



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:05 AM UTC

PDB ID : 2NVZ / pdb_00002nvz
Title : RNA Polymerase II elongation complex with UTP, updated 11/2006
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

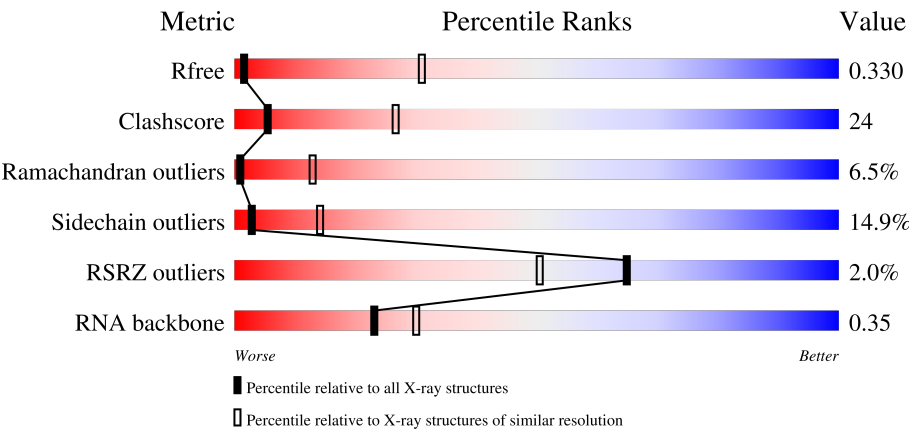
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)
RNA backbone	3983	1036 (5.50-3.10)

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

Mol	Chain	Length	Quality of chain
1	R	10	50%50%
2	T	28	4% 50%50%
3	N	14	86%14%
4	A	1733	% 40%32%7%19%

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1398	Total	C	N	O	S	0	0	0
			10984	6930	1924	2069	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1096	Total	C	N	O	S	0	0	0
			8701	5508	1518	1620	55			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	193	Total	C	N	O	S	0	0	0
			1594	1016	283	287	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

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

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

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

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

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

tide.

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

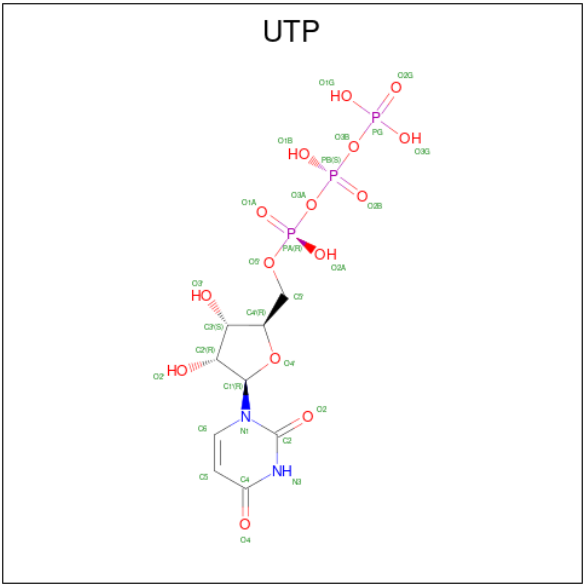
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	2	Total	Mg	0	0
			2	2		

- Molecule 16 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

3 Residue-property plots [i](#)

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

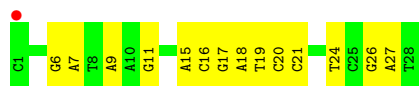
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R: 



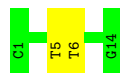
- Molecule 2: 28-MER DNA template strand

Chain T: 



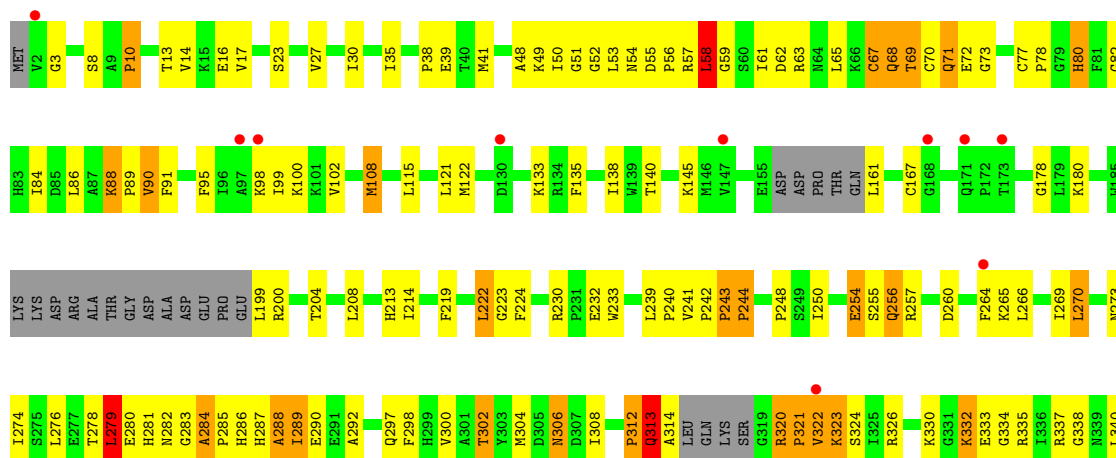
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

Chain N: 

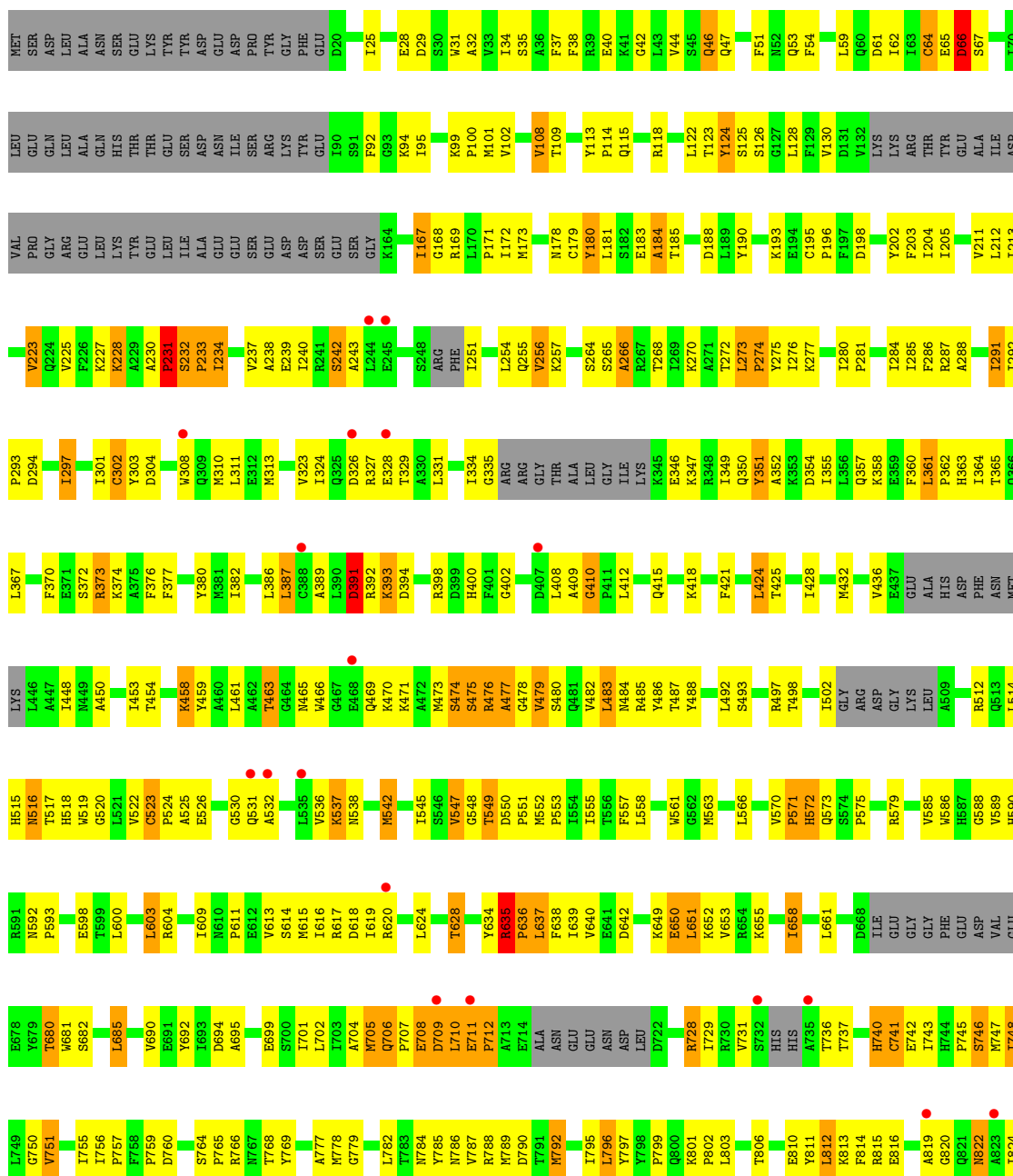
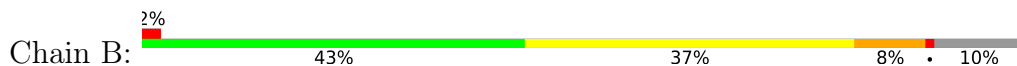


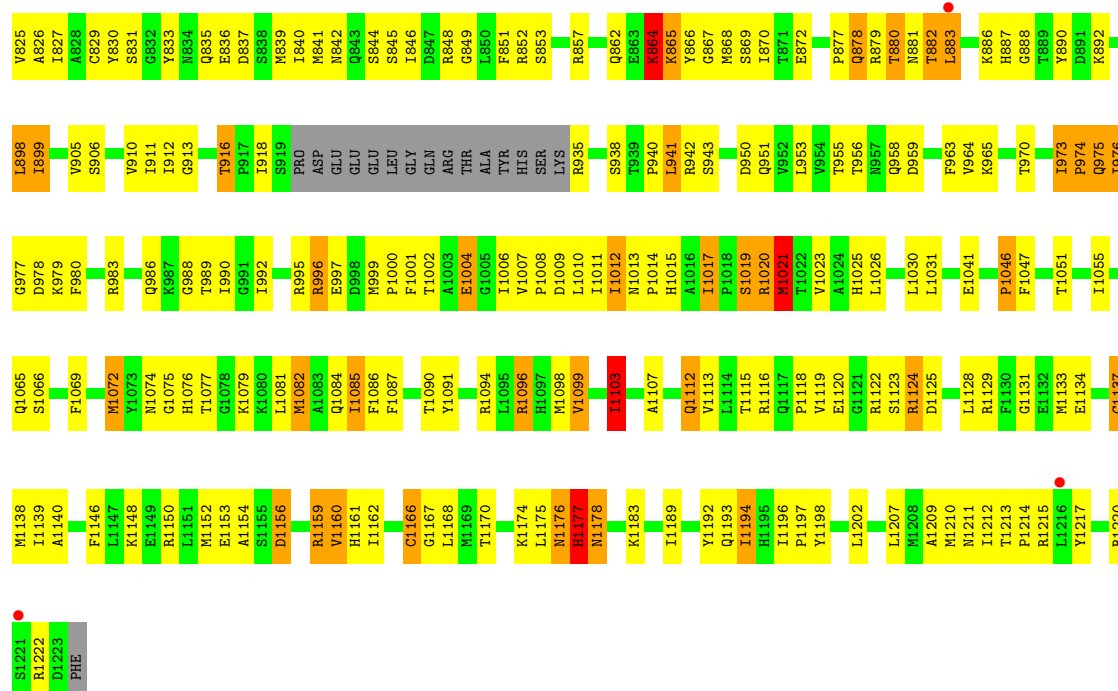
- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

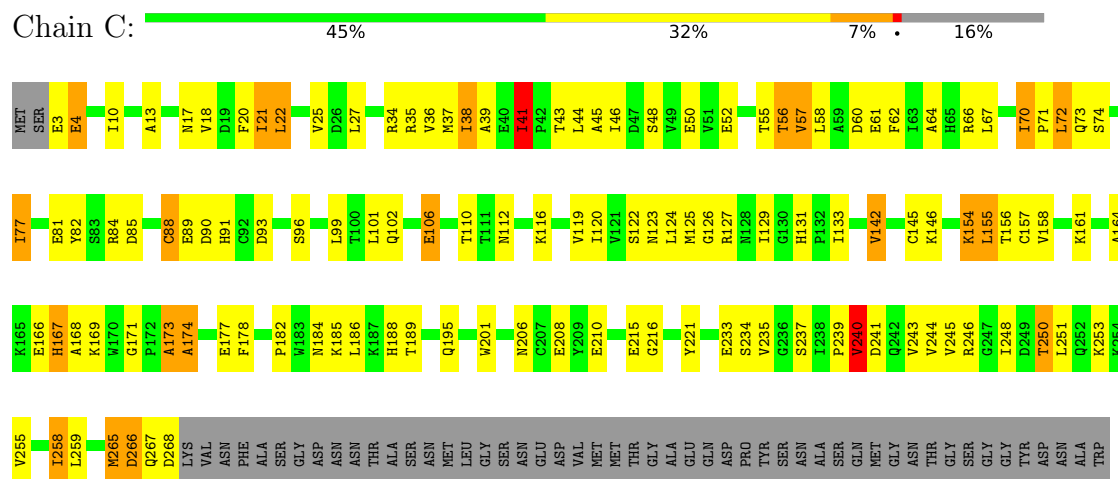




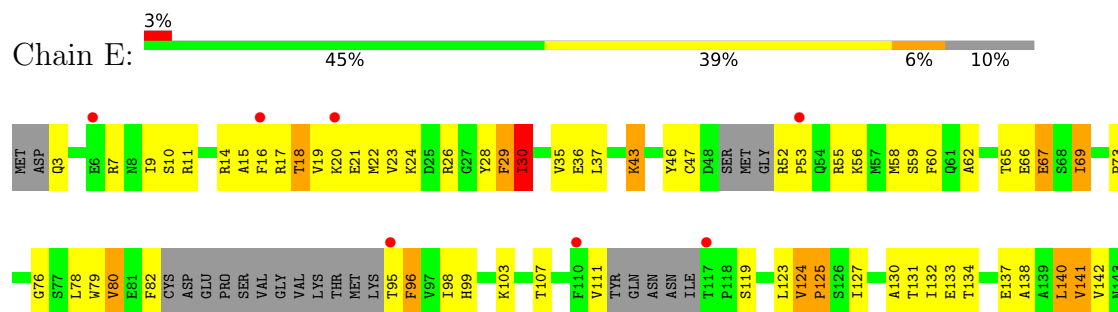


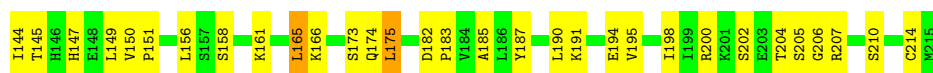


• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

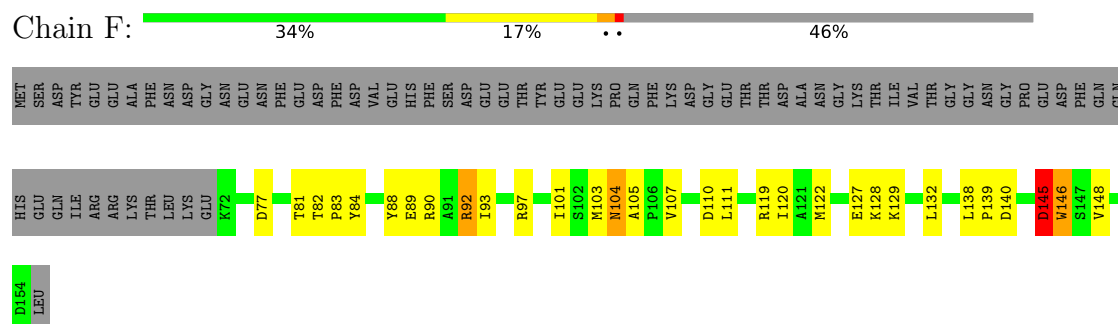


• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

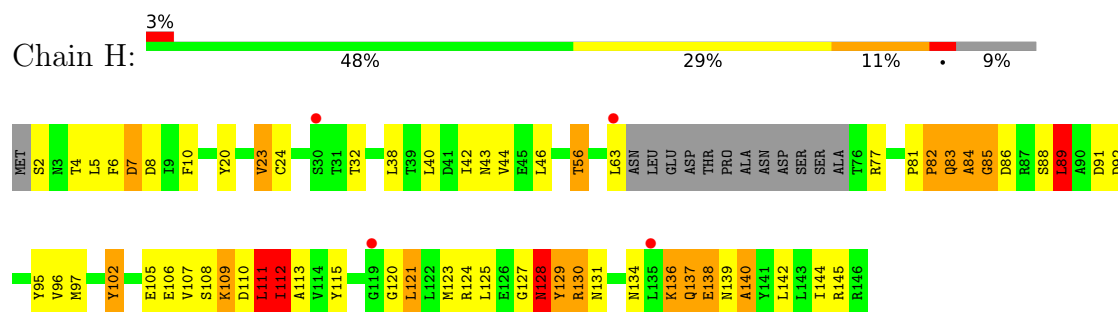




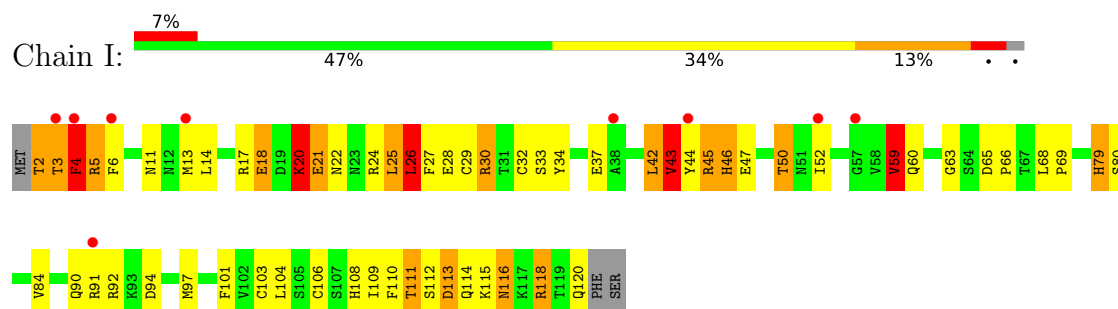
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



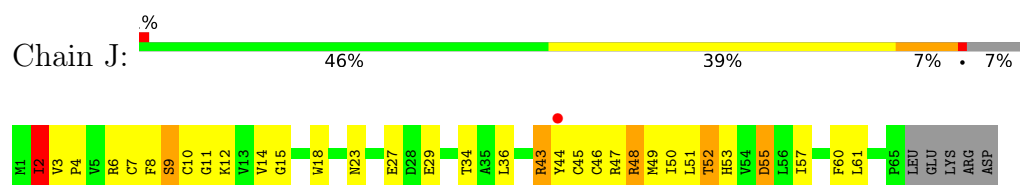
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



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

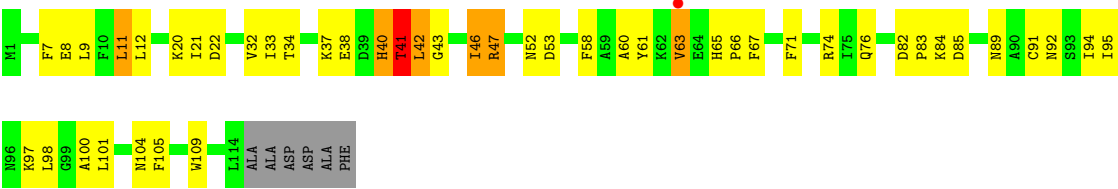


- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

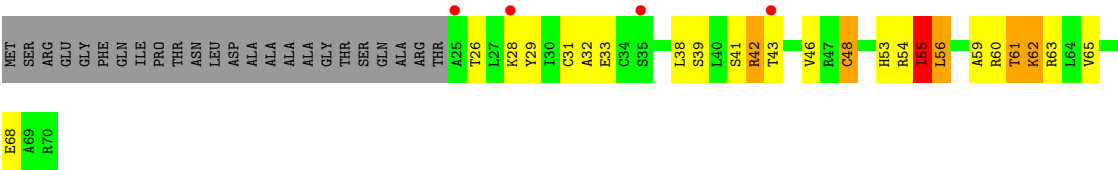
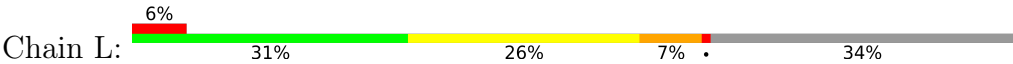


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide





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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.30 40.00 – 4.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.30) 86.3 (40.00-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.332 0.277 , 0.330	Depositor DCC
R_{free} test set	4179 reflections (8.72%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29002	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	R	0.59	0/243	0.97	0/378
2	T	0.35	0/634	0.92	1/975 (0.1%)
3	N	0.29	0/317	0.78	0/488
4	A	0.59	1/11180 (0.0%)	1.01	42/15117 (0.3%)
5	B	0.57	0/8866	0.95	24/11956 (0.2%)
6	C	0.55	0/2133	0.93	8/2891 (0.3%)
7	E	0.55	0/1625	0.92	1/2182 (0.0%)
8	F	0.56	0/682	0.88	0/922
9	H	0.63	0/1086	1.00	8/1470 (0.5%)
10	I	0.64	0/989	1.06	3/1331 (0.2%)
11	J	0.57	0/541	0.89	0/727
12	K	0.58	0/937	0.94	1/1265 (0.1%)
13	L	0.75	0/365	1.01	3/485 (0.6%)
All	All	0.58	1/29598 (0.0%)	0.97	91/40187 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	9
5	B	0	1
9	H	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1158	PRO	CG-CD	5.74	1.70	1.50

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	973	ILE	N-CA-C	8.98	119.02	110.30
4	A	1163	ILE	CA-C-N	8.70	130.72	119.84
4	A	1163	ILE	C-N-CA	8.70	130.72	119.84
9	H	129	TYR	N-CA-C	-8.65	102.73	113.28
12	K	41	THR	N-CA-C	-8.17	103.45	113.50
5	B	635	ARG	CA-C-N	7.65	129.40	119.84
5	B	635	ARG	C-N-CA	7.65	129.40	119.84
4	A	452	LYS	N-CA-C	-7.61	104.52	113.88
5	B	1019	SER	N-CA-C	7.60	120.29	111.02
5	B	709	ASP	N-CA-C	7.40	120.79	111.69
4	A	1071	SER	N-CA-C	6.99	123.83	114.12
4	A	1069	ALA	N-CA-C	-6.73	96.46	110.80
4	A	699	ALA	N-CA-C	6.59	119.80	111.69
4	A	1093	LYS	CA-C-N	6.50	133.41	121.70
4	A	1093	LYS	C-N-CA	6.50	133.41	121.70
4	A	975	HIS	CA-C-N	6.30	133.03	121.70
4	A	975	HIS	C-N-CA	6.30	133.03	121.70
10	I	5	ARG	N-CA-C	6.22	118.95	110.55
4	A	243	PRO	CA-C-N	6.22	126.79	120.38
4	A	243	PRO	C-N-CA	6.22	126.79	120.38
9	H	111	LEU	CA-C-N	6.21	132.88	121.70
9	H	111	LEU	C-N-CA	6.21	132.88	121.70
5	B	1066	SER	N-CA-C	6.19	118.83	111.71
4	A	956	LEU	CA-C-N	6.18	126.10	119.85
4	A	956	LEU	C-N-CA	6.18	126.10	119.85
6	C	70	ILE	CA-C-N	6.13	127.50	119.84
6	C	70	ILE	C-N-CA	6.13	127.50	119.84
4	A	244	PRO	N-CA-C	6.04	118.07	110.70
6	C	41	ILE	N-CA-CB	5.99	116.16	109.99
7	E	67	GLU	N-CA-C	-5.97	106.63	114.04
4	A	1319	VAL	N-CA-C	5.94	114.55	109.02
5	B	1177	HIS	CA-C-N	5.91	132.35	121.70
5	B	1177	HIS	C-N-CA	5.91	132.35	121.70
2	T	15	DA	P-O3'-C3'	5.84	128.96	120.20
5	B	709	ASP	CA-C-N	5.81	132.15	121.70
5	B	709	ASP	C-N-CA	5.81	132.15	121.70
13	L	42	ARG	CA-C-N	5.80	132.15	121.70
13	L	42	ARG	C-N-CA	5.80	132.15	121.70
5	B	389	ALA	N-CA-C	-5.78	106.20	113.72
6	C	155	LEU	N-CA-C	5.73	117.90	109.24
4	A	1070	GLN	N-CA-C	-5.73	94.95	111.00
5	B	231	PRO	CA-C-N	5.73	132.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	231	PRO	C-N-CA	5.73	132.01	121.70
4	A	460	VAL	N-CA-C	5.70	116.00	107.51
4	A	1283	VAL	N-CA-C	5.68	116.05	107.75
4	A	714	PHE	N-CA-C	-5.67	106.19	113.23
6	C	240	VAL	N-CA-C	5.65	117.06	110.62
4	A	1162	VAL	CA-C-N	5.52	131.64	121.70
4	A	1162	VAL	C-N-CA	5.52	131.64	121.70
6	C	60	ASP	N-CA-C	5.52	116.97	111.07
4	A	1071	SER	CA-C-N	5.51	131.63	121.70
4	A	1071	SER	C-N-CA	5.51	131.63	121.70
4	A	281	HIS	N-CA-C	-5.51	105.55	114.09
5	B	523	CYS	CA-C-N	5.50	125.33	119.28
5	B	523	CYS	C-N-CA	5.50	125.33	119.28
4	A	88	LYS	CA-C-N	5.45	126.65	119.84
4	A	88	LYS	C-N-CA	5.45	126.65	119.84
4	A	230	ARG	CA-C-N	5.40	125.48	119.32
4	A	230	ARG	C-N-CA	5.40	125.48	119.32
4	A	1159	ARG	CA-C-N	5.39	131.40	121.70
4	A	1159	ARG	C-N-CA	5.39	131.40	121.70
4	A	524	VAL	N-CA-C	5.39	115.74	107.77
4	A	1191	TRP	CA-C-N	5.34	131.31	121.70
4	A	1191	TRP	C-N-CA	5.34	131.31	121.70
9	H	128	ASN	N-CA-C	5.32	117.31	107.73
5	B	231	PRO	N-CA-C	5.29	123.38	112.47
9	H	109	LYS	CA-C-N	5.28	131.21	121.70
9	H	109	LYS	C-N-CA	5.28	131.21	121.70
9	H	137	GLN	N-CA-C	5.27	116.89	110.41
4	A	242	PRO	CA-C-N	5.26	125.79	120.38
4	A	242	PRO	C-N-CA	5.26	125.79	120.38
5	B	99	LYS	CA-C-N	5.25	126.40	119.84
5	B	99	LYS	C-N-CA	5.25	126.40	119.84
5	B	380	TYR	N-CA-C	-5.21	106.83	114.39
4	A	999	VAL	N-CA-C	-5.20	107.51	111.62
5	B	706	GLN	CA-C-N	5.16	126.86	121.65
5	B	706	GLN	C-N-CA	5.16	126.86	121.65
9	H	5	LEU	N-CA-C	5.15	119.56	113.12
6	C	4	GLU	N-CA-C	5.14	116.74	111.03
5	B	516	ASN	N-CA-C	5.11	117.59	111.71
4	A	1151	GLU	N-CA-C	5.11	117.73	109.40
5	B	1170	THR	N-CA-C	-5.11	108.80	114.62
5	B	1019	SER	CA-C-N	5.10	130.88	121.70
5	B	1019	SER	C-N-CA	5.10	130.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	3	THR	CA-C-N	5.09	130.85	121.70
10	I	3	THR	C-N-CA	5.09	130.85	121.70
4	A	1152	ILE	CA-C-N	5.07	130.83	121.70
4	A	1152	ILE	C-N-CA	5.07	130.83	121.70
6	C	106	GLU	N-CA-C	-5.07	107.64	113.88
13	L	41	SER	N-CA-C	5.03	116.78	108.48
4	A	1155	ASP	N-CA-C	5.02	120.90	109.81

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1068	ALA	Peptide
4	A	1069	ALA	Peptide
4	A	1070	GLN	Peptide
4	A	1079	MET	Peptide
4	A	1084	PHE	Peptide
4	A	1155	ASP	Peptide
4	A	1157	ASP	Peptide
4	A	451	HIS	Peptide
4	A	974	ASP	Peptide
5	B	1176	ASN	Peptide
9	H	128	ASN	Peptide
9	H	130	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	6	0
2	T	566	0	316	19	0
3	N	284	0	161	2	0
4	A	10984	0	11069	605	0
5	B	8701	0	8728	499	0
6	C	2095	0	2051	93	0
7	E	1594	0	1622	57	0
8	F	670	0	690	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1068	0	1040	53	0
10	I	971	0	928	65	0
11	J	532	0	542	39	0
12	K	919	0	929	33	0
13	L	363	0	387	13	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	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	B	29	0	11	2	0
All	All	29002	0	28583	1368	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 24.

All (1368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:701:LEU:HA	4:A:702:LEU:CB	1.68	1.20
4:A:975:HIS:HB3	4:A:976:THR:OG1	1.41	1.19
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.27	1.16
4:A:1167:GLU:CB	4:A:1168:GLU:HA	1.75	1.15
5:B:1019:SER:HB2	5:B:1020:ARG:HB2	1.24	1.15
4:A:707:GLY:HA2	4:A:709:THR:H	0.99	1.14
4:A:712:GLU:H	4:A:713:SER:HB2	0.98	1.14
4:A:709:THR:HA	4:A:710:LEU:HB3	1.19	1.13
5:B:227:LYS:HA	5:B:228:LYS:HB2	1.29	1.12
10:I:3:THR:HA	10:I:4:PHE:CG	1.85	1.11
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.33	1.11
4:A:1167:GLU:HB2	4:A:1168:GLU:CA	1.81	1.09
5:B:705:MET:HB3	5:B:706:GLN:HB2	1.08	1.08
4:A:1080:THR:O	4:A:1082:ASN:N	1.86	1.08
5:B:877:PRO:HA	5:B:878:GLN:CB	1.84	1.07
9:H:85:GLY:HA2	9:H:86:ASP:HB2	1.14	1.06
5:B:868:MET:H	5:B:869:SER:HB3	0.92	1.06
10:I:20:LYS:HA	10:I:21:GLU:O	1.57	1.05
4:A:707:GLY:HA2	4:A:709:THR:N	1.72	1.04
5:B:327:ARG:HB3	5:B:328:GLU:HB2	1.09	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:293:PRO:HA	5:B:294:ASP:HB2	1.40	1.03
4:A:701:LEU:CA	4:A:702:LEU:HB2	1.88	1.03
4:A:1091:SER:HB2	4:A:1092:LYS:C	1.84	1.03
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.04	1.03
13:L:42:ARG:HB2	13:L:43:THR:HB	1.35	1.03
10:I:25:LEU:HA	10:I:26:LEU:CB	1.89	1.02
5:B:256:VAL:HG11	5:B:382:ILE:HD11	1.40	1.02
4:A:712:GLU:N	4:A:713:SER:HB2	1.73	1.02
10:I:45:ARG:HA	10:I:46:HIS:HB2	1.05	1.02
5:B:868:MET:N	5:B:869:SER:HB3	1.74	1.02
5:B:636:PRO:HB2	5:B:637:LEU:HB3	1.43	1.00
5:B:1019:SER:CB	5:B:1020:ARG:HB2	1.91	1.00
5:B:868:MET:H	5:B:869:SER:CB	1.75	1.00
9:H:111:LEU:HB3	9:H:128:ASN:HB2	1.41	0.99
9:H:85:GLY:CA	9:H:86:ASP:HB2	1.91	0.99
4:A:709:THR:HA	4:A:710:LEU:CB	1.92	0.99
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.26	0.99
5:B:877:PRO:HA	5:B:878:GLN:HB2	1.44	0.98
10:I:45:ARG:HA	10:I:46:HIS:CB	1.93	0.98
5:B:635:ARG:CB	5:B:636:PRO:HD2	1.92	0.98
4:A:712:GLU:H	4:A:713:SER:CB	1.76	0.98
10:I:25:LEU:HA	10:I:26:LEU:HB2	1.44	0.98
5:B:635:ARG:HB2	5:B:636:PRO:CD	1.94	0.97
4:A:802:ASN:HD21	5:B:729:ILE:H	0.98	0.97
4:A:67:CYS:CB	4:A:70:CYS:HB2	1.93	0.97
9:H:85:GLY:HA2	9:H:86:ASP:CB	1.94	0.97
4:A:1071:SER:H	4:A:1072:ILE:HB	1.26	0.96
10:I:63:GLY:HA3	10:I:104:LEU:HD21	1.45	0.96
10:I:45:ARG:CA	10:I:46:HIS:HB2	1.95	0.96
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.30	0.95
4:A:1236:LEU:HA	4:A:1237:ILE:HB	1.46	0.95
4:A:782:ARG:HB3	4:A:789:LYS:HA	1.46	0.95
5:B:766:ARG:HH21	5:B:1020:ARG:HA	1.26	0.95
9:H:84:ALA:HA	9:H:85:GLY:C	1.92	0.94
4:A:284:ALA:H	4:A:285:PRO:HD3	1.29	0.94
5:B:350:GLN:HB3	5:B:351:TYR:HB2	1.48	0.94
4:A:284:ALA:H	4:A:285:PRO:CD	1.80	0.94
4:A:701:LEU:HA	4:A:702:LEU:HB2	0.95	0.94
6:C:58:LEU:HD11	11:J:2:ILE:HD12	1.50	0.93
5:B:882:THR:HB	5:B:883:LEU:HA	1.49	0.92
4:A:709:THR:CA	4:A:710:LEU:HB3	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:67:LEU:O	6:C:70:ILE:HG22	1.69	0.91
5:B:327:ARG:CB	5:B:328:GLU:HB2	2.01	0.90
1:R:10:A:H61	2:T:19:DT:H3	1.16	0.90
4:A:282:ASN:HB3	4:A:283:GLY:CA	2.02	0.90
5:B:122:LEU:HD22	5:B:958:GLN:HG3	1.51	0.89
1:R:4:G:H2'	1:R:5:A:H8	1.38	0.89
6:C:74:SER:O	6:C:77:ILE:HB	1.74	0.87
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.55	0.87
5:B:636:PRO:HB2	5:B:637:LEU:CB	2.05	0.86
10:I:20:LYS:HA	10:I:21:GLU:C	2.01	0.86
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.76	0.86
1:R:4:G:H2'	1:R:5:A:C8	2.10	0.85
4:A:108:MET:HE3	4:A:167:CYS:HB2	1.57	0.85
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.56	0.85
4:A:1085:HIS:H	4:A:1085:HIS:CD2	1.88	0.85
4:A:1152:ILE:HA	4:A:1153:TYR:HB2	1.57	0.84
5:B:705:MET:HB3	5:B:706:GLN:CB	2.01	0.84
4:A:630:ILE:HD12	4:A:630:ILE:H	1.43	0.84
5:B:705:MET:CB	5:B:706:GLN:HB2	2.03	0.84
4:A:423:ASP:CG	4:A:424:ILE:H	1.85	0.83
1:R:9:G:N2	2:T:21:DC:H1'	1.92	0.83
4:A:67:CYS:HB2	4:A:70:CYS:HB2	1.59	0.83
4:A:1082:ASN:N	4:A:1083:THR:HA	1.90	0.83
4:A:1191:TRP:HA	4:A:1192:LEU:HB2	1.58	0.83
5:B:782:LEU:HD13	5:B:784:ASN:HD21	1.43	0.83
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.61	0.83
5:B:557:PHE:O	5:B:561:TRP:HB3	1.79	0.83
4:A:1083:THR:OG1	4:A:1084:PHE:HB3	1.79	0.83
4:A:1097:GLY:H	4:A:1100:ARG:HB2	1.41	0.83
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.60	0.83
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.12	0.82
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.59	0.82
7:E:165:LEU:HD21	7:E:175:LEU:HD21	1.61	0.82
10:I:25:LEU:CA	10:I:26:LEU:HB2	2.08	0.82
4:A:335:ARG:HD2	5:B:1202:LEU:CD1	2.06	0.82
6:C:184:ASN:ND2	6:C:189:THR:O	2.13	0.82
5:B:572:HIS:H	5:B:573:GLN:C	1.88	0.81
5:B:877:PRO:HA	5:B:878:GLN:HB3	1.62	0.81
5:B:973:ILE:HG22	5:B:974:PRO:HD2	1.63	0.81
4:A:1191:TRP:HA	4:A:1192:LEU:CB	2.10	0.81
5:B:571:PRO:HB2	5:B:572:HIS:HA	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:498:THR:HB	5:B:537:LYS:O	1.81	0.81
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.60	0.81
6:C:248:ILE:HG23	12:K:98:LEU:HD22	1.61	0.81
5:B:327:ARG:HB3	5:B:328:GLU:CB	2.04	0.81
10:I:43:VAL:HB	10:I:44:TYR:HA	1.61	0.81
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.16	0.80
5:B:349:ILE:HA	5:B:352:ALA:HB2	1.63	0.80
1:R:9:G:H22	2:T:21:DC:H1'	1.46	0.80
4:A:902:LEU:O	4:A:903:ASN:HB2	1.81	0.80
16:B:3000:UTP:O2A	16:B:3000:UTP:H4'	1.79	0.80
4:A:1159:ARG:HB2	4:A:1160:SER:C	2.07	0.79
4:A:1155:ASP:CG	4:A:1190:PRO:HA	2.07	0.79
4:A:1159:ARG:HB2	4:A:1161:THR:N	1.97	0.79
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.65	0.79
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.45	0.79
5:B:955:THR:HG22	5:B:956:THR:H	1.46	0.79
4:A:1083:THR:N	4:A:1084:PHE:O	2.16	0.79
4:A:1089:VAL:N	4:A:1090:ALA:HA	1.98	0.78
5:B:1008:PRO:HB3	5:B:1087:PHE:HE1	1.45	0.78
4:A:707:GLY:CA	4:A:709:THR:H	1.91	0.78
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.64	0.78
5:B:493:SER:OG	5:B:751:VAL:HB	1.83	0.78
5:B:600:LEU:HB3	5:B:615:MET:SD	2.24	0.78
5:B:124:TYR:HH	5:B:179:CYS:HG	1.30	0.77
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.50	0.77
4:A:351:THR:HG22	4:A:352:VAL:N	1.99	0.77
5:B:256:VAL:HG11	5:B:382:ILE:CD1	2.14	0.77
6:C:58:LEU:HD11	11:J:2:ILE:CD1	2.13	0.77
10:I:17:ARG:O	10:I:26:LEU:HB3	1.85	0.77
4:A:834:THR:HG21	4:A:1080:THR:HG21	1.66	0.77
5:B:801:LYS:O	11:J:52:THR:HG22	1.83	0.77
4:A:681:GLU:HA	4:A:684:ALA:HB3	1.66	0.77
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.67	0.77
4:A:278:THR:O	4:A:279:LEU:HB2	1.86	0.76
5:B:705:MET:H	5:B:710:LEU:HD13	1.51	0.76
5:B:277:LYS:HD2	5:B:335:GLY:H	1.50	0.76
13:L:32:ALA:H	13:L:55:ILE:HD13	1.50	0.76
13:L:42:ARG:CB	13:L:43:THR:HB	2.16	0.76
4:A:1228:TRP:HD1	4:A:1228:TRP:O	1.68	0.76
5:B:877:PRO:CA	5:B:878:GLN:CB	2.63	0.75
6:C:93:ASP:OD1	6:C:122:SER:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:675:THR:HG21	4:A:736:ASN:HD21	1.49	0.75
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.68	0.75
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.66	0.75
4:A:1072:ILE:HG22	4:A:1073:GLY:N	2.02	0.75
5:B:572:HIS:H	5:B:573:GLN:CA	1.99	0.75
4:A:701:LEU:CA	4:A:702:LEU:CB	2.58	0.75
4:A:1167:GLU:HB2	4:A:1168:GLU:HA	0.86	0.75
10:I:4:PHE:C	10:I:4:PHE:HD1	1.94	0.75
4:A:265:LYS:HZ1	4:A:323:LYS:HE2	1.51	0.74
4:A:579:SER:HA	4:A:582:ILE:CG1	2.17	0.74
4:A:1427:ASN:HB2	4:A:1434:ALA:HB2	1.69	0.74
4:A:1069:ALA:HB1	4:A:1070:GLN:HA	1.69	0.74
4:A:630:ILE:HD12	4:A:630:ILE:N	2.02	0.74
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.23	0.74
4:A:446:ARG:HH12	4:A:448:PRO:HD2	1.52	0.74
6:C:34:ARG:O	6:C:38:ILE:HG12	1.87	0.74
5:B:227:LYS:HA	5:B:228:LYS:CB	2.15	0.74
10:I:3:THR:HA	10:I:4:PHE:CB	2.17	0.74
9:H:111:LEU:HA	9:H:112:ILE:HB	1.70	0.73
4:A:1071:SER:N	4:A:1072:ILE:HB	2.02	0.73
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.51	0.73
6:C:58:LEU:HD12	6:C:145:CYS:SG	2.28	0.73
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.70	0.73
4:A:1092:LYS:HB3	4:A:1093:LYS:HA	1.70	0.73
4:A:1093:LYS:HB3	4:A:1094:VAL:HB	1.71	0.73
2:T:6:DG:H2"	2:T:7:DA:C8	2.23	0.73
4:A:751:SER:HB2	5:B:1015:HIS:HE1	1.53	0.73
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.53	0.73
5:B:864:LYS:H	5:B:872:GLU:HB2	1.54	0.73
4:A:282:ASN:HB3	4:A:283:GLY:HA3	1.70	0.73
10:I:20:LYS:HG2	10:I:24:ARG:H	1.54	0.73
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.70	0.72
10:I:43:VAL:CB	10:I:44:TYR:HA	2.17	0.72
13:L:42:ARG:HB2	13:L:43:THR:CB	2.16	0.72
4:A:638:GLY:H	4:A:641:VAL:HB	1.54	0.72
4:A:915:SER:HB2	4:A:919:ILE:HG12	1.72	0.72
4:A:1083:THR:N	4:A:1084:PHE:C	2.47	0.72
5:B:636:PRO:CB	5:B:637:LEU:HA	2.18	0.72
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.70	0.72
5:B:1001:PHE:HE1	6:C:178:PHE:HB3	1.53	0.72
4:A:1091:SER:HB2	4:A:1092:LYS:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.52	0.72
11:J:43:ARG:HG3	11:J:46:CYS:SG	2.29	0.72
4:A:975:HIS:HB3	4:A:976:THR:HG1	1.51	0.72
5:B:882:THR:HG21	5:B:935:ARG:HA	1.70	0.72
4:A:579:SER:HA	4:A:582:ILE:HG13	1.71	0.72
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.72	0.72
5:B:705:MET:O	5:B:742:GLU:HB3	1.90	0.72
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.25	0.71
5:B:636:PRO:CB	5:B:637:LEU:CA	2.69	0.71
5:B:126:SER:OG	5:B:172:ILE:HD11	1.90	0.71
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.54	0.71
10:I:4:PHE:C	10:I:4:PHE:CD1	2.69	0.71
5:B:642:ASP:HA	5:B:649:LYS:HA	1.72	0.71
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.72	0.71
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.05	0.71
4:A:288:ALA:HA	4:A:290:GLU:N	2.06	0.70
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.56	0.70
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.74	0.70
4:A:1072:ILE:HG22	4:A:1073:GLY:H	1.56	0.70
5:B:842:ASN:HB3	5:B:845:SER:OG	1.91	0.70
4:A:1075:PRO:O	4:A:1079:MET:N	2.24	0.70
5:B:1156:ASP:HB2	5:B:1198:TYR:H	1.55	0.70
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.73	0.70
5:B:1019:SER:CA	5:B:1020:ARG:HB2	2.22	0.70
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.72	0.69
4:A:802:ASN:HD21	5:B:729:ILE:N	1.83	0.69
5:B:636:PRO:HB2	5:B:637:LEU:CA	2.23	0.69
4:A:288:ALA:HA	4:A:290:GLU:H	1.57	0.69
5:B:1177:HIS:HA	5:B:1178:ASN:HB2	1.74	0.69
6:C:142:VAL:HG13	11:J:15:GLY:HA3	1.73	0.69
5:B:986:GLN:HE21	5:B:1025:HIS:CD2	2.10	0.69
9:H:105:GLU:HG3	9:H:106:GLU:H	1.58	0.69
5:B:168:GLY:H	5:B:450:ALA:HB1	1.57	0.69
5:B:997:GLU:OE1	6:C:39:ALA:HB2	1.92	0.69
4:A:657:LEU:HD21	5:B:829:CYS:HB3	1.75	0.69
10:I:25:LEU:HA	10:I:26:LEU:HB3	1.72	0.69
4:A:1064:VAL:O	4:A:1068:ALA:N	2.26	0.69
10:I:33:SER:HA	10:I:34:TYR:HB3	1.75	0.68
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.76	0.68
5:B:363:HIS:O	5:B:364:ILE:HB	1.93	0.68
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:446:ARG:NH1	4:A:448:PRO:HD2	2.09	0.68
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.74	0.67
4:A:1200:ALA:HB2	4:A:1203:ASN:HB2	1.77	0.67
5:B:65:GLU:O	5:B:66:ASP:HB3	1.95	0.67
5:B:827:ILE:HG12	5:B:1012:ILE:CD1	2.25	0.67
4:A:711:ARG:HA	4:A:713:SER:HB2	1.77	0.67
4:A:834:THR:HG21	4:A:1080:THR:CG2	2.25	0.67
4:A:1084:PHE:CD1	4:A:1085:HIS:HA	2.30	0.67
6:C:21:ILE:HG22	6:C:22:LEU:H	1.59	0.67
4:A:1084:PHE:HA	4:A:1085:HIS:C	2.19	0.67
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.77	0.67
5:B:852:ARG:HG2	5:B:973:ILE:HG23	1.76	0.67
10:I:17:ARG:HB2	10:I:26:LEU:HD12	1.77	0.66
4:A:1085:HIS:H	4:A:1085:HIS:HD2	1.41	0.66
4:A:1085:HIS:CD2	4:A:1085:HIS:N	2.63	0.66
5:B:287:ARG:NH1	5:B:324:ILE:O	2.28	0.66
6:C:101:LEU:HD23	6:C:155:LEU:HD12	1.78	0.66
4:A:1069:ALA:HA	4:A:1072:ILE:HG21	1.77	0.66
4:A:1143:LEU:HB3	4:A:1268:LEU:HA	1.76	0.66
4:A:1228:TRP:O	4:A:1228:TRP:CD1	2.48	0.66
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.78	0.66
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.76	0.65
4:A:630:ILE:H	4:A:630:ILE:CD1	2.09	0.65
5:B:230:ALA:N	5:B:231:PRO:HD3	2.12	0.65
5:B:1137:CYS:O	5:B:1140:ALA:HB3	1.95	0.65
4:A:1104:ILE:HG22	4:A:1105:LEU:HD12	1.79	0.65
4:A:1159:ARG:HD2	4:A:1161:THR:HG23	1.77	0.65
4:A:994:GLN:HG3	4:A:1019:CYS:SG	2.36	0.65
6:C:171:GLY:C	6:C:173:ALA:H	2.03	0.65
9:H:88:SER:O	9:H:89:LEU:HB3	1.95	0.65
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.78	0.65
4:A:782:ARG:NH2	5:B:699:GLU:O	2.29	0.65
4:A:1080:THR:C	4:A:1082:ASN:H	2.00	0.65
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.79	0.65
5:B:709:ASP:HB3	5:B:710:LEU:HD12	1.79	0.65
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.78	0.65
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.62	0.65
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.78	0.64
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.78	0.64
4:A:381:THR:HG22	4:A:382:PRO:HD2	1.79	0.64
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:407:ARG:HD2	4:A:413:ILE:HD13	1.79	0.64
6:C:112:ASN:HD21	6:C:146:LYS:HE2	1.62	0.64
8:F:145:ASP:O	8:F:146:TRP:HB2	1.97	0.64
4:A:545:GLN:O	4:A:549:MET:HG3	1.97	0.64
5:B:421:PHE:O	5:B:424:LEU:HD23	1.96	0.64
5:B:572:HIS:N	5:B:573:GLN:HB3	2.12	0.64
5:B:711:GLU:H	5:B:712:PRO:CD	2.09	0.64
5:B:728:ARG:NH1	5:B:760:ASP:OD2	2.28	0.64
4:A:1092:LYS:HB3	4:A:1093:LYS:CA	2.26	0.64
4:A:1197:LEU:HA	4:A:1198:ASP:HB3	1.78	0.64
5:B:848:ARG:NH1	11:J:8:PHE:O	2.30	0.64
4:A:802:ASN:ND2	5:B:729:ILE:H	1.82	0.64
5:B:124:TYR:OH	5:B:179:CYS:SG	2.49	0.64
5:B:474:SER:HB2	5:B:476:ARG:HG3	1.79	0.64
5:B:886:LYS:HG2	5:B:940:PRO:HG3	1.78	0.64
6:C:84:ARG:HD2	12:K:11:LEU:HD11	1.79	0.64
5:B:572:HIS:H	5:B:573:GLN:HB3	1.61	0.64
5:B:579:ARG:HA	5:B:589:VAL:HA	1.80	0.64
4:A:849:MET:HB3	4:A:1063:MET:SD	2.38	0.64
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.79	0.64
4:A:845:LEU:HB2	4:A:1065:GLY:O	1.98	0.63
5:B:287:ARG:HH21	5:B:294:ASP:CG	2.06	0.63
4:A:282:ASN:CB	4:A:283:GLY:HA3	2.28	0.63
5:B:286:PHE:HB3	5:B:297:ILE:HD11	1.81	0.63
4:A:10:PRO:HG2	5:B:1192:TYR:HA	1.81	0.63
5:B:882:THR:CG2	5:B:935:ARG:HA	2.28	0.63
4:A:472:LEU:HD13	5:B:835:GLN:NE2	2.13	0.63
7:E:65:THR:C	7:E:67:GLU:H	2.06	0.63
4:A:868:TYR:HE2	4:A:1366:ARG:HE	1.45	0.63
4:A:975:HIS:CB	4:A:976:THR:OG1	2.34	0.63
4:A:1421:CYS:HA	4:A:1426:GLU:HG2	1.81	0.62
5:B:67:SER:HB2	5:B:92:PHE:H	1.63	0.62
5:B:572:HIS:H	5:B:573:GLN:CB	2.12	0.62
4:A:282:ASN:HB3	4:A:283:GLY:HA2	1.79	0.62
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.80	0.62
5:B:913:GLY:HA2	5:B:938:SER:HB3	1.81	0.62
4:A:269:ILE:HD11	4:A:300:VAL:HG23	1.81	0.62
5:B:785:TYR:HE2	11:J:60:PHE:CE1	2.17	0.62
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.34	0.62
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.35	0.62
5:B:524:PRO:HG3	5:B:748:ILE:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:785:TYR:CE2	11:J:60:PHE:CE1	2.87	0.62
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.64	0.62
5:B:782:LEU:HD13	5:B:784:ASN:ND2	2.13	0.62
4:A:466:SER:O	5:B:1103:ILE:HD11	1.99	0.62
4:A:845:LEU:O	4:A:848:ILE:HG12	2.00	0.62
5:B:1008:PRO:HB3	5:B:1087:PHE:CE1	2.32	0.62
5:B:1082:MET:HG2	6:C:188:HIS:O	1.99	0.62
6:C:20:PHE:HD1	6:C:21:ILE:O	1.82	0.62
7:E:16:PHE:CE2	7:E:20:LYS:HE2	2.34	0.62
5:B:877:PRO:CA	5:B:878:GLN:HB3	2.29	0.62
4:A:1083:THR:HG23	4:A:1084:PHE:HD2	1.64	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.88	0.62
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.63	0.62
4:A:1093:LYS:H	4:A:1095:THR:H	1.49	0.61
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	1.80	0.61
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.34	0.61
5:B:778:MET:CE	5:B:853:SER:HB3	2.29	0.61
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.82	0.61
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.30	0.61
5:B:955:THR:HG22	5:B:956:THR:N	2.13	0.61
9:H:82:PRO:O	9:H:83:GLN:HB3	2.00	0.61
12:K:47:ARG:HH11	12:K:47:ARG:HB3	1.64	0.61
4:A:1073:GLY:O	4:A:1077:THR:OG1	2.15	0.61
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.35	0.61
6:C:166:GLU:O	6:C:167:HIS:HB2	1.98	0.61
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.83	0.61
12:K:20:LYS:HB3	12:K:34:THR:HB	1.81	0.61
4:A:68:GLN:O	4:A:68:GLN:HG2	2.01	0.61
9:H:111:LEU:HD12	9:H:127:GLY:HA2	1.82	0.61
4:A:320:ARG:HB2	4:A:321:PRO:HA	1.83	0.61
4:A:840:ARG:HG2	4:A:1402:PHE:HZ	1.65	0.61
4:A:1162:VAL:HA	4:A:1163:ILE:O	2.00	0.61
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.82	0.61
5:B:351:TYR:H	5:B:354:ASP:HB2	1.66	0.61
4:A:596:THR:C	4:A:598:LEU:H	2.09	0.61
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.82	0.61
4:A:523:ILE:HD13	4:A:622:VAL:HG22	1.83	0.60
5:B:803:LEU:N	5:B:822:ASN:HD21	1.99	0.60
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.81	0.60
9:H:109:LYS:CG	9:H:110:ASP:HB2	2.31	0.60
2:T:24:DT:H5'	5:B:792:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:785:TYR:CE2	11:J:60:PHE:HE1	2.18	0.60
4:A:961:ARG:NH1	4:A:965:GLN:HE22	2.00	0.60
5:B:123:THR:HG23	5:B:205:ILE:HA	1.81	0.60
6:C:56:THR:HG21	6:C:145:CYS:SG	2.40	0.60
4:A:1070:GLN:O	4:A:1074:GLU:HB2	2.01	0.60
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.66	0.60
5:B:549:THR:HB	5:B:628:THR:CG2	2.31	0.60
5:B:779:GLY:O	5:B:795:ILE:HA	2.01	0.60
4:A:834:THR:OG1	4:A:1077:THR:HA	2.02	0.60
4:A:901:LEU:H	4:A:926:GLN:NE2	1.99	0.60
6:C:45:ALA:HA	6:C:72:LEU:HD13	1.83	0.60
9:H:109:LYS:H	9:H:110:ASP:C	2.10	0.60
11:J:43:ARG:HH11	11:J:43:ARG:HB3	1.66	0.60
2:T:6:DG:H2"	2:T:7:DA:H8	1.65	0.60
4:A:68:GLN:HE22	4:A:80:HIS:CE1	2.20	0.60
1:R:10:A:N6	2:T:19:DT:H3	1.92	0.60
4:A:440:ASP:O	4:A:460:VAL:HG23	2.02	0.60
4:A:675:THR:CG2	4:A:736:ASN:HD21	2.14	0.60
9:H:83:GLN:HG3	9:H:83:GLN:O	2.01	0.60
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.67	0.59
5:B:1176:ASN:O	5:B:1177:HIS:CG	2.55	0.59
4:A:855:THR:HG23	4:A:857:ARG:HE	1.65	0.59
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.68	0.59
5:B:977:GLY:HA3	5:B:1099:VAL:CG1	2.32	0.59
5:B:1156:ASP:OD2	5:B:1156:ASP:N	2.34	0.59
5:B:391:ASP:CA	5:B:392:ARG:HB2	2.32	0.59
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.84	0.59
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.31	0.59
5:B:706:GLN:HB3	5:B:709:ASP:HB2	1.85	0.59
5:B:806:THR:HG22	5:B:1046:PRO:HD3	1.83	0.59
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.84	0.59
4:A:451:HIS:HB3	4:A:453:MET:N	2.16	0.59
5:B:801:LYS:O	11:J:52:THR:CG2	2.50	0.59
9:H:84:ALA:HA	9:H:86:ASP:N	2.16	0.59
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.85	0.59
4:A:567:LYS:O	4:A:569:LYS:N	2.34	0.59
5:B:424:LEU:O	5:B:428:ILE:HG12	2.02	0.59
5:B:882:THR:CB	5:B:883:LEU:HA	2.23	0.59
8:F:81:THR:HG22	8:F:82:THR:H	1.67	0.59
4:A:1223:ASP:O	4:A:1224:LEU:HB2	2.02	0.59
5:B:25:ILE:HD12	5:B:651:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:213:ILE:HD13	5:B:497:ARG:HB3	1.85	0.59
4:A:90:VAL:HG13	4:A:297:GLN:OE1	2.03	0.59
4:A:579:SER:OG	4:A:612:ILE:HG22	2.02	0.59
4:A:699:ALA:N	4:A:700:ASN:HA	2.17	0.59
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.84	0.59
5:B:1031:LEU:HD13	5:B:1055:ILE:HD12	1.85	0.59
7:E:35:VAL:C	7:E:37:LEU:H	2.11	0.59
4:A:1093:LYS:HB3	4:A:1094:VAL:CB	2.33	0.59
7:E:111:VAL:HG12	7:E:137:GLU:HG2	1.84	0.59
5:B:558:LEU:HB3	5:B:563:MET:SD	2.42	0.58
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.03	0.58
4:A:449:SER:HB2	5:B:1137:CYS:SG	2.43	0.58
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.38	0.58
4:A:455:MET:HE3	5:B:1134:GLU:HG3	1.84	0.58
4:A:579:SER:HA	4:A:582:ILE:HG12	1.85	0.58
5:B:292:ILE:HD12	5:B:326:ASP:HA	1.84	0.58
5:B:709:ASP:HB3	5:B:710:LEU:HB2	1.85	0.58
5:B:831:SER:HB2	5:B:833:TYR:HD1	1.66	0.58
4:A:364:VAL:HG12	4:A:459:ARG:O	2.02	0.58
5:B:239:GLU:HG3	5:B:255:GLN:HG2	1.84	0.58
5:B:351:TYR:CD2	5:B:355:ILE:HD11	2.38	0.58
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.38	0.58
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.18	0.58
5:B:1162:ILE:HG12	5:B:1194:ILE:HD12	1.85	0.58
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.69	0.58
4:A:909:ASP:C	4:A:911:SER:H	2.11	0.58
4:A:1084:PHE:HD1	4:A:1086:PHE:HA	1.69	0.58
5:B:1072:MET:HE2	5:B:1085:ILE:HG21	1.84	0.58
5:B:35:SER:HA	5:B:811:TYR:HE2	1.69	0.58
5:B:115:GLN:CD	5:B:118:ARG:HH21	2.12	0.58
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.85	0.58
8:F:127:GLU:O	8:F:129:LYS:N	2.36	0.58
4:A:800:VAL:HG11	4:A:808:LEU:HG	1.86	0.58
4:A:928:LEU:HA	4:A:931:GLU:HB2	1.86	0.58
2:T:27:DA:H2'	2:T:27:DA:N3	2.19	0.58
4:A:794:PRO:C	4:A:796:SER:H	2.12	0.58
5:B:313:MET:HE2	5:B:386:LEU:HD22	1.86	0.58
7:E:198:ILE:HB	7:E:210:SER:HB3	1.86	0.58
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.86	0.57
4:A:1154:TYR:O	4:A:1192:LEU:HG	2.04	0.57
5:B:975:GLN:O	5:B:990:ILE:HD12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1168:LEU:HD21	5:B:1214:PRO:HD2	1.86	0.57
4:A:482:PHE:C	4:A:484:GLY:H	2.12	0.57
6:C:251:LEU:O	6:C:255:VAL:HG23	2.05	0.57
9:H:56:THR:O	9:H:144:ILE:HA	2.05	0.57
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.85	0.57
7:E:144:ILE:HG13	7:E:145:THR:H	1.69	0.57
4:A:115:LEU:HD11	4:A:145:LYS:HD2	1.87	0.57
5:B:1177:HIS:CA	5:B:1178:ASN:HB2	2.34	0.57
11:J:57:ILE:O	11:J:61:LEU:HG	2.05	0.57
4:A:423:ASP:CG	4:A:424:ILE:N	2.59	0.57
5:B:391:ASP:N	5:B:392:ARG:HB2	2.20	0.57
5:B:941:LEU:HD23	5:B:942:ARG:H	1.70	0.57
5:B:977:GLY:HA3	5:B:1099:VAL:HG13	1.87	0.57
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.86	0.57
4:A:623:GLY:C	4:A:625:SER:H	2.13	0.57
5:B:270:LYS:HA	5:B:281:PRO:HA	1.86	0.57
4:A:534:LEU:O	4:A:574:GLY:HA3	2.05	0.57
4:A:847:ASP:HA	4:A:1063:MET:HE1	1.87	0.57
4:A:901:LEU:HA	4:A:907:THR:HG23	1.87	0.57
5:B:525:ALA:O	5:B:768:THR:HG23	2.03	0.57
4:A:1077:THR:O	4:A:1081:LEU:HB3	2.05	0.56
4:A:313:GLN:HE21	4:A:322:VAL:HG11	1.70	0.56
4:A:1092:LYS:CB	4:A:1093:LYS:HB2	2.35	0.56
4:A:1200:ALA:HA	4:A:1201:ALA:C	2.29	0.56
5:B:1019:SER:CA	5:B:1020:ARG:CB	2.82	0.56
10:I:20:LYS:HG2	10:I:24:ARG:N	2.20	0.56
4:A:648:ASN:O	4:A:652:VAL:HG23	2.05	0.56
4:A:698:GLN:HA	10:I:97:MET:O	2.06	0.56
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.40	0.56
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.88	0.56
4:A:95:PHE:O	4:A:99:ILE:HG13	2.05	0.56
10:I:14:LEU:HD23	10:I:27:PHE:HB3	1.87	0.56
10:I:92:ARG:HA	10:I:92:ARG:NE	2.20	0.56
4:A:663:SER:CB	5:B:827:ILE:O	2.54	0.56
5:B:354:ASP:O	5:B:358:LYS:HB2	2.05	0.56
4:A:969:GLN:HA	4:A:972:HIS:HB3	1.88	0.56
4:A:351:THR:HG22	4:A:352:VAL:H	1.70	0.56
4:A:1433:MET:HE3	4:A:1439:GLY:HA2	1.87	0.56
10:I:3:THR:HA	10:I:4:PHE:CD2	2.37	0.56
4:A:731:ARG:CG	4:A:755:PHE:HE1	2.19	0.56
5:B:764:SER:N	5:B:765:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:974:PRO:HA	5:B:1094:ARG:HH21	1.70	0.56
4:A:855:THR:CG2	4:A:857:ARG:HE	2.18	0.56
4:A:1096:SER:N	4:A:1097:GLY:HA3	2.21	0.56
5:B:180:TYR:HD1	5:B:180:TYR:H	1.54	0.56
7:E:15:ALA:HA	7:E:141:VAL:H	1.70	0.56
11:J:53:HIS:HE1	11:J:55:ASP:OD1	1.89	0.56
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.41	0.55
4:A:596:THR:HB	4:A:598:LEU:HB2	1.88	0.55
4:A:731:ARG:HG3	4:A:755:PHE:CZ	2.40	0.55
4:A:1092:LYS:HB3	4:A:1093:LYS:CB	2.36	0.55
5:B:778:MET:HE1	5:B:853:SER:HB3	1.87	0.55
5:B:1019:SER:N	5:B:1020:ARG:HB3	2.20	0.55
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.71	0.55
4:A:1319:VAL:HB	4:A:1322:ILE:HD12	1.88	0.55
5:B:469:GLN:HE21	5:B:470:LYS:HE3	1.71	0.55
5:B:1120:GLU:HB3	5:B:1124:ARG:HH12	1.71	0.55
4:A:1105:LEU:HB3	4:A:1384:VAL:HB	1.89	0.55
5:B:485:ARG:NH2	5:B:782:LEU:HD11	2.21	0.55
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.88	0.55
4:A:284:ALA:N	4:A:285:PRO:CD	2.56	0.55
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.71	0.55
4:A:442:VAL:HG12	4:A:491:VAL:HG22	1.88	0.55
4:A:868:TYR:CE1	4:A:1064:VAL:HG21	2.41	0.55
5:B:708:GLU:HA	5:B:711:GLU:HG2	1.88	0.55
5:B:879:ARG:O	5:B:880:THR:HG22	2.06	0.55
6:C:18:VAL:HG12	6:C:20:PHE:CD2	2.41	0.55
6:C:82:TYR:HB2	6:C:85:ASP:HB2	1.88	0.55
11:J:3:VAL:HG22	11:J:53:HIS:CE1	2.42	0.55
4:A:456:MET:HB2	4:A:478:TYR:OH	2.06	0.55
4:A:1151:GLU:HA	10:I:45:ARG:HB3	1.89	0.55
4:A:389:THR:OG1	4:A:426:LEU:HD12	2.07	0.55
4:A:667:GLY:HA2	4:A:670:ILE:HG13	1.89	0.55
4:A:1171:GLN:C	4:A:1173:HIS:N	2.64	0.55
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.71	0.55
4:A:351:THR:CG2	4:A:352:VAL:N	2.68	0.55
4:A:617:VAL:HG12	4:A:622:VAL:HB	1.89	0.55
4:A:683:ILE:HG22	4:A:687:LYS:HG3	1.88	0.55
5:B:518:HIS:CE1	5:B:537:LYS:HE2	2.42	0.55
5:B:614:SER:HB3	5:B:694:ASP:OD1	2.07	0.55
5:B:878:GLN:HG3	5:B:881:ASN:HB2	1.87	0.55
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:219:PHE:O	4:A:222:LEU:O	2.24	0.55
5:B:303:TYR:HH	5:B:586:TRP:HH2	1.55	0.55
5:B:512:ARG:NH2	5:B:532:ALA:HA	2.21	0.55
10:I:42:LEU:CD2	10:I:43:VAL:H	2.20	0.55
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.88	0.55
4:A:1157:ASP:C	4:A:1159:ARG:N	2.65	0.55
7:E:29:PHE:O	7:E:30:ILE:HB	2.07	0.55
10:I:101:PHE:HB2	10:I:110:PHE:CZ	2.41	0.55
4:A:1075:PRO:O	4:A:1079:MET:HG3	2.07	0.54
5:B:350:GLN:HB3	5:B:351:TYR:CB	2.31	0.54
4:A:438:ASP:HA	4:A:460:VAL:O	2.07	0.54
4:A:1092:LYS:HB2	4:A:1093:LYS:HB2	1.90	0.54
4:A:1093:LYS:CB	4:A:1094:VAL:HB	2.36	0.54
5:B:391:ASP:HA	5:B:392:ARG:HB2	1.88	0.54
5:B:707:PRO:HA	5:B:741:CYS:SG	2.47	0.54
5:B:851:PHE:CD2	5:B:1094:ARG:HB2	2.42	0.54
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.72	0.54
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.31	0.54
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.42	0.54
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.88	0.54
4:A:629:LEU:O	4:A:633:VAL:HG23	2.08	0.54
4:A:1082:ASN:C	4:A:1084:PHE:O	2.51	0.54
4:A:1287:TYR:HD2	4:A:1305:VAL:HB	1.72	0.54
9:H:84:ALA:CA	9:H:85:GLY:C	2.76	0.54
11:J:6:ARG:HA	11:J:12:LYS:O	2.07	0.54
4:A:1227:ILE:HA	4:A:1228:TRP:CG	2.42	0.54
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.07	0.54
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.37	0.54
4:A:827:THR:OG1	4:A:1083:THR:HG21	2.07	0.54
6:C:173:ALA:O	6:C:233:GLU:O	2.24	0.54
4:A:232:GLU:HG3	4:A:233:TRP:CD1	2.43	0.54
4:A:350:ARG:HD3	4:A:488:ASN:OD1	2.07	0.54
4:A:375:THR:HA	4:A:434:ARG:O	2.08	0.54
6:C:66:ARG:NH2	11:J:4:PRO:HA	2.23	0.54
4:A:8:SER:O	4:A:10:PRO:HD3	2.08	0.53
5:B:515:HIS:H	5:B:518:HIS:CD2	2.25	0.53
10:I:17:ARG:HA	10:I:18:GLU:HB3	1.90	0.53
5:B:237:VAL:HG22	5:B:257:LYS:HG2	1.90	0.53
5:B:573:GLN:O	5:B:575:PRO:HD3	2.07	0.53
4:A:1194:ARG:O	4:A:1195:LEU:HB2	2.08	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:973:ILE:CG2	5:B:974:PRO:HD2	2.37	0.53
9:H:96:VAL:HA	9:H:142:LEU:O	2.09	0.53
4:A:278:THR:O	4:A:279:LEU:CB	2.57	0.53
4:A:930:ASP:HA	4:A:933:TYR:HB3	1.91	0.53
4:A:973:ILE:HG23	4:A:974:ASP:HA	1.90	0.53
4:A:987:VAL:C	4:A:989:GLY:H	2.16	0.53
4:A:1264:GLU:HA	4:A:1267:MET:HB2	1.91	0.53
5:B:789:MET:HE2	5:B:965:LYS:HB3	1.89	0.53
5:B:230:ALA:C	5:B:232:SER:HB3	2.33	0.53
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.42	0.53
9:H:81:PRO:HB2	9:H:82:PRO:CD	2.39	0.53
5:B:515:HIS:H	5:B:518:HIS:HD2	1.57	0.53
6:C:182:PRO:HG3	6:C:206:ASN:O	2.09	0.53
10:I:43:VAL:CG1	10:I:44:TYR:HA	2.38	0.53
4:A:573:SER:O	4:A:576:GLN:HB2	2.08	0.53
6:C:64:ALA:HA	6:C:67:LEU:HD12	1.90	0.53
7:E:7:ARG:HA	7:E:10:SER:HB3	1.91	0.53
4:A:332:LYS:C	4:A:334:GLY:H	2.17	0.53
4:A:847:ASP:HB3	4:A:1424:VAL:HG23	1.90	0.53
4:A:1115:SER:HA	4:A:1308:THR:O	2.08	0.53
6:C:13:ALA:HA	6:C:17:ASN:O	2.09	0.53
13:L:60:ARG:HG3	13:L:61:THR:H	1.73	0.53
4:A:1236:LEU:CA	4:A:1237:ILE:HB	2.30	0.53
5:B:223:VAL:HG22	5:B:240:ILE:HD12	1.91	0.53
7:E:35:VAL:O	7:E:37:LEU:N	2.38	0.53
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.91	0.53
5:B:637:LEU:HA	5:B:743:ILE:HD11	1.91	0.53
5:B:1159:ARG:HE	5:B:1193:GLN:NE2	2.08	0.53
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.44	0.53
4:A:380:VAL:HG22	4:A:430:TRP:H	1.74	0.52
4:A:818:MET:HG2	5:B:514:LEU:HD23	1.91	0.52
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.92	0.52
4:A:1067:LEU:O	4:A:1069:ALA:O	2.28	0.52
5:B:122:LEU:CD2	5:B:958:GLN:HG3	2.32	0.52
5:B:293:PRO:HA	5:B:294:ASP:CB	2.25	0.52
5:B:785:TYR:HE2	11:J:60:PHE:CZ	2.25	0.52
7:E:194:GLU:O	7:E:214:CYS:HB2	2.08	0.52
4:A:1091:SER:CB	4:A:1092:LYS:C	2.72	0.52
5:B:408:LEU:HD23	5:B:545:ILE:HG21	1.92	0.52
5:B:589:VAL:HG12	5:B:590:HIS:N	2.24	0.52
10:I:17:ARG:HB3	10:I:18:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.90	0.52
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.37	0.52
4:A:1069:ALA:C	4:A:1071:SER:N	2.65	0.52
4:A:1261:LYS:C	4:A:1263:ILE:H	2.17	0.52
5:B:649:LYS:HE2	5:B:737:THR:HA	1.92	0.52
9:H:109:LYS:HG2	9:H:110:ASP:HB2	1.90	0.52
4:A:266:LEU:O	4:A:269:ILE:HG22	2.09	0.52
4:A:579:SER:HB3	4:A:611:GLN:HA	1.91	0.52
5:B:557:PHE:O	5:B:561:TRP:CB	2.53	0.52
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.91	0.52
12:K:82:ASP:OD1	12:K:83:PRO:HD2	2.10	0.52
4:A:98:LYS:O	4:A:102:VAL:HG23	2.09	0.52
4:A:446:ARG:HD2	4:A:480:ALA:HB2	1.92	0.52
5:B:571:PRO:N	5:B:572:HIS:HB2	2.25	0.52
6:C:62:PHE:O	6:C:66:ARG:HG3	2.08	0.52
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.90	0.52
5:B:708:GLU:O	5:B:712:PRO:HD3	2.09	0.52
10:I:21:GLU:O	10:I:22:ASN:HB3	2.10	0.52
4:A:681:GLU:HA	4:A:684:ALA:CB	2.39	0.52
4:A:1156:PRO:O	4:A:1157:ASP:HB2	2.09	0.52
6:C:3:GLU:HG3	6:C:4:GLU:H	1.75	0.52
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.91	0.52
2:T:26:DG:C2	2:T:27:DA:H1'	2.44	0.52
4:A:1100:ARG:O	4:A:1103:GLU:HB2	2.10	0.52
4:A:1364:ASN:C	4:A:1364:ASN:HD22	2.18	0.52
5:B:498:THR:O	5:B:536:VAL:HA	2.10	0.52
4:A:642:CYS:O	4:A:645:LEU:HB3	2.10	0.52
4:A:751:SER:CB	5:B:1015:HIS:CE1	2.93	0.52
4:A:768:GLN:NE2	4:A:1087:ALA:HB1	2.25	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.10	0.52
4:A:1093:LYS:HB3	4:A:1094:VAL:CG2	2.39	0.52
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.91	0.52
5:B:471:LYS:O	5:B:474:SER:HB3	2.10	0.52
5:B:570:VAL:C	5:B:572:HIS:HB2	2.35	0.52
6:C:124:LEU:C	6:C:126:GLY:H	2.17	0.52
9:H:63:LEU:C	9:H:89:LEU:HB2	2.35	0.52
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.92	0.52
5:B:40:GLU:OE1	5:B:682:SER:HB2	2.10	0.51
6:C:37:MET:HA	6:C:41:ILE:HD11	1.92	0.51
9:H:129:TYR:O	9:H:130:ARG:HG2	2.09	0.51
4:A:387:ARG:O	4:A:391:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:663:SER:HA	5:B:1014:PRO:HG3	1.91	0.51
11:J:6:ARG:HB3	11:J:11:GLY:O	2.10	0.51
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.92	0.51
4:A:407:ARG:HD3	4:A:411:ASP:HB2	1.93	0.51
5:B:603:LEU:HB3	5:B:609:ILE:HG12	1.93	0.51
5:B:1177:HIS:HA	5:B:1178:ASN:CB	2.38	0.51
6:C:48:SER:HB3	6:C:158:VAL:HB	1.92	0.51
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.93	0.51
5:B:638:PHE:O	5:B:740:HIS:HB2	2.10	0.51
5:B:1075:GLY:O	6:C:35:ARG:HD2	2.11	0.51
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.43	0.51
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.39	0.51
13:L:55:ILE:HD12	13:L:56:LEU:H	1.76	0.51
2:T:16:DC:C6	2:T:17:DG:C8	2.98	0.51
4:A:546:VAL:HG21	4:A:572:TRP:CE3	2.46	0.51
4:A:550:LEU:HD12	4:A:556:TRP:NE1	2.25	0.51
4:A:1156:PRO:HG2	4:A:1163:ILE:HG12	1.93	0.51
5:B:613:VAL:HG22	5:B:628:THR:HG23	1.93	0.51
5:B:1209:ALA:C	5:B:1211:ASN:H	2.19	0.51
6:C:66:ARG:NH2	11:J:3:VAL:O	2.43	0.51
4:A:710:LEU:HA	4:A:713:SER:HB2	1.92	0.51
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.11	0.51
5:B:288:ALA:HB1	5:B:331:LEU:HG	1.93	0.51
5:B:518:HIS:HE1	5:B:537:LYS:HE2	1.75	0.51
5:B:815:ARG:HD3	5:B:1041:GLU:OE2	2.11	0.51
5:B:1019:SER:N	5:B:1020:ARG:CB	2.74	0.51
4:A:873:MET:HE3	4:A:957:PRO:HG2	1.93	0.51
4:A:1391:ARG:O	4:A:1393:ASN:N	2.43	0.51
4:A:1411:GLU:HA	4:A:1414:ALA:HB3	1.92	0.51
4:A:1434:ALA:O	4:A:1436:ILE:N	2.44	0.51
5:B:1156:ASP:CB	5:B:1198:TYR:H	2.21	0.51
4:A:403:LYS:O	4:A:433:GLU:O	2.29	0.51
4:A:731:ARG:HG2	4:A:755:PHE:HE1	1.76	0.51
4:A:834:THR:O	4:A:837:ILE:HB	2.11	0.51
5:B:637:LEU:O	5:B:690:VAL:HG13	2.10	0.51
5:B:745:PRO:O	5:B:747:MET:N	2.44	0.51
5:B:983:ARG:HH11	5:B:1091:TYR:HB3	1.76	0.51
10:I:29:CYS:H	10:I:33:SER:HB2	1.76	0.51
10:I:43:VAL:HB	10:I:44:TYR:CA	2.38	0.51
11:J:43:ARG:HB3	11:J:43:ARG:NH1	2.26	0.51
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:814:PHE:HB2	5:B:519:TRP:HZ3	1.76	0.50
4:A:1071:SER:H	4:A:1072:ILE:CB	2.11	0.50
5:B:552:MET:HB2	5:B:553:PRO:HD3	1.93	0.50
6:C:66:ARG:HH21	11:J:4:PRO:HA	1.75	0.50
9:H:115:TYR:HE2	9:H:124:ARG:HG3	1.76	0.50
12:K:65:HIS:O	12:K:67:PHE:N	2.44	0.50
4:A:330:LYS:O	4:A:334:GLY:HA3	2.10	0.50
4:A:663:SER:HB2	5:B:827:ILE:O	2.11	0.50
4:A:1091:SER:HB2	4:A:1093:LYS:N	2.26	0.50
6:C:57:VAL:HG11	11:J:60:PHE:CD1	2.46	0.50
6:C:133:ILE:HD11	6:C:237:SER:HA	1.92	0.50
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.52	0.50
5:B:364:ILE:O	5:B:365:THR:HB	2.11	0.50
6:C:36:VAL:HG21	6:C:251:LEU:HD13	1.93	0.50
9:H:6:PHE:O	9:H:7:ASP:HB3	2.11	0.50
9:H:105:GLU:CG	9:H:106:GLU:H	2.23	0.50
13:L:29:TYR:HB3	13:L:56:LEU:HD22	1.93	0.50
4:A:374:LEU:O	4:A:436:ILE:HG13	2.11	0.50
4:A:407:ARG:HD2	4:A:413:ILE:CD1	2.42	0.50
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.93	0.50
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.11	0.50
6:C:77:ILE:HD12	6:C:161:LYS:HE3	1.93	0.50
8:F:103:MET:O	8:F:105:ALA:N	2.45	0.50
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.24	0.50
4:A:1390:ASN:ND2	4:A:1402:PHE:HB3	2.26	0.50
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.42	0.50
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.93	0.50
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.77	0.50
4:A:667:GLY:HA2	4:A:670:ILE:CG1	2.42	0.50
4:A:1167:GLU:CB	4:A:1168:GLU:CA	2.62	0.50
5:B:635:ARG:O	5:B:636:PRO:O	2.30	0.50
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.10	0.50
10:I:33:SER:HA	10:I:34:TYR:CB	2.39	0.50
4:A:407:ARG:CD	4:A:413:ILE:HD13	2.41	0.50
4:A:712:GLU:H	4:A:713:SER:CA	2.24	0.50
4:A:822:GLU:O	4:A:825:ILE:HB	2.11	0.50
4:A:1068:ALA:C	4:A:1069:ALA:O	2.53	0.50
4:A:452:LYS:HB3	5:B:1140:ALA:HB1	1.93	0.50
5:B:54:PHE:HB2	5:B:410:GLY:HA2	1.93	0.50
5:B:190:TYR:CZ	5:B:196:PRO:HG3	2.47	0.50
10:I:111:THR:HG22	10:I:112:SER:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:350:ARG:O	4:A:351:THR:OG1	2.26	0.49
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.46	0.49
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.93	0.49
4:A:528:LEU:HD23	4:A:751:SER:HA	1.94	0.49
4:A:868:TYR:C	4:A:868:TYR:CD2	2.90	0.49
4:A:1083:THR:H	4:A:1084:PHE:C	2.17	0.49
12:K:7:PHE:C	12:K:9:LEU:H	2.19	0.49
13:L:28:LYS:HB2	13:L:39:SER:HA	1.94	0.49
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	2.15	0.49
5:B:108:VAL:HG12	5:B:109:THR:H	1.77	0.49
5:B:179:CYS:SG	5:B:181:LEU:HG	2.52	0.49
5:B:549:THR:HG22	5:B:550:ASP:H	1.76	0.49
5:B:572:HIS:N	5:B:573:GLN:C	2.64	0.49
9:H:102:TYR:CD2	9:H:102:TYR:N	2.80	0.49
10:I:3:THR:HG22	10:I:4:PHE:CE2	2.47	0.49
10:I:42:LEU:HD22	10:I:43:VAL:H	1.76	0.49
4:A:455:MET:CE	5:B:1134:GLU:HG3	2.42	0.49
4:A:1086:PHE:N	4:A:1086:PHE:CD1	2.79	0.49
5:B:579:ARG:HB3	5:B:589:VAL:HG22	1.94	0.49
5:B:708:GLU:O	5:B:708:GLU:HG2	2.12	0.49
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.93	0.49
5:B:1177:HIS:CB	5:B:1178:ASN:HB2	2.42	0.49
10:I:5:ARG:HG2	10:I:6:PHE:H	1.77	0.49
4:A:575:LYS:HD2	9:H:120:GLY:HA3	1.94	0.49
4:A:754:SER:N	4:A:757:ASN:HD22	2.11	0.49
4:A:826:ASP:HA	4:A:830:LYS:H	1.76	0.49
4:A:961:ARG:O	4:A:965:GLN:NE2	2.45	0.49
5:B:814:PHE:C	5:B:816:GLU:H	2.20	0.49
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.94	0.49
4:A:903:ASN:O	4:A:907:THR:OG1	2.30	0.49
4:A:976:THR:H	4:A:1036:ARG:NH1	2.11	0.49
4:A:1436:ILE:HG22	4:A:1437:GLY:N	2.27	0.49
5:B:59:LEU:HA	5:B:62:ILE:HD12	1.93	0.49
5:B:476:ARG:O	5:B:477:ALA:C	2.55	0.49
5:B:549:THR:HB	5:B:628:THR:HG21	1.95	0.49
5:B:955:THR:CG2	5:B:956:THR:H	2.23	0.49
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.48	0.49
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.95	0.49
4:A:853:ASP:OD2	4:A:855:THR:HG22	2.12	0.49
5:B:976:ILE:HD11	5:B:992:ILE:HA	1.94	0.49
6:C:265:MET:C	6:C:267:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:731:ARG:CG	4:A:755:PHE:CE1	2.95	0.49
5:B:291:ILE:HD12	5:B:291:ILE:H	1.78	0.49
5:B:1074:ASN:C	5:B:1074:ASN:OD1	2.54	0.49
4:A:1152:ILE:CA	4:A:1153:TYR:HB2	2.36	0.49
5:B:880:THR:H	5:B:883:LEU:HD12	1.77	0.49
4:A:788:SER:HB3	10:I:69:PRO:HD3	1.93	0.49
4:A:1070:GLN:O	4:A:1074:GLU:N	2.46	0.49
4:A:1161:THR:O	4:A:1163:ILE:HG12	2.12	0.49
5:B:811:TYR:N	5:B:811:TYR:CD1	2.80	0.49
8:F:81:THR:HG22	8:F:82:THR:N	2.27	0.49
13:L:62:LYS:H	13:L:62:LYS:HD2	1.78	0.49
4:A:1171:GLN:C	4:A:1173:HIS:H	2.21	0.49
4:A:1311:VAL:HG22	4:A:1329:THR:HG21	1.95	0.49
4:A:1341:ILE:HB	7:E:182:ASP:OD1	2.13	0.49
5:B:302:CYS:HB2	5:B:310:MET:HG2	1.95	0.49
5:B:1124:ARG:O	5:B:1125:ASP:C	2.55	0.49
11:J:23:ASN:O	11:J:27:GLU:HB3	2.11	0.49
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.43	0.48
4:A:1411:GLU:O	4:A:1415:SER:N	2.38	0.48
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.78	0.48
6:C:239:PRO:O	6:C:243:VAL:HG23	2.13	0.48
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.43	0.48
4:A:320:ARG:CB	4:A:321:PRO:HA	2.43	0.48
4:A:707:GLY:CA	4:A:709:THR:N	2.62	0.48
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.95	0.48
5:B:101:MET:HE3	5:B:169:ARG:HH12	1.79	0.48
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.31	0.48
5:B:487:THR:HG22	5:B:488:TYR:N	2.27	0.48
5:B:825:VAL:HG21	5:B:1090:THR:HB	1.95	0.48
5:B:872:GLU:HG2	5:B:916:THR:HB	1.94	0.48
8:F:90:ARG:NH2	8:F:122:MET:HE3	2.28	0.48
4:A:517:ASN:ND2	4:A:1364:ASN:OD1	2.44	0.48
4:A:663:SER:HB3	5:B:827:ILE:O	2.14	0.48
4:A:873:MET:C	4:A:1058:VAL:HG13	2.38	0.48
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.95	0.48
5:B:640:VAL:HG13	5:B:650:GLU:O	2.14	0.48
4:A:442:VAL:CG1	4:A:491:VAL:HG22	2.43	0.48
4:A:491:VAL:H	5:B:1150:ARG:NH2	2.11	0.48
4:A:775:ILE:HB	4:A:797:LYS:O	2.13	0.48
4:A:821:ARG:O	4:A:825:ILE:HG12	2.13	0.48
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:43:LYS:O	7:E:47:CYS:HB3	2.12	0.48
4:A:492:PRO:O	4:A:493:GLN:NE2	2.46	0.48
4:A:754:SER:H	4:A:757:ASN:HD22	1.60	0.48
4:A:768:GLN:HE22	4:A:1087:ALA:HB1	1.79	0.48
6:C:173:ALA:O	6:C:174:ALA:HB3	2.13	0.48
12:K:38:GLU:HG3	12:K:42:LEU:HD22	1.96	0.48
4:A:350:ARG:HH11	4:A:488:ASN:HD21	1.60	0.48
4:A:515:GLN:HG3	4:A:1071:SER:HB3	1.96	0.48
4:A:1082:ASN:HB3	4:A:1084:PHE:O	2.12	0.48
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.95	0.48
5:B:636:PRO:CB	5:B:637:LEU:HB3	2.29	0.48
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.46	0.48
5:B:1175:LEU:HB2	5:B:1176:ASN:HA	1.94	0.48
6:C:3:GLU:HG2	12:K:104:ASN:OD1	2.13	0.48
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.94	0.48
4:A:702:LEU:HG	4:A:704:ALA:HB2	1.96	0.48
4:A:1030:ARG:HD3	4:A:1034:GLU:HG3	1.94	0.48
5:B:520:GLY:HA2	5:B:748:ILE:HA	1.94	0.48
2:T:17:DG:H5"	2:T:18:DA:OP1	2.13	0.48
4:A:332:LYS:H	4:A:337:ARG:HB2	1.79	0.48
4:A:897:TYR:CD2	4:A:936:LEU:HD21	2.48	0.48
4:A:1209:MET:HE2	4:A:1231:ASP:H	1.79	0.48
5:B:571:PRO:HB2	5:B:572:HIS:CA	2.36	0.48
10:I:103:CYS:SG	10:I:106:CYS:CB	3.00	0.48
4:A:56:PRO:HA	4:A:57:ARG:HA	1.62	0.47
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.14	0.47
5:B:95:ILE:HD12	5:B:130:VAL:HG22	1.96	0.47
5:B:839:MET:O	5:B:990:ILE:HA	2.14	0.47
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.79	0.47
4:A:623:GLY:O	4:A:625:SER:N	2.44	0.47
4:A:818:MET:CG	5:B:514:LEU:HD23	2.43	0.47
4:A:819:GLY:O	4:A:820:GLY:C	2.57	0.47
5:B:996:ARG:HH12	6:C:173:ALA:CB	2.27	0.47
6:C:35:ARG:HH12	12:K:41:THR:N	2.13	0.47
7:E:55:ARG:HB3	7:E:82:PHE:HB3	1.96	0.47
12:K:65:HIS:C	12:K:67:PHE:H	2.22	0.47
4:A:1159:ARG:CB	4:A:1160:SER:C	2.83	0.47
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.14	0.47
7:E:18:THR:HG21	7:E:140:LEU:HB2	1.96	0.47
4:A:707:GLY:O	4:A:1283:VAL:HG21	2.14	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1081:LEU:O	4:A:1083:THR:HG22	2.13	0.47
4:A:1343:ALA:HB2	7:E:150:VAL:HG22	1.97	0.47
5:B:294:ASP:H	5:B:297:ILE:HB	1.78	0.47
5:B:459:TYR:C	5:B:459:TYR:CD2	2.91	0.47
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.47	0.47
5:B:1209:ALA:C	5:B:1211:ASN:N	2.71	0.47
2:T:26:DG:C6	2:T:27:DA:C8	3.02	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.95	0.47
4:A:446:ARG:HB2	4:A:487:MET:HE3	1.96	0.47
4:A:490:HIS:ND1	5:B:1150:ARG:NH1	2.63	0.47
5:B:638:PHE:O	5:B:740:HIS:CB	2.63	0.47
5:B:841:MET:HA	5:B:1009:ASP:O	2.13	0.47
6:C:173:ALA:O	6:C:174:ALA:CB	2.63	0.47
7:E:144:ILE:HG13	7:E:145:THR:N	2.30	0.47
10:I:30:ARG:HB2	10:I:30:ARG:NH1	2.29	0.47
4:A:380:VAL:HG21	4:A:427:GLN:O	2.15	0.47
4:A:420:ARG:O	4:A:424:ILE:HG13	2.14	0.47
4:A:833:GLU:O	4:A:837:ILE:HG12	2.14	0.47
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.95	0.47
4:A:1069:ALA:CB	4:A:1070:GLN:HA	2.41	0.47
5:B:95:ILE:HD12	5:B:130:VAL:CG2	2.45	0.47
7:E:131:THR:HG21	7:E:191:LYS:HD3	1.96	0.47
7:E:140:LEU:HA	7:E:141:VAL:HB	1.96	0.47
4:A:350:ARG:NH1	4:A:488:ASN:HD21	2.11	0.47
4:A:867:ILE:HG22	4:A:872:GLY:CA	2.45	0.47
4:A:1076:ALA:O	4:A:1080:THR:HG22	2.15	0.47
4:A:1084:PHE:CD1	4:A:1086:PHE:HA	2.49	0.47
5:B:38:PHE:O	5:B:42:GLY:N	2.47	0.47
5:B:256:VAL:CG1	5:B:382:ILE:HD11	2.29	0.47
4:A:399:HIS:O	4:A:435:HIS:HD2	1.97	0.47
4:A:503:GLN:O	4:A:504:LEU:HD12	2.14	0.47
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.80	0.47
4:A:1083:THR:C	4:A:1084:PHE:O	2.57	0.47
5:B:51:PHE:CD2	5:B:173:MET:HB3	2.50	0.47
7:E:10:SER:O	7:E:14:ARG:HG3	2.15	0.47
4:A:975:HIS:HB3	4:A:976:THR:CB	2.39	0.47
5:B:243:ALA:HB2	5:B:251:ILE:HD13	1.96	0.47
10:I:43:VAL:HG12	10:I:44:TYR:HA	1.97	0.47
11:J:9:SER:CB	11:J:45:CYS:HB2	2.45	0.47
4:A:61:ILE:HG13	4:A:62:ASP:N	2.30	0.47
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:32:ALA:O	5:B:35:SER:HB2	2.15	0.47
5:B:979:LYS:HA	5:B:989:THR:HG22	1.96	0.47
4:A:792:TYR:OH	10:I:91:ARG:NH2	2.48	0.46
5:B:777:ALA:HB1	5:B:819:ALA:HB1	1.97	0.46
7:E:205:SER:O	7:E:207:ARG:N	2.47	0.46
10:I:101:PHE:HB2	10:I:110:PHE:CE1	2.50	0.46
4:A:457:ALA:O	4:A:507:VAL:HG23	2.16	0.46
4:A:1342:GLU:HG3	7:E:198:ILE:HG21	1.98	0.46
5:B:1120:GLU:HB3	5:B:1124:ARG:NH1	2.30	0.46
4:A:58:LEU:HD22	4:A:244:PRO:HD2	1.97	0.46
4:A:298:PHE:O	4:A:302:THR:OG1	2.33	0.46
4:A:416:ARG:HG3	4:A:417:TYR:CD1	2.49	0.46
4:A:793:SER:CB	4:A:794:PRO:HD2	2.45	0.46
4:A:1191:TRP:CA	4:A:1192:LEU:CB	2.90	0.46
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.97	0.46
5:B:265:SER:O	5:B:266:ALA:HB3	2.14	0.46
5:B:785:TYR:HA	5:B:788:ARG:HB2	1.96	0.46
4:A:254:GLU:HA	4:A:255:SER:HA	1.70	0.46
4:A:482:PHE:C	4:A:484:GLY:N	2.73	0.46
4:A:617:VAL:CG1	4:A:622:VAL:HB	2.45	0.46
4:A:1364:ASN:O	4:A:1365:TYR:C	2.57	0.46
9:H:23:VAL:HA	9:H:43:ASN:HA	1.95	0.46
9:H:139:ASN:O	9:H:140:ALA:HB2	2.15	0.46
4:A:370:ILE:HG22	4:A:374:LEU:CD1	2.45	0.46
4:A:396:PRO:HB3	4:A:403:LYS:HG2	1.96	0.46
4:A:445:ASN:CB	4:A:455:MET:HG2	2.46	0.46
4:A:666:ILE:HD12	4:A:666:ILE:H	1.79	0.46
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.45	0.46
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.96	0.46
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.98	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:CZ	2.45	0.46
4:A:575:LYS:O	4:A:576:GLN:C	2.59	0.46
4:A:794:PRO:C	4:A:796:SER:N	2.73	0.46
4:A:1170:ILE:HA	4:A:1171:GLN:O	2.16	0.46
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.97	0.46
5:B:328:GLU:HA	5:B:329:THR:HA	1.63	0.46
5:B:950:ASP:O	5:B:951:GLN:HG3	2.16	0.46
10:I:114:GLN:HA	10:I:115:LYS:HA	1.69	0.46
4:A:312:PRO:O	4:A:313:GLN:HB2	2.15	0.46
4:A:767:GLN:NE2	4:A:774:ARG:HB2	2.31	0.46
4:A:1414:ALA:C	4:A:1416:ALA:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1441:PHE:HZ	8:F:88:TYR:C	2.24	0.46
5:B:227:LYS:CA	5:B:228:LYS:HB2	2.18	0.46
5:B:471:LYS:O	5:B:471:LYS:HG2	2.16	0.46
5:B:704:ALA:HB1	5:B:710:LEU:HB3	1.98	0.46
5:B:892:LYS:O	5:B:899:ILE:HG23	2.16	0.46
6:C:50:GLU:HB2	6:C:156:THR:OG1	2.15	0.46
9:H:6:PHE:HZ	9:H:134:ASN:HB2	1.81	0.46
9:H:106:GLU:HA	9:H:112:ILE:H	1.81	0.46
4:A:838:GLN:O	4:A:840:ARG:N	2.49	0.46
5:B:213:ILE:CD1	5:B:497:ARG:HB3	2.45	0.46
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.79	0.46
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.98	0.46
4:A:345:VAL:HA	5:B:1154:ALA:O	2.16	0.46
4:A:892:ALA:O	4:A:896:ARG:HB2	2.16	0.46
4:A:1050:GLU:O	4:A:1054:LEU:HD13	2.16	0.46
4:A:1116:LEU:HB3	4:A:1308:THR:HB	1.98	0.46
5:B:230:ALA:O	5:B:232:SER:O	2.34	0.46
2:T:9:DA:H61	3:N:6:DT:H3	1.63	0.46
4:A:637:LYS:HA	4:A:638:GLY:HA2	1.65	0.46
4:A:909:ASP:C	4:A:911:SER:N	2.74	0.46
5:B:125:SER:HB2	5:B:169:ARG:HB3	1.97	0.46
5:B:707:PRO:HB3	5:B:741:CYS:SG	2.55	0.46
5:B:955:THR:HG23	13:L:54:ARG:O	2.16	0.46
6:C:41:ILE:CG2	6:C:246:ARG:HB3	2.46	0.46
4:A:282:ASN:CB	4:A:283:GLY:CA	2.78	0.45
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.97	0.45
4:A:513:SER:HB3	4:A:518:LYS:O	2.16	0.45
4:A:722:LEU:HD11	4:A:794:PRO:HB3	1.98	0.45
4:A:824:LEU:HD21	5:B:769:TYR:HE1	1.81	0.45
4:A:901:LEU:H	4:A:926:GLN:HE21	1.62	0.45
4:A:1015:VAL:O	4:A:1017:LEU:N	2.49	0.45
5:B:709:ASP:CB	5:B:710:LEU:HB2	2.46	0.45
5:B:845:SER:HB2	11:J:8:PHE:HB3	1.96	0.45
5:B:997:GLU:C	5:B:999:MET:H	2.24	0.45
2:T:11:DG:N2	3:N:5:DT:O2	2.49	0.45
4:A:10:PRO:HD2	5:B:1193:GLN:HB2	1.96	0.45
4:A:452:LYS:HD2	4:A:510:GLN:HE22	1.81	0.45
4:A:858:ASN:C	4:A:858:ASN:HD22	2.24	0.45
5:B:372:SER:O	5:B:376:PHE:HD1	1.99	0.45
5:B:492:LEU:HD13	5:B:812:LEU:HD12	1.98	0.45
5:B:996:ARG:CG	5:B:1007:VAL:HG21	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:79:HIS:HA	10:I:80:SER:O	2.16	0.45
4:A:563:PRO:HD3	4:A:572:TRP:CZ2	2.52	0.45
4:A:712:GLU:N	4:A:713:SER:CB	2.53	0.45
4:A:741:ASN:HD22	4:A:744:LYS:H	1.62	0.45
4:A:907:THR:HG22	4:A:908:LEU:N	2.31	0.45
5:B:61:ASP:HA	5:B:64:CYS:HB2	1.98	0.45
5:B:212:LEU:HA	5:B:479:VAL:O	2.15	0.45
5:B:331:LEU:HB3	5:B:352:ALA:HB1	1.97	0.45
5:B:680:THR:HB	5:B:681:TRP:H	1.56	0.45
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.51	0.45
6:C:88:CYS:SG	6:C:89:GLU:N	2.89	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.45
5:B:1076:HIS:ND1	12:K:40:HIS:NE2	2.64	0.45
5:B:1098:MET:O	5:B:1099:VAL:C	2.57	0.45
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.99	0.45
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.99	0.45
12:K:37:LYS:O	12:K:38:GLU:HG2	2.16	0.45
4:A:663:SER:OG	5:B:1085:ILE:HA	2.16	0.45
5:B:831:SER:HB2	5:B:833:TYR:CD1	2.49	0.45
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.81	0.45
6:C:124:LEU:C	6:C:126:GLY:N	2.75	0.45
6:C:215:GLU:HG3	6:C:216:GLY:H	1.81	0.45
4:A:199:LEU:HB3	4:A:200:ARG:H	1.56	0.45
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.98	0.45
4:A:959:ASN:OD1	4:A:961:ARG:HB3	2.17	0.45
4:A:1191:TRP:HA	4:A:1192:LEU:HB3	1.96	0.45
4:A:1394:THR:HG22	4:A:1398:MET:HE1	1.99	0.45
8:F:93:ILE:HG12	8:F:148:VAL:HG21	1.98	0.45
10:I:59:VAL:HG12	10:I:60:GLN:H	1.81	0.45
4:A:1080:THR:HG23	4:A:1081:LEU:H	1.81	0.45
5:B:1177:HIS:HB2	5:B:1178:ASN:HB2	1.98	0.45
7:E:69:ILE:HD13	7:E:73:PRO:HA	1.99	0.45
9:H:108:SER:HB3	9:H:111:LEU:H	1.81	0.45
4:A:894:GLU:C	4:A:896:ARG:H	2.25	0.45
4:A:975:HIS:NE2	9:H:136:LYS:CB	2.80	0.45
5:B:1166:CYS:O	5:B:1168:LEU:N	2.48	0.45
5:B:1175:LEU:HA	5:B:1177:HIS:O	2.16	0.45
12:K:97:LYS:O	12:K:100:ALA:HB3	2.16	0.45
13:L:32:ALA:H	13:L:55:ILE:CD1	2.26	0.45
4:A:630:ILE:N	4:A:630:ILE:CD1	2.72	0.45
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:579:ARG:HA	5:B:589:VAL:HG13	1.97	0.45
6:C:127:ARG:HG3	6:C:129:ILE:HG22	1.99	0.45
4:A:783:THR:O	5:B:516:ASN:OD1	2.35	0.45
5:B:600:LEU:HD22	5:B:615:MET:SD	2.57	0.45
5:B:812:LEU:O	5:B:813:LYS:C	2.59	0.45
4:A:68:GLN:O	4:A:68:GLN:CG	2.65	0.44
4:A:1069:ALA:CB	4:A:1070:GLN:CA	2.95	0.44
4:A:1072:ILE:CG2	4:A:1073:GLY:N	2.72	0.44
5:B:651:LEU:C	5:B:653:VAL:H	2.25	0.44
5:B:1020:ARG:O	5:B:1021:MET:C	2.59	0.44
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.64	0.44
10:I:50:THR:HB	10:I:90:GLN:HE22	1.81	0.44
4:A:324:SER:O	4:A:326:ARG:N	2.45	0.44
4:A:1069:ALA:HA	4:A:1072:ILE:CG2	2.45	0.44
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.17	0.44
5:B:459:TYR:O	5:B:463:THR:OG1	2.35	0.44
5:B:1148:LYS:O	5:B:1152:MET:HB2	2.17	0.44
9:H:88:SER:O	9:H:89:LEU:CB	2.63	0.44
4:A:1197:LEU:HA	4:A:1198:ASP:CB	2.47	0.44
6:C:124:LEU:O	6:C:127:ARG:HG2	2.17	0.44
7:E:7:ARG:C	7:E:9:ILE:N	2.75	0.44
4:A:222:LEU:O	4:A:224:PHE:N	2.50	0.44
4:A:915:SER:HB2	4:A:919:ILE:CG1	2.45	0.44
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.48	0.44
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.46	0.44
5:B:1176:ASN:O	5:B:1177:HIS:ND1	2.51	0.44
7:E:46:TYR:CD2	7:E:58:MET:HG3	2.53	0.44
7:E:173:SER:O	7:E:175:LEU:N	2.51	0.44
4:A:351:THR:HB	4:A:468:PHE:CD1	2.52	0.44
4:A:692:ASP:O	4:A:695:LYS:HG2	2.17	0.44
4:A:1327:ILE:O	7:E:147:HIS:HE1	2.01	0.44
5:B:638:PHE:HB3	5:B:651:LEU:HD21	1.99	0.44
6:C:46:ILE:O	6:C:169:LYS:HE3	2.18	0.44
10:I:21:GLU:O	10:I:22:ASN:CB	2.65	0.44
5:B:487:THR:CG2	5:B:488:TYR:N	2.80	0.44
5:B:999:MET:CE	5:B:1000:PRO:HD2	2.47	0.44
6:C:101:LEU:HB3	6:C:155:LEU:HB2	2.00	0.44
4:A:451:HIS:HB3	4:A:453:MET:H	1.81	0.44
4:A:541:ILE:CD1	4:A:577:ILE:HD11	2.48	0.44
4:A:855:THR:HG23	4:A:855:THR:O	2.18	0.44
4:A:1162:VAL:HG23	4:A:1163:ILE:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:756:ILE:O	5:B:759:PRO:HD3	2.17	0.44
8:F:145:ASP:O	8:F:146:TRP:CB	2.65	0.44
9:H:129:TYR:O	9:H:130:ARG:CG	2.65	0.44
10:I:63:GLY:CA	10:I:104:LEU:HD21	2.32	0.44
4:A:304:MET:SD	5:B:1210:MET:HG3	2.58	0.44
4:A:344:ARG:HB3	5:B:1118:PRO:HD2	1.99	0.44
4:A:1150:SER:HB3	10:I:46:HIS:CD2	2.53	0.44
4:A:1325:THR:HG23	4:A:1326:ARG:HG3	2.00	0.44
5:B:408:LEU:O	5:B:409:ALA:C	2.60	0.44
16:B:3000:UTP:H5'1	16:B:3000:UTP:H6	1.83	0.44
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.00	0.44
4:A:366:VAL:O	4:A:463:ILE:HG13	2.18	0.44
4:A:722:LEU:C	4:A:724:GLU:N	2.75	0.44
4:A:838:GLN:C	4:A:840:ARG:N	2.74	0.44
4:A:1327:ILE:O	7:E:147:HIS:CE1	2.71	0.44
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.99	0.44
5:B:387:LEU:HD13	5:B:392:ARG:HD2	1.99	0.44
5:B:458:LYS:O	5:B:459:TYR:C	2.61	0.44
5:B:547:VAL:CG1	5:B:548:GLY:N	2.81	0.44
5:B:865:LYS:HB2	5:B:865:LYS:HE3	1.81	0.44
4:A:365:GLY:HA3	4:A:469:ARG:HB2	2.00	0.43
4:A:479:ASN:ND2	4:A:1078:GLN:OE1	2.50	0.43
4:A:1070:GLN:O	4:A:1074:GLU:CB	2.64	0.43
5:B:242:SER:HB2	5:B:362:PRO:HD2	2.00	0.43
5:B:357:GLN:HA	5:B:374:LYS:HZ1	1.80	0.43
6:C:43:THR:HG22	6:C:44:LEU:H	1.83	0.43
6:C:71:PRO:HB2	6:C:133:ILE:HB	1.98	0.43
7:E:9:ILE:C	7:E:11:ARG:N	2.76	0.43
7:E:19:VAL:O	7:E:23:VAL:HG23	2.17	0.43
11:J:43:ARG:HD2	11:J:46:CYS:SG	2.58	0.43
12:K:65:HIS:C	12:K:67:PHE:N	2.76	0.43
4:A:413:ILE:HG22	4:A:413:ILE:O	2.18	0.43
4:A:451:HIS:O	4:A:1070:GLN:NE2	2.52	0.43
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.50	0.43
4:A:956:LEU:HA	4:A:957:PRO:HD3	1.68	0.43
5:B:273:LEU:HD21	5:B:360:PHE:HB2	1.99	0.43
5:B:572:HIS:N	5:B:573:GLN:CB	2.77	0.43
5:B:986:GLN:HE21	5:B:1025:HIS:HD2	1.64	0.43
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.46	0.43
7:E:52:ARG:HA	7:E:53:PRO:HD3	1.74	0.43
4:A:668:ASP:HB3	4:A:743:VAL:CG2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:870:GLU:OE2	7:E:200:ARG:NH1	2.51	0.43
5:B:46:GLN:OE1	5:B:47:GLN:HG2	2.18	0.43
5:B:563:MET:HA	5:B:590:HIS:ND1	2.33	0.43
5:B:1194:ILE:HD13	5:B:1194:ILE:H	1.84	0.43
7:E:16:PHE:O	7:E:17:ARG:C	2.62	0.43
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.83	0.43
9:H:105:GLU:HB3	9:H:113:ALA:HB3	1.99	0.43
5:B:898:LEU:HD22	5:B:964:VAL:HG11	2.00	0.43
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.99	0.43
4:A:383:TYR:OH	8:F:107:VAL:HG21	2.19	0.43
4:A:751:SER:CB	5:B:1015:HIS:HE1	2.26	0.43
4:A:816:HIS:CD2	5:B:764:SER:H	2.36	0.43
4:A:1089:VAL:H	4:A:1090:ALA:HA	1.77	0.43
4:A:1313:LEU:O	4:A:1314:SER:C	2.61	0.43
5:B:31:TRP:O	5:B:34:ILE:HB	2.17	0.43
5:B:53:GLN:O	5:B:53:GLN:HG3	2.16	0.43
6:C:102:GLN:CD	6:C:154:LYS:HD2	2.43	0.43
10:I:113:ASP:CG	10:I:116:ASN:HB2	2.44	0.43
12:K:58:PHE:HE2	12:K:74:ARG:HB3	1.84	0.43
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.48	0.43
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.54	0.43
5:B:463:THR:HB	5:B:465:ASN:H	1.84	0.43
5:B:790:ASP:N	5:B:790:ASP:OD1	2.52	0.43
7:E:55:ARG:O	7:E:56:LYS:C	2.61	0.43
10:I:2:THR:OG1	10:I:43:VAL:HG13	2.18	0.43
11:J:2:ILE:HG13	11:J:57:ILE:HG21	1.99	0.43
4:A:135:PHE:HA	4:A:138:ILE:HD12	2.00	0.43
4:A:304:MET:SD	5:B:1210:MET:HA	2.59	0.43
4:A:313:GLN:HB3	4:A:314:ALA:H	1.66	0.43
4:A:374:LEU:CB	4:A:436:ILE:HD11	2.49	0.43
4:A:567:LYS:HD2	9:H:46:LEU:HD13	2.01	0.43
4:A:596:THR:C	4:A:598:LEU:N	2.77	0.43
4:A:1277:GLU:H	4:A:1277:GLU:HG2	1.70	0.43
5:B:124:TYR:HB2	5:B:204:ILE:HB	2.01	0.43
5:B:172:ILE:HG22	5:B:173:MET:O	2.19	0.43
5:B:230:ALA:N	5:B:231:PRO:CD	2.81	0.43
12:K:40:HIS:CE1	12:K:63:VAL:HG11	2.53	0.43
2:T:19:DT:H2'	2:T:20:DC:C6	2.54	0.43
4:A:88:LYS:HA	4:A:89:PRO:HD3	1.91	0.43
4:A:353:ILE:HA	4:A:468:PHE:O	2.19	0.43
4:A:1092:LYS:CB	4:A:1093:LYS:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:555:ILE:HA	5:B:558:LEU:HD12	2.00	0.43
5:B:1010:LEU:HD12	5:B:1010:LEU:HA	1.75	0.43
5:B:1213:THR:HB	5:B:1215:ARG:NH1	2.34	0.43
6:C:91:HIS:HB2	6:C:96:SER:OG	2.19	0.43
7:E:138:ALA:HA	7:E:140:LEU:N	2.33	0.43
8:F:93:ILE:HD11	8:F:132:LEU:HB2	2.00	0.43
9:H:43:ASN:ND2	9:H:46:LEU:HD12	2.34	0.43
4:A:77:CYS:SG	4:A:80:HIS:NE2	2.91	0.43
4:A:826:ASP:HB2	4:A:830:LYS:HB3	2.01	0.43
4:A:1171:GLN:O	4:A:1173:HIS:N	2.52	0.43
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.54	0.43
5:B:890:TYR:CE2	5:B:910:VAL:HG11	2.54	0.43
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.19	0.43
4:A:38:PRO:CB	4:A:39:GLU:HA	2.47	0.43
4:A:82:GLY:C	4:A:241:VAL:HG22	2.44	0.43
4:A:774:ARG:O	4:A:775:ILE:C	2.61	0.43
4:A:961:ARG:HH11	4:A:965:GLN:HE22	1.65	0.43
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	2.01	0.43
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	2.01	0.42
4:A:867:ILE:HG22	4:A:872:GLY:HA3	2.01	0.42
4:A:979:SER:OG	4:A:980:ASP:N	2.53	0.42
5:B:802:PRO:HA	5:B:1091:TYR:CD1	2.54	0.42
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.24	0.42
5:B:846:ILE:HG23	5:B:974:PRO:HG2	2.01	0.42
5:B:886:LYS:C	5:B:888:GLY:H	2.26	0.42
7:E:59:SER:HB3	7:E:80:VAL:O	2.18	0.42
10:I:3:THR:CA	10:I:4:PHE:CB	2.93	0.42
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.42
4:A:502:SER:HA	4:A:506:ALA:HB2	2.01	0.42
5:B:37:PHE:O	5:B:38:PHE:HB2	2.19	0.42
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.49	0.42
5:B:820:GLY:N	5:B:1091:TYR:OH	2.49	0.42
10:I:4:PHE:HD1	10:I:5:ARG:N	2.17	0.42
12:K:40:HIS:HB3	12:K:61:TYR:HE1	1.84	0.42
12:K:82:ASP:OD2	12:K:84:LYS:HB2	2.20	0.42
4:A:332:LYS:C	4:A:334:GLY:N	2.77	0.42
4:A:562:THR:HA	4:A:563:PRO:HD2	1.81	0.42
4:A:647:GLY:O	4:A:651:LYS:HG3	2.19	0.42
4:A:711:ARG:CA	4:A:713:SER:HB2	2.48	0.42
5:B:31:TRP:HA	5:B:34:ILE:HG13	2.01	0.42
5:B:408:LEU:C	5:B:412:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:82:THR:HA	8:F:83:PRO:HD3	1.87	0.42
12:K:32:VAL:HG22	12:K:74:ARG:HG3	2.00	0.42
2:T:18:DA:H2'	2:T:19:DT:C6	2.55	0.42
4:A:465:TYR:HB3	5:B:976:ILE:HG21	2.01	0.42
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.84	0.42
5:B:1176:ASN:C	5:B:1177:HIS:CG	2.97	0.42
7:E:141:VAL:HG12	7:E:142:VAL:HG23	2.00	0.42
13:L:60:ARG:HG3	13:L:61:THR:N	2.34	0.42
4:A:503:GLN:C	4:A:504:LEU:HD12	2.43	0.42
4:A:1155:ASP:OD1	4:A:1190:PRO:HA	2.18	0.42
5:B:254:LEU:HD12	5:B:272:THR:O	2.20	0.42
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.02	0.42
5:B:886:LYS:O	5:B:888:GLY:N	2.42	0.42
6:C:43:THR:HG22	6:C:44:LEU:N	2.34	0.42
11:J:8:PHE:H	11:J:49:MET:HE3	1.83	0.42
4:A:351:THR:CG2	4:A:352:VAL:H	2.32	0.42
4:A:589:GLN:HB3	4:A:961:ARG:HH22	1.84	0.42
4:A:900:ASP:O	4:A:907:THR:OG1	2.31	0.42
4:A:1078:GLN:O	4:A:1082:ASN:HB2	2.20	0.42
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.85	0.42
5:B:483:LEU:HD22	5:B:484:ASN:H	1.85	0.42
5:B:745:PRO:HB2	5:B:1047:PHE:HD1	1.84	0.42
5:B:973:ILE:H	5:B:973:ILE:HG13	1.47	0.42
6:C:21:ILE:O	6:C:22:LEU:HB2	2.18	0.42
10:I:115:LYS:C	10:I:116:ASN:HD22	2.27	0.42
4:A:1015:VAL:O	4:A:1016:THR:C	2.63	0.42
5:B:620:ARG:HH21	10:I:68:LEU:HD21	1.84	0.42
5:B:867:GLY:HA2	5:B:868:MET:HA	1.65	0.42
5:B:1011:ILE:HD12	5:B:1011:ILE:N	2.34	0.42
5:B:1077:THR:C	5:B:1079:LYS:H	2.28	0.42
5:B:1139:ILE:H	5:B:1139:ILE:HG13	1.66	0.42
4:A:14:VAL:HG21	4:A:1430:LEU:HD22	2.01	0.42
4:A:538:ASP:HB2	9:H:20:TYR:CD2	2.54	0.42
4:A:606:LEU:HD23	4:A:613:ILE:HG21	2.01	0.42
4:A:841:LEU:HD22	4:A:1072:ILE:HG21	2.01	0.42
5:B:232:SER:HA	5:B:233:PRO:HD3	2.00	0.42
5:B:681:TRP:O	5:B:682:SER:C	2.63	0.42
5:B:911:ILE:HG22	5:B:912:ILE:CG1	2.43	0.42
7:E:22:MET:HG3	7:E:187:TYR:CD1	2.54	0.42
7:E:65:THR:C	7:E:67:GLU:N	2.76	0.42
9:H:111:LEU:HB2	9:H:112:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:42:LEU:HD22	10:I:43:VAL:N	2.34	0.42
4:A:817:ALA:O	4:A:818:MET:C	2.62	0.42
4:A:964:ILE:O	4:A:968:GLN:HG2	2.20	0.42
4:A:1012:ARG:C	4:A:1014:ALA:H	2.28	0.42
4:A:1197:LEU:HB3	4:A:1198:ASP:O	2.19	0.42
5:B:265:SER:O	5:B:266:ALA:CB	2.68	0.42
6:C:61:GLU:HA	6:C:64:ALA:HB3	2.01	0.42
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.49	0.42
4:A:582:ILE:HG22	4:A:610:GLY:HA2	2.02	0.42
4:A:745:GLN:H	4:A:745:GLN:HG2	1.62	0.42
4:A:1057:VAL:HG12	4:A:1058:VAL:O	2.19	0.42
5:B:211:VAL:O	5:B:480:SER:HA	2.20	0.42
5:B:796:LEU:HD22	5:B:799:PRO:HA	2.02	0.42
5:B:802:PRO:HA	5:B:822:ASN:ND2	2.35	0.42
5:B:826:ALA:O	5:B:1011:ILE:HA	2.20	0.42
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.66	0.42
4:A:704:ALA:HB1	4:A:710:LEU:HD22	2.01	0.41
4:A:858:ASN:ND2	4:A:860:LEU:H	2.18	0.41
5:B:67:SER:HB2	5:B:92:PHE:CD1	2.55	0.41
5:B:123:THR:O	5:B:125:SER:N	2.43	0.41
6:C:18:VAL:HG23	6:C:240:VAL:HB	2.02	0.41
7:E:161:LYS:HG3	7:E:195:VAL:HG21	2.02	0.41
7:E:202:SER:OG	7:E:204:THR:HG22	2.20	0.41
4:A:563:PRO:C	4:A:565:ILE:H	2.28	0.41
4:A:831:THR:O	4:A:834:THR:HG23	2.20	0.41
4:A:987:VAL:C	4:A:989:GLY:N	2.78	0.41
4:A:1096:SER:O	4:A:1100:ARG:HG3	2.21	0.41
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.52	0.41
5:B:831:SER:CB	5:B:833:TYR:HD1	2.32	0.41
5:B:977:GLY:HA3	5:B:1099:VAL:HG11	2.02	0.41
5:B:1013:ASN:C	5:B:1015:HIS:H	2.28	0.41
5:B:1021:MET:HE3	5:B:1021:MET:HB2	1.91	0.41
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.55	0.41
4:A:810:PRO:O	4:A:811:GLN:C	2.63	0.41
4:A:812:GLU:O	4:A:813:PHE:C	2.64	0.41
5:B:125:SER:HA	5:B:171:PRO:HA	2.01	0.41
5:B:475:SER:O	5:B:476:ARG:C	2.63	0.41
4:A:537:ARG:HG2	4:A:575:LYS:HE3	2.00	0.41
4:A:567:LYS:O	4:A:568:PRO:C	2.63	0.41
4:A:657:LEU:O	4:A:658:LEU:C	2.62	0.41
4:A:754:SER:H	4:A:757:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:777:PHE:CE2	4:A:782:ARG:HA	2.55	0.41
5:B:363:HIS:O	5:B:364:ILE:CB	2.66	0.41
5:B:1150:ARG:HA	5:B:1150:ARG:HD3	1.90	0.41
6:C:234:SER:HB3	6:C:240:VAL:HG13	2.02	0.41
6:C:245:VAL:HA	6:C:248:ILE:HD12	2.03	0.41
6:C:250:THR:HA	6:C:253:LYS:HB2	2.02	0.41
7:E:149:LEU:O	7:E:151:PRO:HD3	2.20	0.41
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.83	0.41
4:A:323:LYS:N	4:A:323:LYS:HD3	2.35	0.41
4:A:365:GLY:N	4:A:469:ARG:O	2.50	0.41
4:A:722:LEU:C	4:A:724:GLU:H	2.28	0.41
5:B:195:CYS:HB3	5:B:198:ASP:HB2	2.02	0.41
5:B:391:ASP:HA	5:B:393:LYS:N	2.36	0.41
5:B:586:TRP:CD1	5:B:588:GLY:H	2.39	0.41
5:B:757:PRO:HD3	5:B:983:ARG:HE	1.85	0.41
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.55	0.41
2:T:20:DC:OP1	5:B:1131:GLY:HA3	2.19	0.41
4:A:23:SER:O	4:A:27:VAL:HG23	2.21	0.41
5:B:128:LEU:HB2	5:B:167:ILE:O	2.21	0.41
5:B:183:GLU:CA	5:B:184:ALA:HB3	2.51	0.41
5:B:636:PRO:HB3	5:B:743:ILE:CG1	2.51	0.41
8:F:138:LEU:O	8:F:139:PRO:C	2.63	0.41
9:H:23:VAL:HG11	9:H:121:LEU:HD22	2.02	0.41
12:K:42:LEU:O	12:K:46:ILE:HB	2.21	0.41
4:A:395:GLY:C	4:A:397:ASN:H	2.29	0.41
4:A:552:TRP:CE3	4:A:651:LYS:HB3	2.55	0.41
4:A:919:ILE:O	4:A:920:LEU:C	2.64	0.41
4:A:1083:THR:CA	4:A:1084:PHE:O	2.68	0.41
5:B:273:LEU:HD23	5:B:274:PRO:HD2	2.01	0.41
5:B:549:THR:HB	5:B:628:THR:HG22	2.02	0.41
5:B:833:TYR:C	5:B:835:GLN:H	2.29	0.41
5:B:1103:ILE:O	5:B:1103:ILE:HG22	2.21	0.41
5:B:1177:HIS:CA	5:B:1178:ASN:CB	2.98	0.41
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.51	0.41
6:C:34:ARG:HG3	6:C:35:ARG:N	2.34	0.41
6:C:73:GLN:HB3	6:C:131:HIS:H	1.86	0.41
6:C:102:GLN:OE1	6:C:154:LYS:HD2	2.20	0.41
9:H:92:ASP:O	9:H:145:ARG:HD3	2.20	0.41
10:I:103:CYS:SG	10:I:106:CYS:HB2	2.60	0.41
4:A:16:GLU:HB2	5:B:1217:TYR:HB2	2.03	0.41
4:A:453:MET:HE1	4:A:514:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:LEU:HD11	4:A:649:ILE:HD11	2.02	0.41
4:A:710:LEU:HA	4:A:712:GLU:N	2.36	0.41
4:A:1064:VAL:O	4:A:1065:GLY:C	2.63	0.41
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	2.03	0.41
4:A:1193:LEU:HD21	4:A:1264:GLU:HB3	2.03	0.41
4:A:1265:ASN:C	4:A:1267:MET:H	2.29	0.41
5:B:51:PHE:CE1	5:B:203:PHE:HE2	2.39	0.41
5:B:523:CYS:SG	5:B:750:GLY:N	2.94	0.41
5:B:1023:VAL:O	5:B:1026:LEU:HB2	2.21	0.41
9:H:105:GLU:HG3	9:H:106:GLU:N	2.30	0.41
11:J:3:VAL:HA	11:J:4:PRO:HD3	1.88	0.41
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.56	0.41
4:A:619:LYS:O	4:A:623:GLY:HA3	2.21	0.41
4:A:857:ARG:HA	4:A:864:ILE:HG12	2.03	0.41
4:A:1364:ASN:C	4:A:1364:ASN:ND2	2.79	0.41
4:A:1438:THR:CG2	8:F:92:ARG:HB2	2.51	0.41
5:B:29:ASP:HB3	5:B:658:ILE:HD13	2.03	0.41
7:E:140:LEU:HA	7:E:142:VAL:H	1.84	0.41
12:K:40:HIS:HB3	12:K:61:TYR:CE1	2.56	0.41
4:A:61:ILE:HG13	4:A:62:ASP:H	1.86	0.41
4:A:452:LYS:HB3	5:B:1140:ALA:CB	2.50	0.41
4:A:675:THR:HG21	4:A:736:ASN:ND2	2.26	0.41
4:A:962:ARG:C	4:A:964:ILE:N	2.77	0.41
4:A:1072:ILE:HD13	4:A:1072:ILE:HA	1.86	0.41
4:A:1200:ALA:CB	4:A:1203:ASN:HB2	2.50	0.41
4:A:1371:LEU:O	4:A:1372:VAL:C	2.63	0.41
5:B:634:TYR:HE1	5:B:692:TYR:CD1	2.36	0.41
5:B:746:SER:C	5:B:748:ILE:H	2.29	0.41
5:B:999:MET:HE3	5:B:999:MET:HA	2.03	0.41
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.02	0.41
6:C:258:ILE:H	6:C:258:ILE:HG13	1.60	0.41
4:A:86:LEU:HD23	4:A:273:ASN:HD22	1.86	0.40
4:A:256:GLN:HE21	4:A:256:GLN:HB3	1.62	0.40
4:A:347:PHE:H	5:B:1107:ALA:HA	1.86	0.40
4:A:481:ASP:HA	5:B:836:GLU:HG2	2.03	0.40
4:A:527:THR:HG23	4:A:650:GLN:HA	2.04	0.40
4:A:814:PHE:O	4:A:817:ALA:HB3	2.22	0.40
4:A:1323:ASP:CG	4:A:1325:THR:HG22	2.45	0.40
5:B:183:GLU:N	5:B:184:ALA:HB3	2.36	0.40
5:B:212:LEU:HD21	5:B:461:LEU:CD1	2.50	0.40
5:B:238:ALA:HB3	5:B:256:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:293:PRO:CA	5:B:294:ASP:HB2	2.29	0.40
5:B:550:ASP:HA	5:B:551:PRO:HD3	1.97	0.40
10:I:118:ARG:C	10:I:120:GLN:H	2.29	0.40
4:A:764:CYS:HA	4:A:802:ASN:O	2.21	0.40
4:A:1192:LEU:HD13	4:A:1193:LEU:N	2.35	0.40
4:A:1366:ARG:HG2	4:A:1366:ARG:H	1.77	0.40
7:E:59:SER:O	7:E:60:PHE:HB3	2.21	0.40
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.56	0.40
2:T:18:DA:H8	4:A:832:ALA:HA	1.87	0.40
4:A:977:LYS:HD3	4:A:977:LYS:HA	1.69	0.40
4:A:993:LEU:HA	4:A:996:ASN:HD21	1.86	0.40
5:B:421:PHE:HA	5:B:453:ILE:HD11	2.03	0.40
5:B:1138:MET:HE2	5:B:1146:PHE:CD2	2.56	0.40
7:E:21:GLU:O	7:E:24:LYS:HG2	2.21	0.40
7:E:79:TRP:CZ2	7:E:99:HIS:NE2	2.90	0.40
9:H:137:GLN:HG2	9:H:138:GLU:H	1.85	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.90	0.40
4:A:505:CYS:O	4:A:506:ALA:C	2.65	0.40
4:A:560:ILE:H	4:A:560:ILE:HG12	1.58	0.40
4:A:809:THR:O	4:A:810:PRO:C	2.64	0.40
4:A:1189:SER:HB2	4:A:1242:VAL:O	2.22	0.40
4:A:1271:ILE:HD13	4:A:1271:ILE:HA	1.99	0.40
5:B:327:ARG:O	5:B:331:LEU:HD12	2.21	0.40
5:B:745:PRO:O	5:B:746:SER:C	2.65	0.40
6:C:166:GLU:O	6:C:167:HIS:CB	2.69	0.40
4:A:38:PRO:HG3	4:A:270:LEU:HB3	2.04	0.40
4:A:71:GLN:O	4:A:73:GLY:N	2.53	0.40
4:A:380:VAL:HG12	4:A:388:LEU:HD13	2.03	0.40
4:A:818:MET:HA	5:B:514:LEU:HB3	2.03	0.40
4:A:841:LEU:O	4:A:845:LEU:HG	2.22	0.40
4:A:975:HIS:NE2	9:H:136:LYS:HB2	2.36	0.40
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	2.03	0.40
5:B:108:VAL:HG12	5:B:109:THR:N	2.37	0.40
8:F:82:THR:HG22	8:F:84:TYR:HB2	2.04	0.40
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.56	0.40
9:H:111:LEU:HD12	9:H:127:GLY:CA	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1384/1733 (80%)	1055 (76%)	224 (16%)	105 (8%)	1	10
5	B	1074/1224 (88%)	855 (80%)	161 (15%)	58 (5%)	1	15
6	C	264/318 (83%)	217 (82%)	35 (13%)	12 (4%)	2	17
7	E	185/215 (86%)	146 (79%)	26 (14%)	13 (7%)	1	11
8	F	81/155 (52%)	62 (76%)	15 (18%)	4 (5%)	1	16
9	H	129/146 (88%)	87 (67%)	30 (23%)	12 (9%)	0	8
10	I	117/122 (96%)	73 (62%)	32 (27%)	12 (10%)	0	6
11	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2	16
12	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	14	49
13	L	44/70 (63%)	29 (66%)	11 (25%)	4 (9%)	0	8
All	All	3453/4173 (83%)	2678 (78%)	551 (16%)	224 (6%)	1	13

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	63	ARG
4	A	223	GLY
4	A	284	ALA
4	A	313	GLN
4	A	404	TYR
4	A	517	ASN
4	A	525	GLN
4	A	568	PRO
4	A	702	LEU
4	A	710	LEU
4	A	903	ASN
4	A	998	LEU
4	A	1016	THR
4	A	1081	LEU

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Mol	Chain	Res	Type
4	A	1084	PHE
4	A	1085	HIS
4	A	1156	PRO
4	A	1158	PRO
4	A	1163	ILE
4	A	1165	GLU
4	A	1172	LEU
4	A	1191	TRP
4	A	1365	TYR
4	A	1392	SER
4	A	1393	ASN
5	B	66	ASP
5	B	184	ALA
5	B	231	PRO
5	B	274	PRO
5	B	636	PRO
5	B	711	GLU
5	B	878	GLN
5	B	882	THR
5	B	1178	ASN
6	C	110	THR
6	C	167	HIS
6	C	173	ALA
6	C	174	ALA
7	E	130	ALA
8	F	104	ASN
8	F	128	LYS
9	H	77	ARG
9	H	84	ALA
10	I	21	GLU
10	I	26	LEU
10	I	46	HIS
10	I	47	GLU
13	L	26	THR
4	A	55	ASP
4	A	71	GLN
4	A	250	ILE
4	A	279	LEU
4	A	288	ALA
4	A	312	PRO
4	A	423	ASP
4	A	424	ILE

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Mol	Chain	Res	Type
4	A	479	ASN
4	A	543	LEU
4	A	576	GLN
4	A	624	SER
4	A	637	LYS
4	A	713	SER
4	A	1069	ALA
4	A	1072	ILE
4	A	1094	VAL
4	A	1127	ASP
4	A	1153	TYR
4	A	1154	TYR
4	A	1160	SER
4	A	1167	GLU
4	A	1192	LEU
4	A	1224	LEU
4	A	1391	ARG
5	B	228	LYS
5	B	266	ALA
5	B	276	ILE
5	B	301	ILE
5	B	391	ASP
5	B	410	GLY
5	B	474	SER
5	B	478	GLY
5	B	705	MET
5	B	708	GLU
5	B	864	LYS
5	B	996	ARG
5	B	1020	ARG
5	B	1021	MET
5	B	1167	GLY
5	B	1177	HIS
6	C	22	LEU
6	C	142	VAL
6	C	266	ASP
7	E	30	ILE
7	E	36	GLU
7	E	141	VAL
7	E	174	GLN
7	E	206	GLY
8	F	145	ASP

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Mol	Chain	Res	Type
9	H	82	PRO
9	H	85	GLY
9	H	89	LEU
9	H	107	VAL
9	H	112	ILE
9	H	140	ALA
4	A	48	ALA
4	A	72	GLU
4	A	214	ILE
4	A	257	ARG
4	A	289	ILE
4	A	465	TYR
4	A	741	ASN
4	A	972	HIS
4	A	1206	ASP
5	B	477	ALA
5	B	482	VAL
5	B	531	GLN
5	B	792	MET
6	C	88	CYS
6	C	90	ASP
9	H	91	ASP
9	H	131	ASN
10	I	4	PHE
13	L	56	LEU
4	A	54	ASN
4	A	287	HIS
4	A	321	PRO
4	A	591	PHE
4	A	651	LYS
4	A	708	MET
4	A	775	ILE
4	A	975	HIS
4	A	1003	LYS
4	A	1262	LYS
4	A	1270	ASN
4	A	1435	PRO
5	B	100	PRO
5	B	124	TYR
5	B	458	LYS
5	B	572	HIS
5	B	635	ARG

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Mol	Chain	Res	Type
5	B	710	LEU
5	B	865	LYS
5	B	887	HIS
5	B	1017	ILE
5	B	1046	PRO
5	B	1103	ILE
5	B	1112	GLN
7	E	125	PRO
8	F	146	TRP
10	I	20	LYS
10	I	113	ASP
11	J	10	CYS
11	J	29	GLU
12	K	66	PRO
4	A	10	PRO
4	A	58	LEU
4	A	178	GLY
4	A	213	HIS
4	A	254	GLU
4	A	306	ASN
4	A	332	LYS
4	A	333	GLU
4	A	639	PRO
4	A	650	GLN
4	A	673	GLY
4	A	870	GLU
4	A	902	LEU
4	A	910	PRO
4	A	920	LEU
4	A	922	ASP
4	A	958	VAL
4	A	969	GLN
4	A	1013	ASP
4	A	1155	ASP
4	A	1164	PRO
4	A	1366	ARG
5	B	64	CYS
5	B	232	SER
5	B	476	ARG
5	B	652	LYS
5	B	786	ASN
5	B	870	ILE

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Mol	Chain	Res	Type
5	B	974	PRO
6	C	21	ILE
6	C	38	ILE
7	E	29	PHE
7	E	66	GLU
7	E	96	PHE
7	E	166	LYS
9	H	7	ASP
9	H	23	VAL
10	I	11	ASN
10	I	18	GLU
11	J	2	ILE
13	L	59	ALA
4	A	248	PRO
4	A	707	GLY
4	A	883	LEU
4	A	886	ILE
4	A	1388	GLY
5	B	233	PRO
5	B	275	TYR
5	B	436	VAL
5	B	571	PRO
5	B	712	PRO
5	B	731	VAL
5	B	746	SER
6	C	168	ALA
7	E	76	GLY
10	I	118	ARG
4	A	1107	VAL
4	A	1237	ILE
13	L	55	ILE
4	A	35	ILE
4	A	1157	ASP
4	A	52	GLY
5	B	592	ASN
10	I	59	VAL
4	A	3	GLY
7	E	124	VAL
10	I	43	VAL
4	A	396	PRO
5	B	234	ILE
5	B	751	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1218/1520 (80%)	1026 (84%)	192 (16%)	2	13
5	B	951/1061 (90%)	817 (86%)	134 (14%)	3	15
6	C	234/274 (85%)	205 (88%)	29 (12%)	4	18
7	E	177/197 (90%)	157 (89%)	20 (11%)	5	21
8	F	73/137 (53%)	64 (88%)	9 (12%)	4	18
9	H	117/128 (91%)	103 (88%)	14 (12%)	5	19
10	I	113/116 (97%)	90 (80%)	23 (20%)	1	8
11	J	60/65 (92%)	50 (83%)	10 (17%)	2	12
12	K	99/102 (97%)	82 (83%)	17 (17%)	2	11
13	L	40/57 (70%)	29 (72%)	11 (28%)	0	3
All	All	3082/3657 (84%)	2623 (85%)	459 (15%)	3	14

All (459) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	13	THR
4	A	30	ILE
4	A	41	MET
4	A	49	LYS
4	A	50	ILE
4	A	53	LEU
4	A	58	LEU
4	A	65	LEU
4	A	67	CYS
4	A	68	GLN
4	A	69	THR
4	A	80	HIS
4	A	84	ILE
4	A	90	VAL
4	A	100	LYS
4	A	108	MET

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Mol	Chain	Res	Type
4	A	121	LEU
4	A	122	MET
4	A	133	LYS
4	A	140	THR
4	A	161	LEU
4	A	180	LYS
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	256	GLN
4	A	260	ASP
4	A	264	PHE
4	A	270	LEU
4	A	274	ILE
4	A	279	LEU
4	A	280	GLU
4	A	286	HIS
4	A	289	ILE
4	A	302	THR
4	A	306	ASN
4	A	308	ILE
4	A	313	GLN
4	A	320	ARG
4	A	322	VAL
4	A	323	LYS
4	A	348	SER
4	A	352	VAL
4	A	373	THR
4	A	379	VAL
4	A	381	THR
4	A	391	LEU
4	A	443	LEU
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	466	SER
4	A	469	ARG
4	A	470	LEU
4	A	481	ASP
4	A	487	MET
4	A	494	SER

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Mol	Chain	Res	Type
4	A	501	LEU
4	A	509	LEU
4	A	535	THR
4	A	541	ILE
4	A	544	ASP
4	A	560	ILE
4	A	566	ILE
4	A	576	GLN
4	A	577	ILE
4	A	582	ILE
4	A	596	THR
4	A	618	GLU
4	A	630	ILE
4	A	635	ARG
4	A	645	LEU
4	A	652	VAL
4	A	660	ASN
4	A	666	ILE
4	A	675	THR
4	A	680	THR
4	A	687	LYS
4	A	710	LEU
4	A	714	PHE
4	A	721	PHE
4	A	728	LYS
4	A	735	VAL
4	A	738	LYS
4	A	739	ASP
4	A	740	LEU
4	A	743	VAL
4	A	745	GLN
4	A	756	ILE
4	A	758	ILE
4	A	765	VAL
4	A	795	GLU
4	A	821	ARG
4	A	829	VAL
4	A	834	THR
4	A	839	ARG
4	A	841	LEU
4	A	856	THR
4	A	858	ASN

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Mol	Chain	Res	Type
4	A	859	SER
4	A	867	ILE
4	A	881	GLN
4	A	896	ARG
4	A	902	LEU
4	A	913	LEU
4	A	915	SER
4	A	918	GLU
4	A	920	LEU
4	A	927	VAL
4	A	929	LEU
4	A	941	LYS
4	A	945	GLU
4	A	949	ASP
4	A	964	ILE
4	A	971	PHE
4	A	972	HIS
4	A	973	ILE
4	A	974	ASP
4	A	988	LEU
4	A	994	GLN
4	A	996	ASN
4	A	998	LEU
4	A	1015	VAL
4	A	1016	THR
4	A	1017	LEU
4	A	1025	ARG
4	A	1028	THR
4	A	1034	GLU
4	A	1035	TYR
4	A	1048	ASN
4	A	1054	LEU
4	A	1058	VAL
4	A	1078	GLN
4	A	1083	THR
4	A	1085	HIS
4	A	1086	PHE
4	A	1104	ILE
4	A	1109	LYS
4	A	1113	THR
4	A	1116	LEU
4	A	1127	ASP

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Mol	Chain	Res	Type
4	A	1128	GLN
4	A	1129	GLU
4	A	1141	THR
4	A	1142	THR
4	A	1152	ILE
4	A	1156	PRO
4	A	1158	PRO
4	A	1159	ARG
4	A	1161	THR
4	A	1162	VAL
4	A	1166	ASP
4	A	1167	GLU
4	A	1170	ILE
4	A	1172	LEU
4	A	1187	GLN
4	A	1188	GLN
4	A	1192	LEU
4	A	1215	ARG
4	A	1224	LEU
4	A	1227	ILE
4	A	1228	TRP
4	A	1242	VAL
4	A	1262	LYS
4	A	1266	THR
4	A	1271	ILE
4	A	1276	VAL
4	A	1281	ARG
4	A	1284	MET
4	A	1295	THR
4	A	1297	GLU
4	A	1322	ILE
4	A	1329	THR
4	A	1333	ILE
4	A	1334	ASP
4	A	1335	ILE
4	A	1336	MET
4	A	1356	ILE
4	A	1358	SER
4	A	1364	ASN
4	A	1366	ARG
4	A	1371	LEU
4	A	1376	THR

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Mol	Chain	Res	Type
4	A	1385	THR
4	A	1391	ARG
4	A	1394	THR
4	A	1407	GLU
4	A	1426	GLU
4	A	1428	VAL
4	A	1442	ASP
4	A	1443	VAL
5	B	28	GLU
5	B	44	VAL
5	B	46	GLN
5	B	66	ASP
5	B	94	LYS
5	B	102	VAL
5	B	108	VAL
5	B	167	ILE
5	B	178	ASN
5	B	180	TYR
5	B	185	THR
5	B	188	ASP
5	B	223	VAL
5	B	225	VAL
5	B	234	ILE
5	B	242	SER
5	B	256	VAL
5	B	264	SER
5	B	268	THR
5	B	273	LEU
5	B	284	ILE
5	B	291	ILE
5	B	297	ILE
5	B	302	CYS
5	B	304	ASP
5	B	323	VAL
5	B	334	ILE
5	B	346	GLU
5	B	347	LYS
5	B	351	TYR
5	B	361	LEU
5	B	367	LEU
5	B	373	ARG
5	B	387	LEU

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Mol	Chain	Res	Type
5	B	391	ASP
5	B	393	LYS
5	B	394	ASP
5	B	398	ARG
5	B	415	GLN
5	B	424	LEU
5	B	425	THR
5	B	432	MET
5	B	448	ILE
5	B	463	THR
5	B	466	TRP
5	B	473	MET
5	B	475	SER
5	B	479	VAL
5	B	483	LEU
5	B	502	ILE
5	B	522	VAL
5	B	537	LYS
5	B	542	MET
5	B	547	VAL
5	B	549	THR
5	B	598	GLU
5	B	603	LEU
5	B	604	ARG
5	B	616	ILE
5	B	618	ASP
5	B	624	LEU
5	B	628	THR
5	B	635	ARG
5	B	637	LEU
5	B	650	GLU
5	B	651	LEU
5	B	655	LYS
5	B	658	ILE
5	B	680	THR
5	B	685	LEU
5	B	701	ILE
5	B	702	LEU
5	B	728	ARG
5	B	736	THR
5	B	740	HIS
5	B	741	CYS

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Mol	Chain	Res	Type
5	B	748	ILE
5	B	755	ILE
5	B	787	VAL
5	B	796	LEU
5	B	797	TYR
5	B	812	LEU
5	B	822	ASN
5	B	837	ASP
5	B	844	SER
5	B	864	LYS
5	B	866	TYR
5	B	880	THR
5	B	883	LEU
5	B	898	LEU
5	B	899	ILE
5	B	905	VAL
5	B	906	SER
5	B	916	THR
5	B	918	ILE
5	B	941	LEU
5	B	943	SER
5	B	953	LEU
5	B	959	ASP
5	B	970	THR
5	B	973	ILE
5	B	975	GLN
5	B	976	ILE
5	B	1004	GLU
5	B	1012	ILE
5	B	1017	ILE
5	B	1021	MET
5	B	1051	THR
5	B	1065	GLN
5	B	1072	MET
5	B	1082	MET
5	B	1085	ILE
5	B	1096	ARG
5	B	1099	VAL
5	B	1103	ILE
5	B	1113	VAL
5	B	1115	THR
5	B	1116	ARG

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Mol	Chain	Res	Type
5	B	1122	ARG
5	B	1123	SER
5	B	1124	ARG
5	B	1133	MET
5	B	1137	CYS
5	B	1153	GLU
5	B	1156	ASP
5	B	1159	ARG
5	B	1160	VAL
5	B	1166	CYS
5	B	1183	LYS
5	B	1189	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1220	ARG
5	B	1222	ARG
6	C	10	ILE
6	C	27	LEU
6	C	41	ILE
6	C	55	THR
6	C	56	THR
6	C	57	VAL
6	C	72	LEU
6	C	77	ILE
6	C	81	GLU
6	C	106	GLU
6	C	116	LYS
6	C	119	VAL
6	C	120	ILE
6	C	123	ASN
6	C	125	MET
6	C	154	LYS
6	C	185	LYS
6	C	195	GLN
6	C	208	GLU
6	C	210	GLU
6	C	221	TYR
6	C	235	VAL
6	C	240	VAL
6	C	250	THR
6	C	258	ILE
6	C	259	LEU

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Mol	Chain	Res	Type
6	C	265	MET
6	C	266	ASP
6	C	268	ASP
7	E	3	GLN
7	E	18	THR
7	E	30	ILE
7	E	43	LYS
7	E	69	ILE
7	E	80	VAL
7	E	95	THR
7	E	98	ILE
7	E	103	LYS
7	E	107	THR
7	E	119	SER
7	E	123	LEU
7	E	127	ILE
7	E	132	ILE
7	E	134	THR
7	E	140	LEU
7	E	156	LEU
7	E	158	SER
7	E	165	LEU
7	E	175	LEU
8	F	77	ASP
8	F	92	ARG
8	F	97	ARG
8	F	104	ASN
8	F	110	ASP
8	F	111	LEU
8	F	119	ARG
8	F	140	ASP
8	F	145	ASP
9	H	2	SER
9	H	4	THR
9	H	24	CYS
9	H	32	THR
9	H	44	VAL
9	H	56	THR
9	H	83	GLN
9	H	89	LEU
9	H	102	TYR
9	H	111	LEU

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Mol	Chain	Res	Type
9	H	112	ILE
9	H	121	LEU
9	H	136	LYS
9	H	138	GLU
10	I	2	THR
10	I	4	PHE
10	I	13	MET
10	I	20	LYS
10	I	25	LEU
10	I	26	LEU
10	I	28	GLU
10	I	30	ARG
10	I	32	CYS
10	I	37	GLU
10	I	42	LEU
10	I	43	VAL
10	I	45	ARG
10	I	50	THR
10	I	52	ILE
10	I	59	VAL
10	I	79	HIS
10	I	84	VAL
10	I	94	ASP
10	I	108	HIS
10	I	109	ILE
10	I	111	THR
10	I	116	ASN
11	J	2	ILE
11	J	7	CYS
11	J	9	SER
11	J	34	THR
11	J	36	LEU
11	J	43	ARG
11	J	48	ARG
11	J	51	LEU
11	J	52	THR
11	J	55	ASP
12	K	8	GLU
12	K	11	LEU
12	K	12	LEU
12	K	22	ASP
12	K	40	HIS

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Mol	Chain	Res	Type
12	K	41	THR
12	K	42	LEU
12	K	46	ILE
12	K	47	ARG
12	K	52	ASN
12	K	53	ASP
12	K	63	VAL
12	K	85	ASP
12	K	89	ASN
12	K	91	CYS
12	K	94	ILE
12	K	101	LEU
13	L	31	CYS
13	L	33	GLU
13	L	46	VAL
13	L	48	CYS
13	L	53	HIS
13	L	55	ILE
13	L	61	THR
13	L	62	LYS
13	L	63	ARG
13	L	65	VAL
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	64	ASN
4	A	68	GLN
4	A	83	HIS
4	A	92	HIS
4	A	109	HIS
4	A	225	ASN
4	A	256	GLN
4	A	273	ASN
4	A	313	GLN
4	A	390	GLN
4	A	397	ASN
4	A	399	HIS
4	A	435	HIS
4	A	488	ASN
4	A	503	GLN

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Mol	Chain	Res	Type
4	A	510	GLN
4	A	517	ASN
4	A	576	GLN
4	A	660	ASN
4	A	700	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	802	ASN
4	A	838	GLN
4	A	858	ASN
4	A	926	GLN
4	A	965	GLN
4	A	968	GLN
4	A	996	ASN
4	A	1085	HIS
4	A	1110	ASN
4	A	1222	ASN
4	A	1312	ASN
4	A	1364	ASN
4	A	1390	ASN
4	A	1393	ASN
5	B	121	ASN
5	B	215	GLN
5	B	350	GLN
5	B	357	GLN
5	B	363	HIS
5	B	366	GLN
5	B	469	GLN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	531	GLN
5	B	686	ASN
5	B	744	HIS
5	B	776	GLN
5	B	822	ASN
5	B	835	GLN
5	B	975	GLN
5	B	984	HIS
5	B	986	GLN

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Mol	Chain	Res	Type
5	B	1013	ASN
5	B	1015	HIS
5	B	1084	GLN
5	B	1193	GLN
5	B	1205	GLN
6	C	112	ASN
6	C	135	GLN
6	C	224	GLN
6	C	231	ASN
6	C	242	GLN
7	E	8	ASN
7	E	101	GLN
7	E	147	HIS
9	H	33	GLN
10	I	90	GLN
10	I	116	ASN
11	J	53	HIS
12	K	29	ASN
12	K	44	ASN

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 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	UTP	B	3000	15	29,30,30	1.66	4 (13%)	43,47,47	1.57	6 (13%)

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	UTP	B	3000	15	-	6/22/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	3000	UTP	PA-O3A	3.65	1.63	1.59
16	B	3000	UTP	PG-O2G	3.46	1.61	1.50
16	B	3000	UTP	PB-O3A	3.21	1.63	1.59
16	B	3000	UTP	C2-N1	2.25	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	3000	UTP	C4-N3-C2	-4.87	120.57	126.61
16	B	3000	UTP	C5-C4-N3	3.94	120.32	114.80
16	B	3000	UTP	O4-C4-C5	-3.64	118.89	125.16
16	B	3000	UTP	N3-C2-N1	3.29	119.17	114.89
16	B	3000	UTP	O1G-PG-O3B	2.57	113.25	104.64
16	B	3000	UTP	C5'-C4'-C3'	-2.11	107.63	115.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

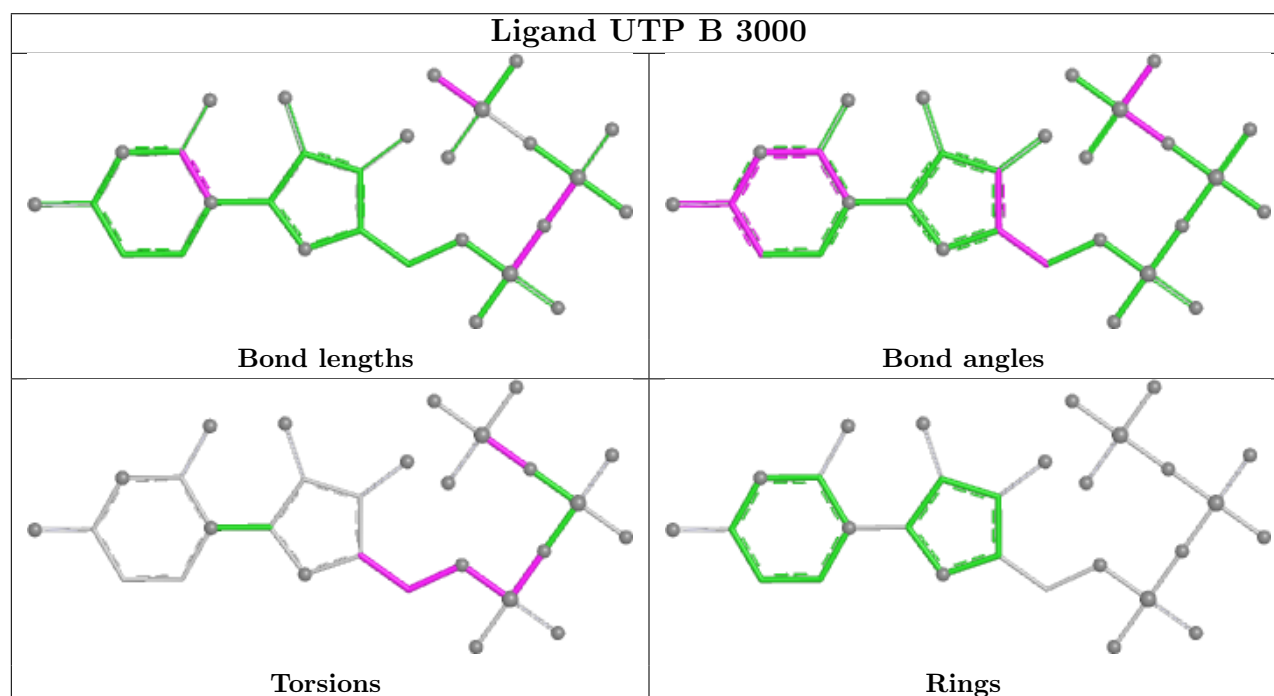
Mol	Chain	Res	Type	Atoms
16	B	3000	UTP	C5'-O5'-PA-O1A
16	B	3000	UTP	C4'-C5'-O5'-PA
16	B	3000	UTP	O4'-C4'-C5'-O5'
16	B	3000	UTP	C3'-C4'-C5'-O5'
16	B	3000	UTP	PB-O3A-PA-O5'
16	B	3000	UTP	PB-O3B-PG-O2G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	3000	UTP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	10/10 (100%)	-0.27	0 100 100	89, 111, 136, 141	0
2	T	28/28 (100%)	0.78	1 (3%) 46 37	81, 200, 281, 291	0
3	N	14/14 (100%)	0.90	0 100 100	265, 273, 290, 292	0
4	A	1398/1733 (80%)	0.36	23 (1%) 70 55	84, 118, 171, 184	0
5	B	1096/1224 (89%)	0.38	21 (1%) 66 51	86, 114, 151, 165	0
6	C	266/318 (83%)	0.19	0 100 100	99, 118, 146, 150	0
7	E	193/215 (89%)	0.37	7 (3%) 46 37	98, 130, 163, 167	0
8	F	83/155 (53%)	0.24	0 100 100	111, 127, 138, 144	0
9	H	133/146 (91%)	0.60	4 (3%) 52 40	120, 141, 176, 181	0
10	I	119/122 (97%)	0.69	9 (7%) 20 22	118, 149, 168, 173	0
11	J	65/70 (92%)	0.10	1 (1%) 72 56	103, 119, 134, 136	0
12	K	114/120 (95%)	0.13	1 (0%) 81 66	99, 118, 134, 136	0
13	L	46/70 (65%)	0.93	4 (8%) 16 19	137, 178, 191, 193	0
All	All	3565/4225 (84%)	0.37	71 (1%) 65 50	81, 120, 168, 292	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1088	GLY	3.7
4	A	785	PRO	3.6
4	A	1090	ALA	3.5
4	A	168	GLY	3.4
5	B	1221	SER	3.1
5	B	709	ASP	3.1
13	L	28	LYS	3.1
13	L	25	ALA	3.0
7	E	95	THR	3.0

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Mol	Chain	Res	Type	RSRZ
5	B	244	LEU	3.0
10	I	6	PHE	3.0
4	A	1176	LEU	2.9
9	H	135	LEU	2.9
5	B	735	ALA	2.9
5	B	532	ALA	2.8
5	B	732	SER	2.8
5	B	711	GLU	2.8
4	A	264	PHE	2.8
5	B	823	ALA	2.7
10	I	91	ARG	2.7
10	I	4	PHE	2.7
5	B	328	GLU	2.6
5	B	819	ALA	2.6
5	B	407	ASP	2.6
5	B	308	TRP	2.5
7	E	20	LYS	2.5
4	A	97	ALA	2.5
9	H	119	GLY	2.5
5	B	326	ASP	2.5
7	E	16	PHE	2.5
4	A	784	LEU	2.5
4	A	2	VAL	2.5
4	A	130	ASP	2.5
7	E	117	THR	2.5
4	A	701	LEU	2.4
4	A	147	VAL	2.4
9	H	63	LEU	2.4
10	I	13	MET	2.4
4	A	1087	ALA	2.4
5	B	883	LEU	2.4
4	A	322	VAL	2.4
5	B	535	LEU	2.3
5	B	388	CYS	2.3
4	A	171	GLN	2.3
7	E	6	GLU	2.3
10	I	52	ILE	2.3
5	B	531	GLN	2.2
9	H	30	SER	2.2
7	E	110	PHE	2.2
4	A	98	LYS	2.2
4	A	752	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
10	I	44	TYR	2.2
10	I	38	ALA	2.2
5	B	245	GLU	2.1
4	A	1071	SER	2.1
5	B	620	ARG	2.1
4	A	595	THR	2.1
10	I	3	THR	2.1
13	L	43	THR	2.1
7	E	53	PRO	2.1
4	A	703	THR	2.0
5	B	1216	LEU	2.0
10	I	57	GLY	2.0
2	T	1	DC	2.0
4	A	708	MET	2.0
4	A	1175	SER	2.0
11	J	44	TYR	2.0
12	K	63	VAL	2.0
4	A	173	THR	2.0
5	B	468	GLU	2.0
13	L	35	SER	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.

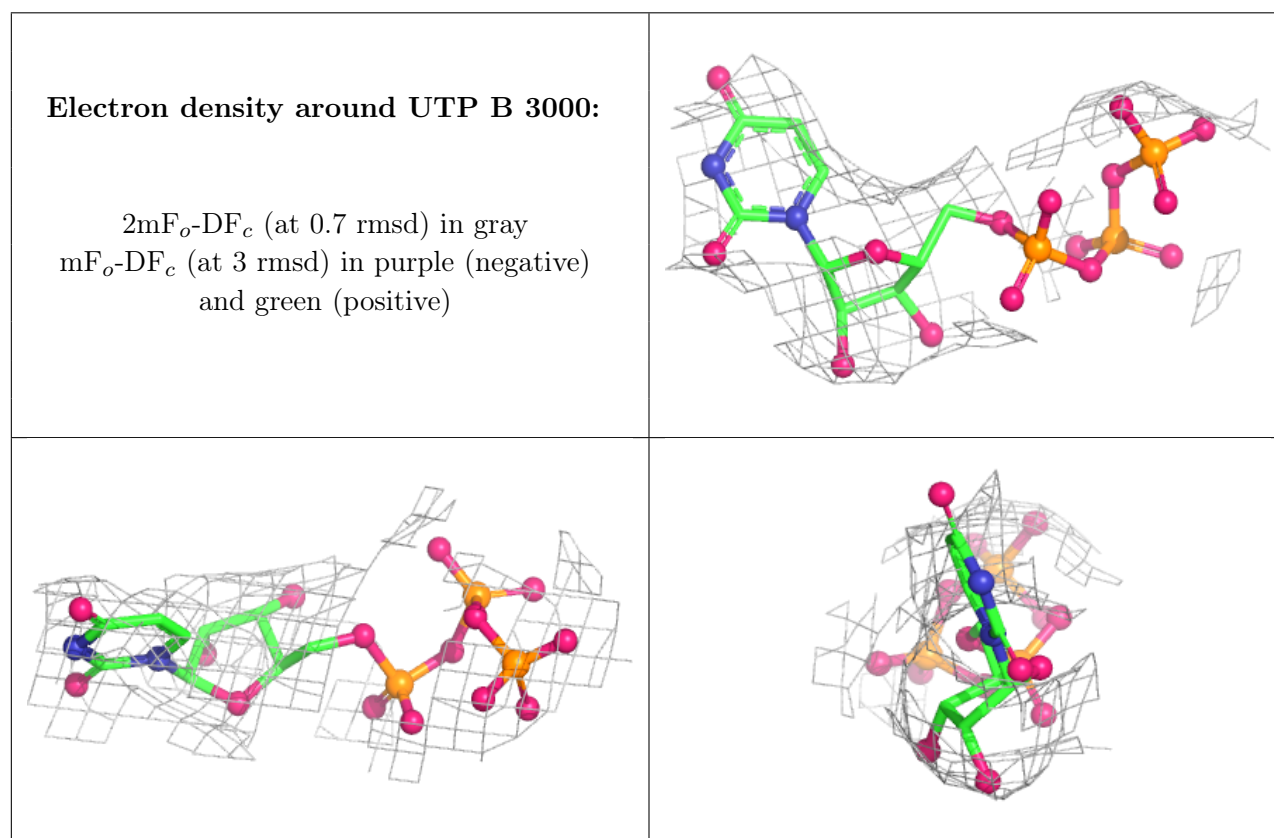
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	A	2002	1/1	0.80	0.16	102,102,102,102	0
14	ZN	A	1734	1/1	0.93	0.06	177,177,177,177	0
15	MG	A	2001	1/1	0.94	0.10	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	UTP	B	3000	29/29	0.96	0.09	110,112,113,113	0
14	ZN	L	105	1/1	0.97	0.08	181,181,181,181	0
14	ZN	A	1735	1/1	0.98	0.03	165,165,165,165	0
14	ZN	B	1307	1/1	0.98	0.04	147,147,147,147	0
14	ZN	I	203	1/1	0.98	0.09	121,121,121,121	0
14	ZN	I	204	1/1	0.98	0.03	157,157,157,157	0
14	ZN	C	319	1/1	0.99	0.03	117,117,117,117	0
14	ZN	J	101	1/1	0.99	0.02	112,112,112,112	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.