS
8	J	48	ARG
8	J	54	VAL
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	6	ARG
9	K	14	GLU
9	K	17	SER
9	K	18	LYS
9	K	20	LYS
9	K	26	LYS
9	K	31	VAL
9	K	32	VAL
9	K	42	LEU
9	K	46	ILE
9	K	51	LEU
9	K	56	VAL
9	K	77	THR
9	K	79	GLU

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Mol	Chain	Res	Type
9	K	82	ASP
9	K	101	LEU
9	K	102	LYS
9	K	103	THR
9	K	106	GLU
9	K	107	THR
10	L	27	LEU
10	L	28	LYS
10	L	31	CYS
10	L	38	LEU
10	L	42	ARG
10	L	55	ILE
10	L	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	68	GLN
1	A	75	ASN
1	A	83	HIS
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	273	ASN
1	A	297	GLN
1	A	311	GLN
1	A	316	GLN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	425	GLN
1	A	435	HIS
1	A	451	HIS
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	589	GLN
1	A	611	GLN
1	A	698	GLN
1	A	736	ASN
1	A	741	ASN

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Mol	Chain	Res	Type
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	906	HIS
1	A	926	GLN
1	A	968	GLN
1	A	1033	GLN
1	A	1110	ASN
1	A	1130	GLN
1	A	1171	GLN
1	A	1203	ASN
1	A	1270	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1393	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	115	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	255	GLN
2	B	325	GLN
2	B	350	GLN
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	433	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	573	GLN
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	686	ASN
2	B	744	HIS

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Mol	Chain	Res	Type
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	835	GLN
2	B	843	GLN
2	B	862	GLN
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1117	GLN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	123	ASN
3	C	128	ASN
3	C	167	HIS
3	C	188	HIS
3	C	206	ASN
3	C	224	GLN
3	C	242	GLN
3	C	264	GLN
3	C	267	GLN
4	E	32	GLN
4	E	63	ASN
4	E	147	HIS
4	E	179	GLN
6	H	11	GLN
6	H	133	ASN
6	H	137	GLN
7	I	12	ASN
7	I	60	GLN
7	I	83	ASN
7	I	114	GLN
9	K	65	HIS
9	K	76	GLN

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Mol	Chain	Res	Type
9	K	89	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	G
11	R	11	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	C7P	T	29	12	5,9,10	1.10	0	2,11,14	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	C7P	T	29	12	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1395/1733 (80%)	0.27	55 (3%)	43	25	47, 104, 216, 308	0
2	B	1106/1224 (90%)	0.03	32 (2%)	53	34	43, 86, 154, 209	0
3	C	266/318 (83%)	-0.15	0	100	100	62, 91, 135, 158	0
4	E	214/215 (99%)	0.52	4 (1%)	66	45	81, 159, 224, 242	0
5	F	84/155 (54%)	-0.00	2 (2%)	59	39	77, 110, 142, 150	0
6	H	133/146 (91%)	0.94	15 (11%)	10	6	101, 153, 199, 211	0
7	I	119/122 (97%)	0.61	5 (4%)	40	23	74, 118, 158, 172	0
8	J	65/70 (92%)	-0.41	0	100	100	56, 73, 100, 116	0
9	K	114/120 (95%)	-0.07	1 (0%)	81	64	59, 103, 131, 141	0
10	L	46/70 (65%)	1.08	6 (13%)	7	5	72, 143, 173, 182	0
11	R	11/11 (100%)	3.64	11 (100%)	0	0	140, 156, 209, 217	0
12	T	28/28 (100%)	2.51	14 (50%)	0	1	146, 280, 387, 396	0
13	N	14/14 (100%)	1.69	2 (14%)	6	4	308, 349, 380, 385	0
All	All	3595/4226 (85%)	0.23	147 (4%)	41	24	43, 103, 202, 396	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	477	ALA	7.5
10	L	27	LEU	5.6
2	B	335	GLY	5.2
1	A	141	LEU	5.1
10	L	28	LYS	4.8
1	A	318	SER	4.8
6	H	63	LEU	4.7
6	H	84	ALA	4.7
12	T	26	DC	4.5

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Mol	Chain	Res	Type	RSRZ
12	T	20	DC	4.5
11	R	8	G	4.4
12	T	21	DC	4.4
11	R	7	A	4.4
11	R	10	A	4.3
1	A	69	THR	4.3
11	R	11	C	4.3
2	B	70	ILE	4.1
6	H	140	ALA	4.0
2	B	643	ASP	4.0
12	T	25	DC	3.9
2	B	509	ALA	3.9
12	T	22	DT	3.9
11	R	6	G	3.9
11	R	9	G	3.8
12	T	24	DT	3.8
10	L	25	ALA	3.7
2	B	709	ASP	3.7
1	A	65	LEU	3.7
12	T	19	DT	3.7
6	H	139	ASN	3.6
12	T	18	DG	3.6
2	B	446	LEU	3.5
1	A	51	GLY	3.5
2	B	646	LEU	3.5
12	T	23	DC	3.4
11	R	2	U	3.4
11	R	5	A	3.4
12	T	27	DA	3.4
6	H	85	GLY	3.3
1	A	250	ILE	3.2
1	A	59	GLY	3.2
10	L	26	THR	3.1
12	T	28	DT	3.1
6	H	31	THR	3.0
1	A	154	SER	3.0
7	I	49	ILE	3.0
6	H	6	PHE	3.0
10	L	45	ALA	3.0
11	R	3	G	3.0
2	B	715	ALA	2.9
2	B	866	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
6	H	134	ASN	2.9
1	A	315	LEU	2.9
2	B	250	PHE	2.9
7	I	82	GLU	2.8
1	A	216	VAL	2.8
6	H	90	ALA	2.8
1	A	144	THR	2.8
6	H	130	ARG	2.8
1	A	317	LYS	2.8
1	A	322	VAL	2.7
2	B	473	MET	2.7
1	A	1081	LEU	2.7
11	R	1	A	2.7
2	B	474	SER	2.7
1	A	174	ILE	2.6
1	A	252	PHE	2.6
12	T	4	DC	2.6
2	B	710	LEU	2.6
5	F	155	LEU	2.6
2	B	816	GLU	2.6
2	B	733	HIS	2.6
11	R	4	G	2.6
6	H	136	LYS	2.5
1	A	1445	ILE	2.5
4	E	98	ILE	2.5
1	A	98	LYS	2.5
1	A	186	LYS	2.5
1	A	58	LEU	2.5
13	N	4	DG	2.4
1	A	121	LEU	2.4
1	A	73	GLY	2.4
2	B	731	VAL	2.4
1	A	126	LEU	2.4
1	A	54	ASN	2.4
2	B	334	ILE	2.4
1	A	64	ASN	2.4
1	A	114	LEU	2.4
1	A	153	PRO	2.4
2	B	865	LYS	2.4
1	A	41	MET	2.4
1	A	249	SER	2.4
2	B	1221	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	145	LYS	2.3
4	E	91	LYS	2.3
1	A	149	GLU	2.3
9	K	14	GLU	2.3
5	F	74	ILE	2.3
2	B	881	ASN	2.3
1	A	161	LEU	2.3
2	B	879	ARG	2.3
2	B	167	ILE	2.3
10	L	30	ILE	2.3
12	T	5	DC	2.3
1	A	234	MET	2.3
1	A	199	LEU	2.3
6	H	7	ASP	2.3
1	A	567	LYS	2.3
1	A	32	VAL	2.3
1	A	1403	GLU	2.3
1	A	148	CYS	2.3
1	A	61	ILE	2.2
2	B	90	ILE	2.2
1	A	568	PRO	2.2
1	A	152	VAL	2.2
7	I	52	ILE	2.2
1	A	1176	LEU	2.2
2	B	447	ALA	2.2
1	A	176	LYS	2.2
4	E	94	LYS	2.2
4	E	16	PHE	2.2
13	N	14	DG	2.2
2	B	870	ILE	2.2
1	A	1330	ASN	2.2
2	B	708	GLU	2.2
7	I	28	GLU	2.2
1	A	177	ASP	2.2
1	A	319	GLY	2.2
12	T	17	DC	2.1
1	A	66	LYS	2.1
1	A	1273	LEU	2.1
6	H	9	ILE	2.1
2	B	472	ALA	2.1
2	B	248	SER	2.1
6	H	86	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	277	LYS	2.1
6	H	58	THR	2.1
1	A	91	PHE	2.1
1	A	38	PRO	2.0
1	A	56	PRO	2.0
1	A	113	LEU	2.0
7	I	107	SER	2.0
1	A	248	PRO	2.0
1	A	316	GLN	2.0
1	A	147	VAL	2.0
2	B	132	VAL	2.0
2	B	883	LEU	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
16	C7P	T	29	9/10	0.88	0.29	205,229,260,269	1
15	MG	A	2001	1/1	0.93	0.09	67,67,67,67	0
14	ZN	A	1734	1/1	0.96	0.09	113,113,113,113	0
14	ZN	L	105	1/1	0.98	0.05	101,101,101,101	1
14	ZN	A	1735	1/1	0.98	0.07	83,83,83,83	0
14	ZN	B	1307	1/1	0.98	0.06	92,92,92,92	0
14	ZN	J	101	1/1	0.99	0.07	61,61,61,61	0
14	ZN	I	204	1/1	0.99	0.11	59,59,59,59	0
14	ZN	I	203	1/1	1.00	0.05	74,74,74,74	0
14	ZN	C	319	1/1	1.00	0.09	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.