



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:28 AM UTC

PDB ID : 2NVT / pdb_00002nvt
Title : RNA Polymerase II Elongation Complex in 150 mM Mg+2 with GMPCPP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-13
Resolution : 3.36 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

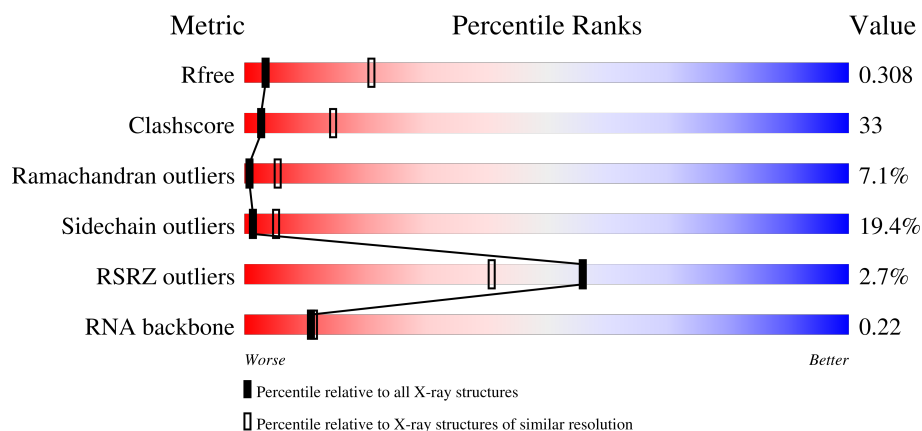
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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

Mol	Chain	Length	Quality of chain
1	R	10	
2	T	21	
3	N	7	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	3%33%41%15%•9%
6	C	318	36%38%9%•16%
7	E	215	%55%35%8%•
8	F	155	%34%18%•45%
9	H	146	3%40%36%11%•9%
10	I	122	4%51%34%11%••
11	J	70	37%37%16%•7%
12	K	120	2%51%37%8%5%
13	L	70	6%21%30%13%•34%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- Molecule 2 is a DNA chain called 5'-D(P*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	21	Total	C	N	O	P	0	0	0
			426	204	72	129	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	7	Total	C	N	O	P	0	0	0
			141	69	24	42	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1411	Total	C	N	O	S	0	0	0
			11090	6993	1942	2094	61			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

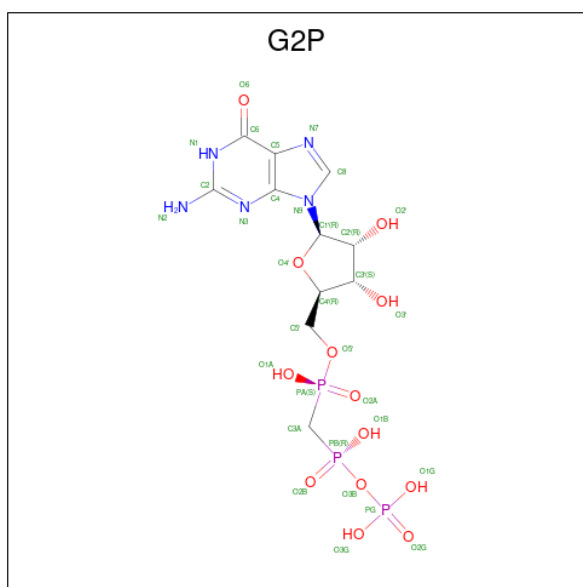
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

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

tide.

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

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

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

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

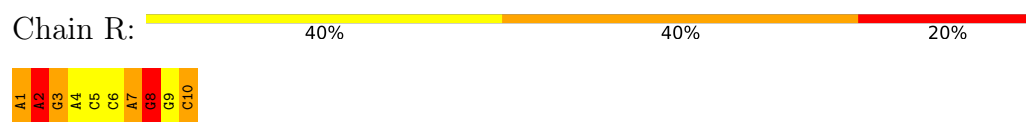
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

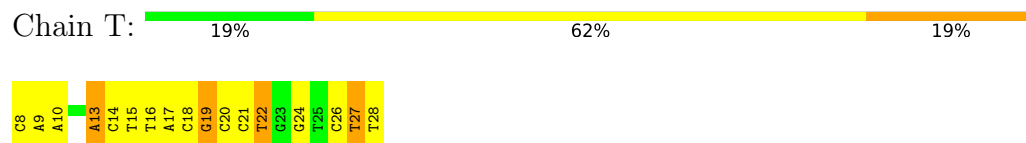
3 Residue-property plots [i](#)

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.

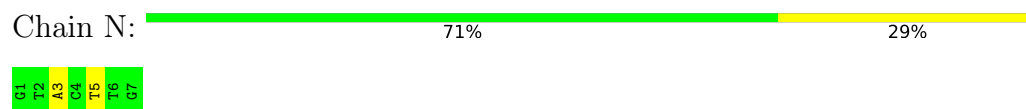
- Molecule 1: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'



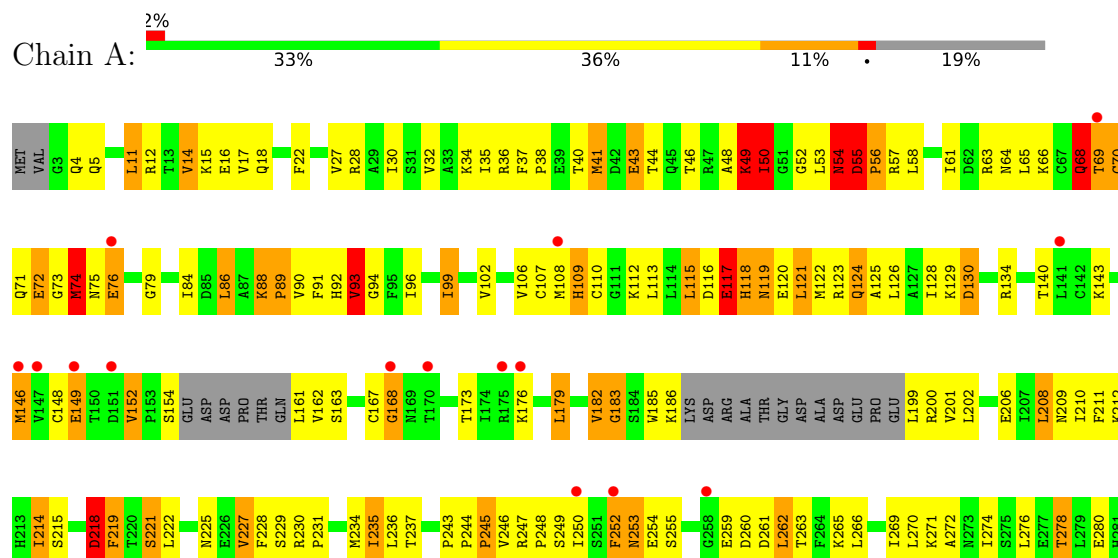
- Molecule 2: 5'-D(P*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*CP*GP*CP*CP*TP*GP*GP*TP*CP*TP*T)-3'

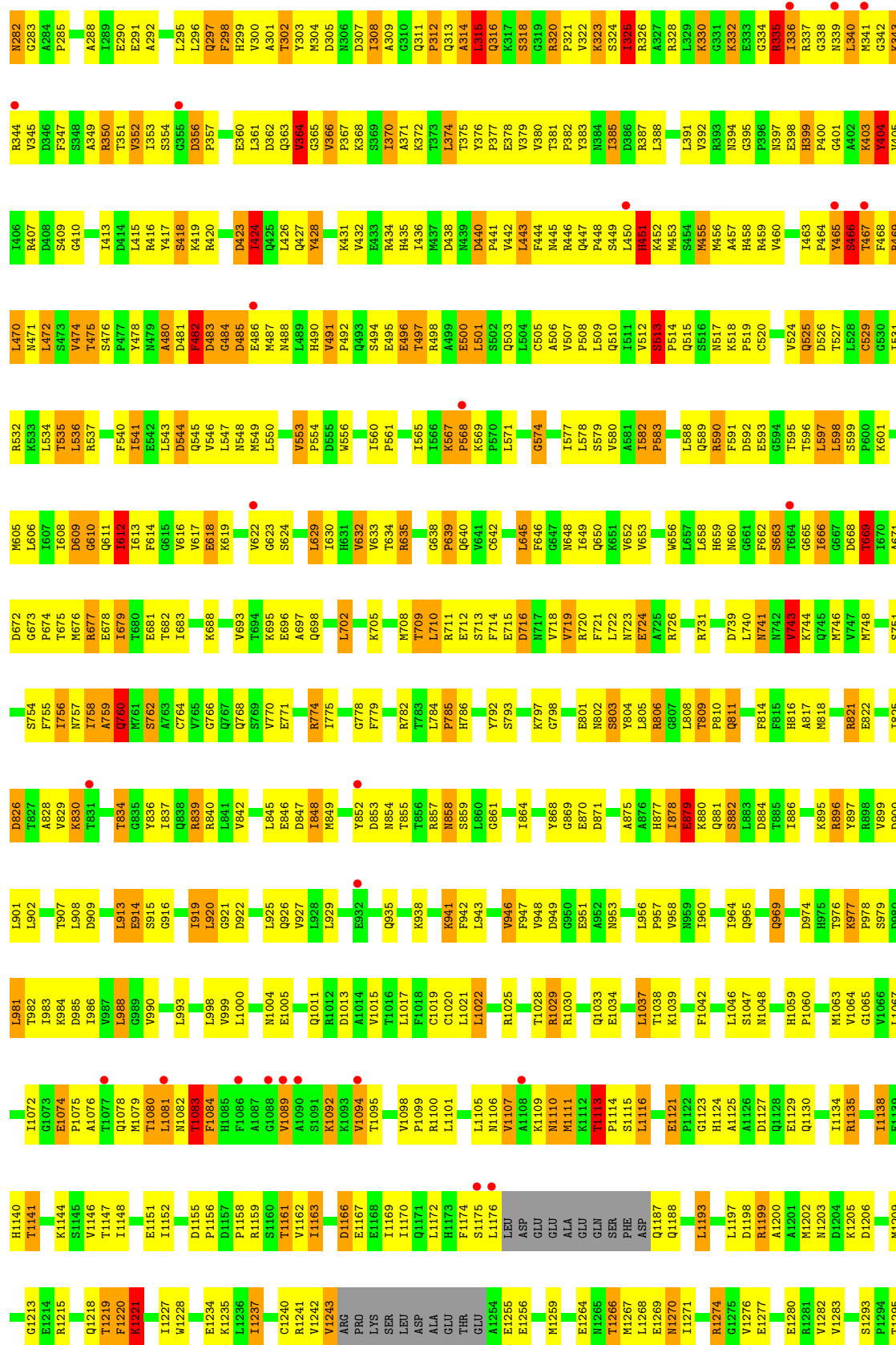


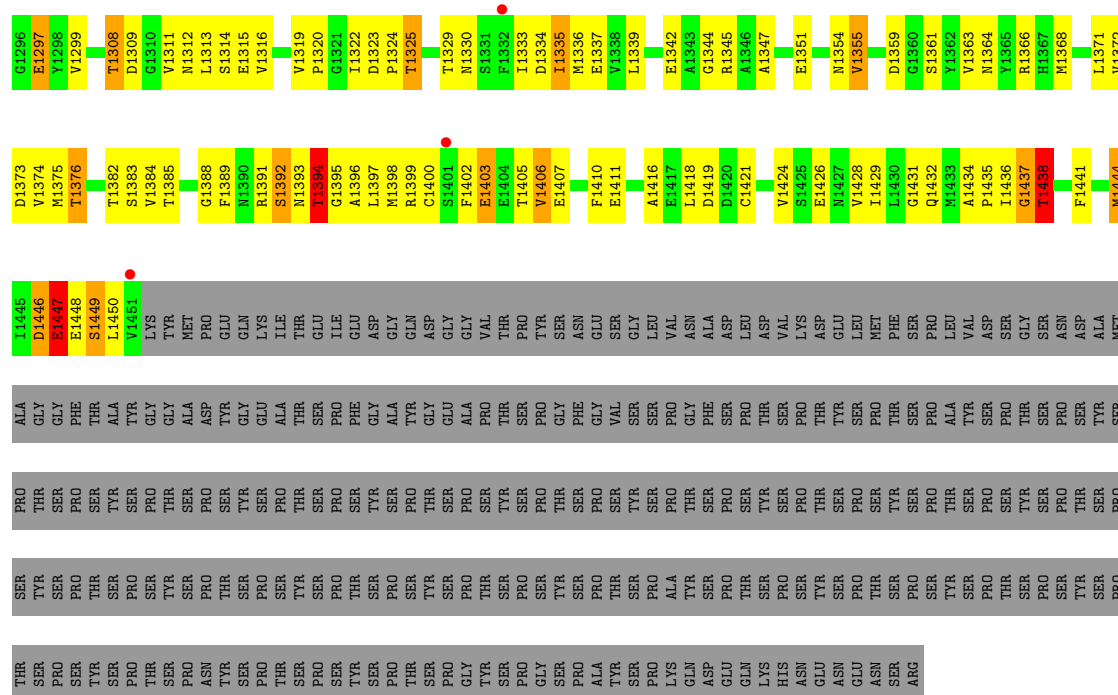
- Molecule 3: 5'-D(*GP*TP*AP*CP*TP*TP*G)-3'



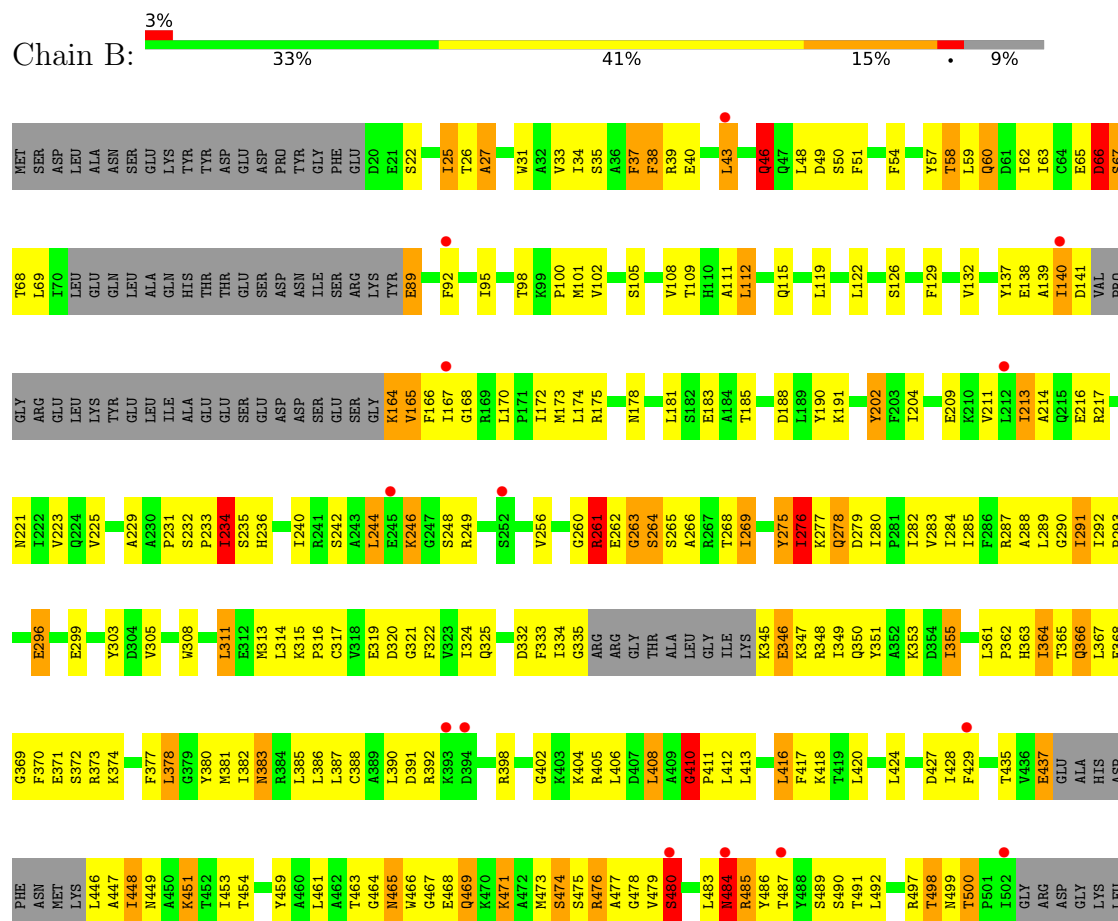
- Molecule 4: DNA-directed RNA polymerase II largest subunit

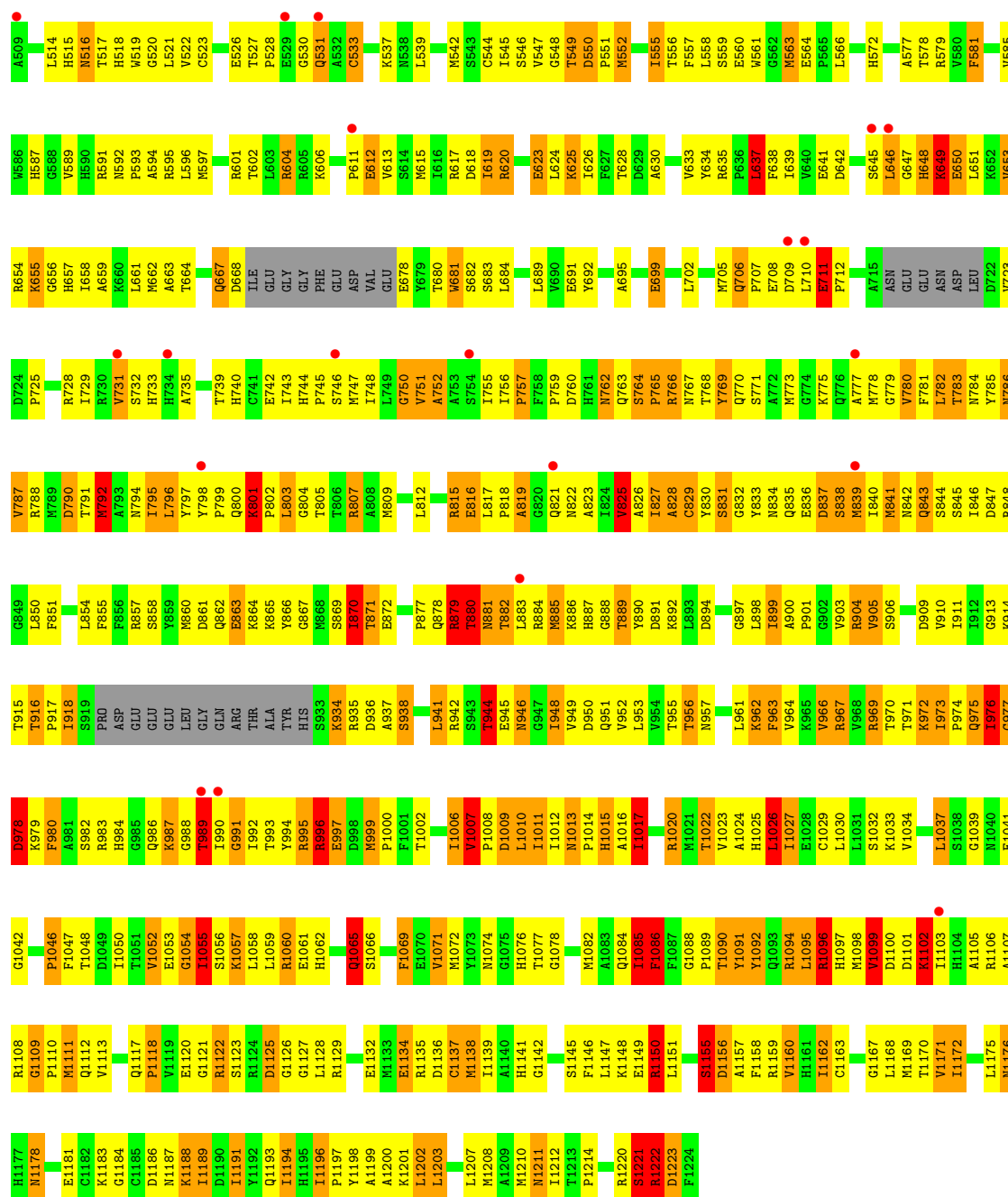






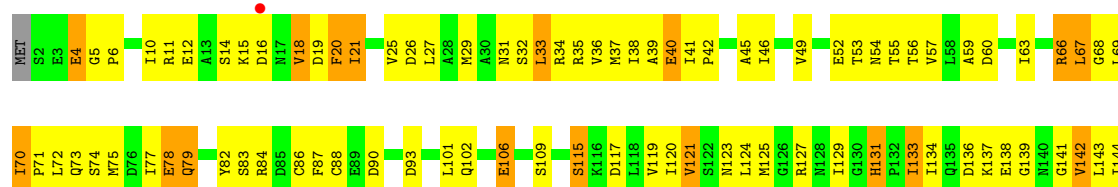
● Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

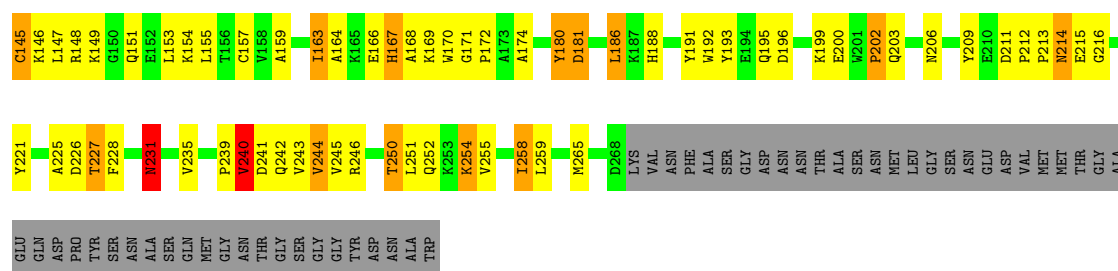




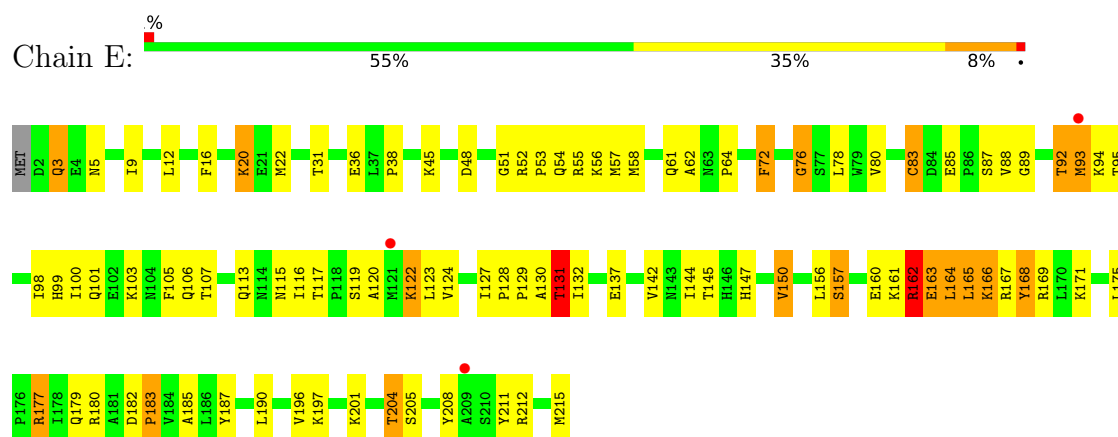
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 36% 38% 9% 16%

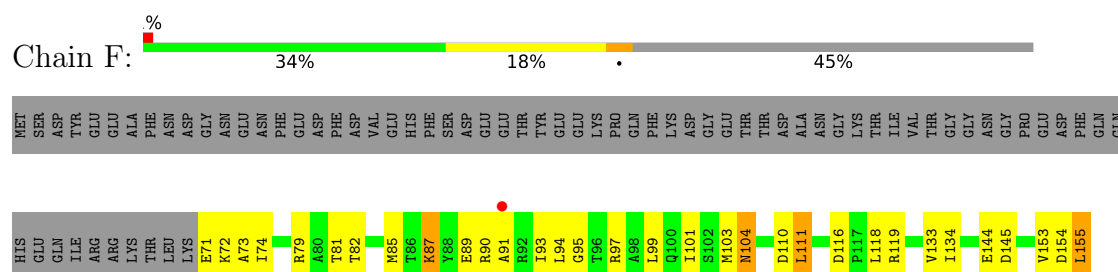




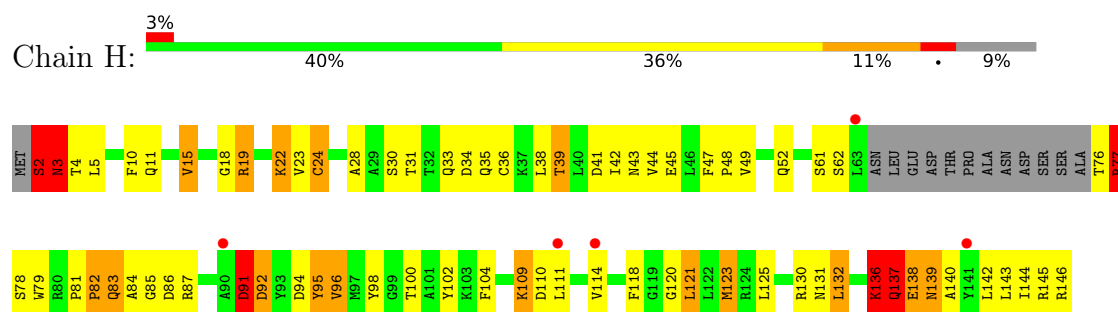
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



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

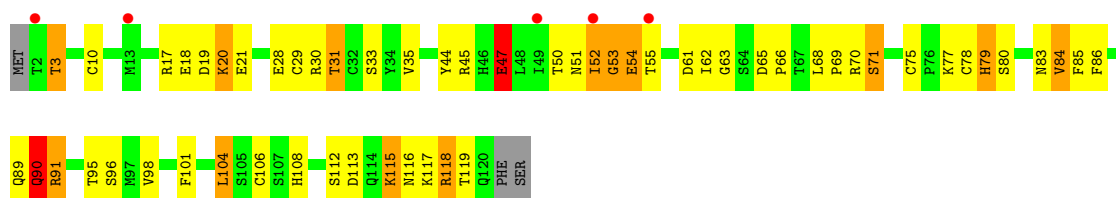


- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



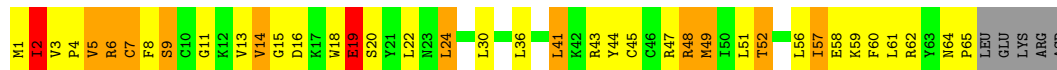
- Molecule 10: DNA-directed RNA polymerase II subunit 9





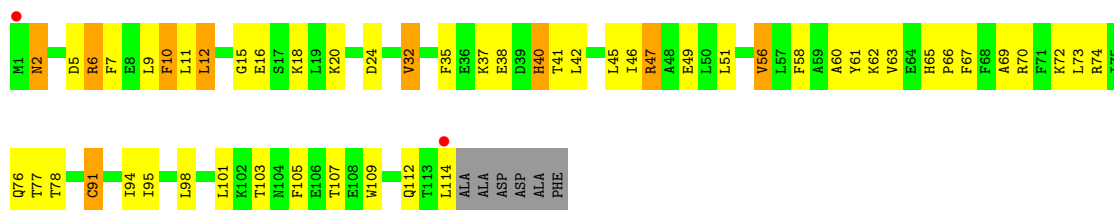
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 37% 37% 16% 7%



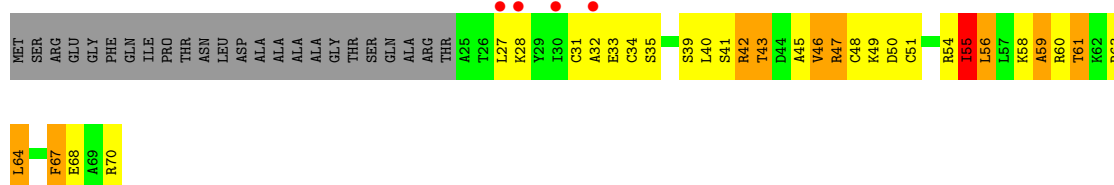
- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 2% 51% 37% 8% 5%



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

Chain L: 6% 21% 30% 13% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.87Å 222.82Å 195.80Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	40.00 – 3.36 40.00 – 3.36	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.36) 97.0 (40.00-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.230 , 0.283 0.258 , 0.308	Depositor DCC
R_{free} test set	4911 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29168	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, G2P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.91	1/240 (0.4%)	1.88	11/373 (2.9%)
2	T	0.55	0/475	1.53	7/730 (1.0%)
3	N	0.40	0/157	1.04	0/241
4	A	0.88	9/11288 (0.1%)	1.17	63/15263 (0.4%)
5	B	1.03	25/9033 (0.3%)	1.26	68/12181 (0.6%)
6	C	0.90	0/2139	1.27	20/2899 (0.7%)
7	E	0.65	0/1788	1.00	1/2406 (0.0%)
8	F	0.68	0/700	0.98	0/945
9	H	0.75	0/1086	1.09	8/1470 (0.5%)
10	I	0.72	1/989 (0.1%)	1.00	2/1331 (0.2%)
11	J	1.05	0/541	1.22	4/727 (0.6%)
12	K	0.81	0/937	1.06	1/1265 (0.1%)
13	L	0.95	0/365	1.24	2/485 (0.4%)
All	All	0.90	36/29738 (0.1%)	1.20	187/40316 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	5
5	B	0	6
9	H	0	1
All	All	0	12

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1086	PHE	C-O	9.00	1.35	1.24
5	B	1055	ILE	CA-CB	8.37	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1222	ARG	CZ-NH1	7.39	1.43	1.32
4	A	343	LYS	C-N	6.67	1.42	1.33
4	A	364	VAL	CA-CB	6.53	1.63	1.54
5	B	752	ALA	CA-CB	6.51	1.64	1.53
5	B	982	SER	C-O	6.37	1.30	1.23
5	B	1011	ILE	C-O	6.28	1.30	1.24
5	B	1091	TYR	CA-C	-6.27	1.44	1.52
5	B	978	ASP	CA-C	6.19	1.61	1.52
5	B	903	VAL	CA-CB	-6.18	1.48	1.54
4	A	352	VAL	CA-C	6.11	1.59	1.52
5	B	978	ASP	C-O	6.04	1.31	1.24
5	B	944	THR	CA-CB	6.00	1.62	1.53
5	B	823	ALA	CA-C	5.92	1.59	1.52
4	A	525	GLN	CA-C	5.91	1.60	1.52
5	B	777	ALA	CA-CB	5.76	1.62	1.53
5	B	972	LYS	CA-C	5.72	1.59	1.52
5	B	1085	ILE	CA-CB	5.71	1.61	1.54
4	A	669	THR	CA-CB	5.57	1.61	1.53
5	B	1099	VAL	CA-CB	5.40	1.62	1.54
5	B	1098	MET	C-O	5.33	1.30	1.23
5	B	818	PRO	CA-C	5.32	1.58	1.52
5	B	996	ARG	CA-C	5.30	1.60	1.52
4	A	349	ALA	CA-C	-5.28	1.46	1.52
5	B	1026	LEU	CA-C	5.20	1.59	1.52
10	I	52	ILE	CA-CB	5.18	1.60	1.54
5	B	1092	TYR	CA-C	-5.17	1.46	1.52
5	B	757	PRO	CB-CG	5.17	1.75	1.49
4	A	362	ASP	N-CA	-5.15	1.40	1.46
4	A	1089	VAL	CA-CB	5.13	1.61	1.54
5	B	1086	PHE	CA-C	5.12	1.59	1.52
5	B	1071	VAL	CA-CB	-5.10	1.47	1.54
4	A	743	VAL	CA-CB	5.10	1.60	1.54
5	B	870	ILE	CA-CB	5.05	1.61	1.54
1	R	10	C	C2'-C1'	5.01	1.60	1.53

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	474	VAL	N-CA-C	-10.05	102.62	112.17
1	R	10	C	P-O5'-C5'	-9.78	106.23	120.90
5	B	751	VAL	N-CA-C	-9.71	103.46	111.81
4	A	88	LYS	CA-C-N	9.27	131.43	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	88	LYS	C-N-CA	9.27	131.43	119.84
5	B	1013	ASN	CA-C-N	9.19	131.33	119.84
5	B	1013	ASN	C-N-CA	9.19	131.33	119.84
1	R	10	C	C5'-C4'-C3'	-8.98	102.53	116.00
2	T	22	DT	C4-C5-C7	-8.92	109.02	122.40
5	B	1009	ASP	N-CA-C	-8.76	101.85	112.54
4	A	491	VAL	N-CA-C	8.68	116.14	107.55
1	R	10	C	C1'-C2'-O2'	8.61	121.31	108.40
5	B	1125	ASP	N-CA-C	-8.54	100.91	110.91
2	T	22	DT	C5'-C4'-O4'	-8.47	96.69	109.40
5	B	966	VAL	CB-CA-C	-8.36	99.61	111.31
12	K	2	ASN	N-CA-C	-8.28	102.49	112.59
4	A	999	VAL	N-CA-C	-8.08	105.36	111.90
5	B	825	VAL	N-CA-C	7.89	119.45	107.77
4	A	356	ASP	CA-C-N	7.82	129.61	119.84
4	A	356	ASP	C-N-CA	7.82	129.61	119.84
1	R	10	C	C4'-C3'-O3'	-7.78	101.33	113.00
10	I	79	HIS	N-CA-C	7.74	120.61	111.71
5	B	1010	LEU	N-CA-C	7.71	121.39	108.13
4	A	314	ALA	N-CA-C	7.68	120.08	109.18
4	A	977	LYS	CA-C-N	7.63	127.62	119.76
4	A	977	LYS	C-N-CA	7.63	127.62	119.76
5	B	1007	VAL	CA-C-N	-7.63	109.95	120.25
5	B	1007	VAL	C-N-CA	-7.63	109.95	120.25
5	B	1017	ILE	CA-C-N	-7.57	110.38	119.84
5	B	1017	ILE	C-N-CA	-7.57	110.38	119.84
5	B	410	GLY	CA-C-N	7.53	129.26	119.84
5	B	410	GLY	C-N-CA	7.53	129.26	119.84
6	C	21	ILE	N-CA-C	-7.48	101.89	110.05
9	H	92	ASP	N-CA-C	-7.30	105.23	112.97
5	B	37	PHE	N-CA-C	-7.20	100.56	110.35
6	C	68	GLY	N-CA-C	-7.19	104.10	112.73
5	B	711	GLU	N-CA-C	7.18	125.69	109.81
5	B	946	ASN	N-CA-C	7.08	119.32	108.42
13	L	60	ARG	N-CA-C	-7.04	98.95	108.24
5	B	1186	ASP	N-CA-C	6.90	121.07	112.24
5	B	839	MET	N-CA-C	6.89	119.91	109.23
1	R	8	G	C1'-O4'-C4'	-6.88	103.02	109.90
4	A	55	ASP	CA-C-N	6.87	128.43	119.84
4	A	55	ASP	C-N-CA	6.87	128.43	119.84
5	B	1065	GLN	N-CA-C	-6.76	98.20	108.96
4	A	497	THR	N-CA-C	-6.75	104.86	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1027	ILE	CA-C-N	6.72	129.58	120.38
5	B	1027	ILE	C-N-CA	6.72	129.58	120.38
9	H	91	ASP	N-CA-C	6.72	119.30	107.61
5	B	168	GLY	N-CA-C	6.69	120.43	112.33
6	C	49	VAL	N-CA-C	6.68	117.92	108.36
5	B	764	SER	CA-C-N	-6.68	111.49	119.84
5	B	764	SER	C-N-CA	-6.68	111.49	119.84
4	A	1113	THR	CA-C-N	-6.66	113.12	119.85
4	A	1113	THR	C-N-CA	-6.66	113.12	119.85
6	C	4	GLU	N-CA-C	6.66	119.15	111.02
5	B	1052	VAL	CA-C-N	6.65	129.43	120.65
5	B	1052	VAL	C-N-CA	6.65	129.43	120.65
1	R	2	A	C4'-C3'-C2'	-6.61	95.99	102.60
6	C	193	TYR	N-CA-C	6.55	117.11	107.88
4	A	879	GLU	N-CA-C	6.54	119.09	108.76
5	B	841	MET	N-CA-C	6.50	119.76	109.81
5	B	819	ALA	N-CA-C	-6.48	97.22	108.69
5	B	1015	HIS	N-CA-C	6.46	120.02	111.75
6	C	131	HIS	CA-C-N	-6.45	112.29	120.23
6	C	131	HIS	C-N-CA	-6.45	112.29	120.23
4	A	218	ASP	N-CA-C	6.31	124.24	110.80
5	B	1156	ASP	N-CA-C	6.31	117.95	111.14
4	A	638	GLY	CA-C-N	-6.29	111.97	119.84
4	A	638	GLY	C-N-CA	-6.29	111.97	119.84
4	A	236	LEU	N-CA-C	6.29	118.99	108.73
4	A	259	GLU	N-CA-C	6.24	118.09	110.41
5	B	170	LEU	CA-C-N	6.24	126.27	119.90
5	B	170	LEU	C-N-CA	6.24	126.27	119.90
6	C	21	ILE	CB-CA-C	-6.23	104.73	111.59
2	T	19	DG	O3'-P-O5'	-6.22	94.67	104.00
5	B	1020	ARG	CA-C-N	6.20	131.62	122.82
5	B	1020	ARG	C-N-CA	6.20	131.62	122.82
4	A	1311	VAL	N-CA-C	6.19	116.93	107.77
4	A	1092	LYS	N-CA-C	-6.17	105.40	113.17
5	B	975	GLN	CB-CA-C	6.07	119.81	109.80
1	R	7	A	C4'-C3'-C2'	-6.06	96.54	102.60
6	C	40	GLU	CA-C-N	-6.06	118.23	122.59
6	C	40	GLU	C-N-CA	-6.06	118.23	122.59
4	A	998	LEU	N-CA-C	6.04	119.12	110.24
4	A	1221	LYS	N-CA-C	6.02	123.63	110.80
5	B	1052	VAL	N-CA-C	-6.01	104.44	111.00
5	B	993	THR	N-CA-C	5.99	118.17	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	8	G	C4'-C3'-C2'	-5.98	96.62	102.60
5	B	234	ILE	N-CA-C	5.96	116.88	108.36
5	B	46	GLN	N-CA-C	5.91	118.48	111.33
4	A	553	VAL	CA-C-N	5.89	126.40	120.04
4	A	553	VAL	C-N-CA	5.89	126.40	120.04
5	B	1048	THR	CB-CA-C	-5.89	99.38	110.51
4	A	802	ASN	N-CA-C	5.83	119.46	110.42
4	A	1013	ASP	N-CA-C	5.81	118.84	111.69
5	B	1142	GLY	N-CA-C	-5.81	107.24	115.43
4	A	288	ALA	N-CA-C	-5.79	106.22	113.28
4	A	229	SER	N-CA-C	5.78	116.85	107.32
4	A	762	SER	N-CA-C	5.78	120.48	112.45
5	B	739	THR	N-CA-C	-5.77	105.51	113.18
5	B	269	ILE	CB-CA-C	-5.75	104.71	111.09
4	A	371	ALA	N-CA-C	-5.74	106.13	113.01
2	T	27	DT	C6-C5-C7	-5.64	115.53	124.00
4	A	1074	GLU	CA-C-N	-5.59	112.84	119.05
4	A	1074	GLU	C-N-CA	-5.59	112.84	119.05
6	C	106	GLU	N-CA-C	-5.59	106.59	113.41
2	T	22	DT	C5'-C4'-C3'	5.59	123.28	114.90
5	B	1091	TYR	CB-CA-C	-5.57	102.95	109.80
2	T	19	DG	N9-C1'-C2'	-5.56	105.16	113.50
6	C	20	PHE	N-CA-C	5.56	117.72	108.99
4	A	524	VAL	N-CA-C	5.55	118.12	108.90
4	A	480	ALA	N-CA-C	5.55	117.69	110.53
4	A	1446	ASP	CA-C-N	5.55	131.68	121.70
4	A	1446	ASP	C-N-CA	5.55	131.68	121.70
9	H	138	GLU	N-CA-C	-5.54	106.40	112.72
5	B	1069	PHE	N-CA-C	5.51	118.01	110.24
4	A	858	ASN	N-CA-C	5.51	115.39	108.45
4	A	340	LEU	CA-C-N	-5.49	115.67	123.03
4	A	340	LEU	C-N-CA	-5.49	115.67	123.03
5	B	816	GLU	N-CA-C	-5.49	106.49	114.12
4	A	218	ASP	CA-C-N	5.48	131.56	121.70
4	A	218	ASP	C-N-CA	5.48	131.56	121.70
1	R	8	G	O4'-C4'-C3'	-5.48	98.52	104.00
5	B	801	LYS	N-CA-C	-5.47	101.61	109.48
9	H	33	GLN	N-CA-C	5.46	117.64	108.96
5	B	479	VAL	N-CA-C	-5.46	102.54	109.58
6	C	174	ALA	N-CA-C	5.42	116.01	108.00
6	C	180	TYR	N-CA-C	5.40	117.20	108.34
10	I	53	GLY	N-CA-C	5.39	128.92	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	980	PHE	N-CA-C	-5.37	100.90	109.07
9	H	2	SER	CA-C-N	5.37	131.36	121.70
9	H	2	SER	C-N-CA	5.37	131.36	121.70
4	A	500	GLU	N-CA-C	-5.37	106.73	113.28
4	A	582	ILE	CA-C-N	5.33	126.51	119.84
4	A	582	ILE	C-N-CA	5.33	126.51	119.84
4	A	451	HIS	CB-CA-C	-5.33	101.41	109.99
4	A	356	ASP	N-CA-C	5.33	120.25	108.27
5	B	550	ASP	CA-C-N	5.32	125.13	119.28
5	B	550	ASP	C-N-CA	5.32	125.13	119.28
5	B	552	MET	N-CA-C	5.32	120.85	113.45
4	A	152	VAL	CA-C-N	5.32	125.25	119.78
4	A	152	VAL	C-N-CA	5.32	125.25	119.78
5	B	1011	ILE	CB-CA-C	-5.31	104.54	110.96
5	B	1127	GLY	CA-C-N	-5.30	113.92	121.50
5	B	1127	GLY	C-N-CA	-5.30	113.92	121.50
2	T	13	DA	O4'-C1'-N9	5.29	116.34	108.40
5	B	787	VAL	CB-CA-C	-5.29	105.47	110.65
5	B	699	GLU	N-CA-C	5.28	117.72	111.33
7	E	157	SER	N-CA-C	5.27	118.32	110.52
9	H	96	VAL	N-CA-C	5.27	115.63	107.78
4	A	366	VAL	N-CA-C	5.26	113.62	107.89
6	C	70	ILE	N-CA-CB	5.26	116.01	110.17
4	A	590	ARG	N-CA-C	5.26	122.00	110.80
5	B	729	ILE	N-CA-C	5.26	115.16	108.12
13	L	67	PHE	N-CA-C	5.25	117.20	107.60
6	C	240	VAL	CB-CA-C	-5.24	102.70	111.29
5	B	637	LEU	N-CA-C	5.21	116.73	108.96
1	R	2	A	C1'-O4'-C4'	-5.21	104.69	109.90
4	A	298	PHE	N-CA-C	-5.21	101.28	109.25
4	A	513	SER	N-CA-C	5.20	118.48	108.45
11	J	57	ILE	N-CA-CB	5.20	116.28	110.51
4	A	884	ASP	N-CA-C	5.19	119.10	112.87
5	B	803	LEU	N-CA-C	-5.18	106.91	113.18
11	J	61	LEU	N-CA-C	-5.18	105.81	111.82
5	B	606	LYS	N-CA-C	-5.16	106.95	114.12
4	A	574	GLY	N-CA-C	-5.15	106.41	112.64
6	C	255	VAL	N-CA-C	-5.15	105.09	112.35
5	B	645	SER	N-CA-C	5.14	116.10	108.60
11	J	15	GLY	N-CA-C	5.11	120.07	113.27
5	B	566	LEU	N-CA-C	5.11	117.24	111.11
9	H	137	GLN	N-CA-C	5.11	118.05	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	345	VAL	N-CA-C	5.09	117.35	108.90
4	A	1324	PRO	N-CA-C	-5.09	108.87	114.92
6	C	67	LEU	N-CA-C	-5.08	107.03	113.18
6	C	115	SER	N-CA-C	-5.07	106.26	112.90
5	B	1006	ILE	N-CA-C	5.06	116.45	109.46
1	R	10	C	C3'-C2'-C1'	5.05	106.35	101.30
4	A	330	LYS	CA-C-N	5.04	124.89	120.10
4	A	330	LYS	C-N-CA	5.04	124.89	120.10
4	A	612	ILE	N-CA-C	5.04	115.56	108.36
5	B	1109	GLY	CA-C-N	5.03	125.31	119.92
5	B	1109	GLY	C-N-CA	5.03	125.31	119.92
6	C	167	HIS	N-CA-C	-5.03	100.87	108.52
5	B	1196	ILE	N-CA-C	5.03	113.42	107.84
4	A	481	ASP	N-CA-C	-5.02	102.12	108.45
11	J	5	VAL	N-CA-C	-5.00	103.04	109.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	115	LEU	Peptide
4	A	117	GLU	Peptide
4	A	342	GLY	Peptide
4	A	482	PHE	Peptide
4	A	484	GLY	Peptide
5	B	1053	GLU	Peptide
5	B	1085	ILE	Peptide
5	B	140	ILE	Peptide
5	B	828	ALA	Peptide
5	B	976	ILE	Peptide
5	B	989	THR	Peptide
9	H	91	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	214	0	111	18	0
2	T	426	0	239	23	0
3	N	141	0	82	2	0
4	A	11090	0	11173	808	1
5	B	8861	0	8884	765	0
6	C	2101	0	2056	157	1
7	E	1752	0	1776	79	0
8	F	688	0	707	27	0
9	H	1068	0	1040	54	0
10	I	971	0	927	39	0
11	J	532	0	542	74	0
12	K	919	0	929	69	0
13	L	363	0	386	28	0
14	T	32	0	14	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29168	0	28866	1922	1

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 33.

All (1922) 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:336:ILE:CD1	4:A:1405:THR:CG2	1.78	1.57
5:B:976:ILE:HD11	5:B:991:GLY:C	1.14	1.53
4:A:341:MET:SD	4:A:1428:VAL:HG12	1.62	1.39
4:A:336:ILE:CD1	4:A:1405:THR:HG21	0.93	1.39
5:B:757:PRO:CB	5:B:757:PRO:CG	1.75	1.38
4:A:336:ILE:HD13	4:A:1405:THR:CG2	1.47	1.34
5:B:839:MET:CE	5:B:990:ILE:HG12	1.55	1.34
4:A:341:MET:HE1	4:A:1428:VAL:CB	1.57	1.33
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.41	1.33
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	1.58	1.32
4:A:117:GLU:N	4:A:118:HIS:HB2	1.41	1.31
5:B:976:ILE:HD11	5:B:991:GLY:O	1.28	1.28
4:A:341:MET:SD	4:A:1428:VAL:CG1	2.20	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:117:GLU:H	4:A:118:HIS:CB	1.46	1.26
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	1.49	1.26
5:B:976:ILE:CD1	5:B:991:GLY:C	2.09	1.24
4:A:341:MET:CE	4:A:1428:VAL:HB	1.69	1.22
5:B:839:MET:HE2	5:B:990:ILE:CG1	1.69	1.21
5:B:647:GLY:HA3	5:B:648:HIS:CB	1.70	1.21
5:B:1122:ARG:HG2	5:B:1122:ARG:HH11	1.05	1.20
5:B:1122:ARG:HH11	5:B:1122:ARG:CG	1.54	1.18
4:A:336:ILE:HD12	4:A:1405:THR:CG2	1.71	1.17
5:B:976:ILE:HD12	5:B:992:ILE:HA	1.20	1.16
10:I:117:LYS:HB3	10:I:118:ARG:HA	1.17	1.16
4:A:343:LYS:CE	5:B:1156:ASP:OD2	1.94	1.15
5:B:839:MET:CG	5:B:989:THR:O	1.95	1.14
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	1.83	1.13
5:B:994:TYR:HB2	5:B:999:MET:HE3	1.24	1.12
4:A:443:LEU:HD21	4:A:455:MET:HG3	1.17	1.11
5:B:976:ILE:HD11	5:B:992:ILE:N	1.63	1.11
5:B:1094:ARG:HG2	5:B:1094:ARG:HH11	1.16	1.11
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	0.94	1.09
9:H:82:PRO:HB2	9:H:83:GLN:HA	1.23	1.09
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.24	1.09
4:A:567:LYS:HB3	9:H:96:VAL:H	1.13	1.09
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.15	1.09
5:B:345:LYS:N	5:B:346:GLU:HA	1.67	1.08
5:B:976:ILE:CD1	5:B:991:GLY:O	2.00	1.08
5:B:976:ILE:CD1	5:B:992:ILE:HA	1.83	1.07
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.35	1.07
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	1.69	1.05
5:B:879:ARG:NH1	5:B:882:THR:HG22	1.69	1.04
4:A:55:ASP:H	4:A:56:PRO:HD2	1.18	1.04
5:B:647:GLY:HA3	5:B:648:HIS:HB3	1.38	1.03
4:A:336:ILE:HD12	4:A:1405:THR:HG21	1.32	1.03
4:A:336:ILE:HD11	4:A:1405:THR:HG21	1.36	1.03
5:B:446:LEU:HG	5:B:447:ALA:H	1.21	1.02
4:A:343:LYS:CD	5:B:1156:ASP:OD2	2.06	1.02
5:B:994:TYR:HB2	5:B:999:MET:CE	1.87	1.02
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.42	1.02
4:A:443:LEU:HD21	4:A:455:MET:CG	1.89	1.02
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.41	1.02
4:A:440:ASP:OD2	4:A:441:PRO:HD2	1.58	1.01
4:A:443:LEU:CD2	4:A:455:MET:HG3	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:48:ALA:HB1	4:A:49:LYS:HB3	1.41	1.01
6:C:57:VAL:HG11	11:J:60:PHE:CB	1.91	1.00
4:A:372:LYS:HA	4:A:435:HIS:CD2	1.96	1.00
4:A:49:LYS:HD2	4:A:55:ASP:OD2	1.61	1.00
11:J:7:CYS:HB2	11:J:49:MET:HG2	1.42	1.00
4:A:760:GLN:HE21	4:A:760:GLN:HA	1.23	1.00
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	1.76	0.99
4:A:447:GLN:HB3	4:A:448:PRO:HA	1.45	0.98
5:B:167:ILE:HG22	5:B:167:ILE:O	1.62	0.98
5:B:879:ARG:HA	5:B:879:ARG:CZ	1.93	0.98
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	0.96	0.97
5:B:822:ASN:HD22	11:J:52:THR:CG2	1.77	0.97
4:A:311:GLN:HB3	4:A:312:PRO:HD2	1.44	0.97
4:A:341:MET:CE	4:A:1428:VAL:CB	2.36	0.97
4:A:343:LYS:HD3	5:B:1156:ASP:OD2	1.64	0.97
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.29	0.96
4:A:853:ASP:OD1	4:A:855:THR:HG22	1.65	0.96
6:C:142:VAL:H	11:J:16:ASP:HB3	1.30	0.96
5:B:1094:ARG:HH11	5:B:1094:ARG:CG	1.79	0.96
4:A:96:ILE:HG21	4:A:176:LYS:HE3	1.47	0.95
4:A:218:ASP:H	4:A:219:PHE:HB3	1.31	0.95
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.06	0.95
5:B:977:GLY:O	5:B:989:THR:HG22	1.68	0.94
6:C:33:LEU:HD23	6:C:37:MET:HE1	1.46	0.94
4:A:341:MET:HE1	4:A:1428:VAL:HB	0.95	0.94
4:A:666:ILE:HD12	5:B:1026:LEU:HB2	1.46	0.94
5:B:778:MET:CE	5:B:1094:ARG:NH1	2.29	0.94
5:B:647:GLY:HA3	5:B:648:HIS:HB2	1.46	0.94
4:A:336:ILE:HG13	4:A:337:ARG:H	1.33	0.93
6:C:33:LEU:CD2	6:C:37:MET:HE1	1.99	0.93
4:A:341:MET:CE	4:A:1428:VAL:CG1	2.47	0.93
4:A:351:THR:HG22	4:A:352:VAL:N	1.81	0.93
5:B:976:ILE:HD12	5:B:992:ILE:CA	1.98	0.93
4:A:48:ALA:CB	4:A:49:LYS:HB3	1.97	0.93
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.48	0.93
5:B:702:LEU:HD21	5:B:735:ALA:HB1	1.49	0.93
4:A:336:ILE:HD12	4:A:1405:THR:HG23	1.47	0.92
5:B:976:ILE:CD1	5:B:992:ILE:CA	2.47	0.92
5:B:778:MET:HE1	5:B:1094:ARG:NH1	1.84	0.92
5:B:1122:ARG:HG2	5:B:1122:ARG:NH1	1.68	0.92
4:A:901:LEU:HA	4:A:907:THR:HG22	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:901:LEU:H	4:A:926:GLN:HE21	1.14	0.91
5:B:31:TRP:HA	5:B:34:ILE:HD12	1.50	0.91
5:B:976:ILE:O	5:B:976:ILE:HG23	1.71	0.91
4:A:323:LYS:HZ3	4:A:324:SER:H	0.91	0.91
4:A:472:LEU:O	4:A:475:THR:HB	1.71	0.91
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.19	0.91
10:I:117:LYS:CB	10:I:118:ARG:HA	2.00	0.90
5:B:1106:ARG:HD2	5:B:1126:GLY:O	1.70	0.90
4:A:809:THR:HG22	4:A:810:PRO:HD2	1.52	0.90
5:B:1029:CYS:SG	5:B:1088:GLY:HA3	2.12	0.90
6:C:57:VAL:CG1	11:J:60:PHE:HB3	2.01	0.90
4:A:455:MET:HG2	5:B:1138:MET:HE1	1.54	0.90
4:A:351:THR:HG23	5:B:1103:ILE:HD13	1.51	0.90
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.06	0.90
6:C:75:MET:HE2	6:C:239:PRO:HD3	1.50	0.90
5:B:839:MET:HE1	5:B:841:MET:CE	2.02	0.90
5:B:1094:ARG:HG2	5:B:1094:ARG:NH1	1.76	0.90
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	1.82	0.89
5:B:879:ARG:HA	5:B:879:ARG:NE	1.84	0.89
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.52	0.89
4:A:323:LYS:HZ3	4:A:324:SER:N	1.71	0.88
4:A:351:THR:HG22	4:A:352:VAL:H	1.34	0.88
4:A:364:VAL:HG12	4:A:459:ARG:O	1.72	0.88
5:B:843:GLN:OE1	5:B:843:GLN:HA	1.71	0.88
4:A:269:ILE:HG22	4:A:299:HIS:HB2	1.54	0.88
4:A:323:LYS:NZ	4:A:324:SER:H	1.71	0.88
4:A:48:ALA:CA	4:A:49:LYS:HB3	2.01	0.88
11:J:19:GLU:OE1	11:J:19:GLU:HA	1.73	0.88
5:B:839:MET:HE1	5:B:841:MET:HE2	1.56	0.88
4:A:803:SER:OG	4:A:806:ARG:HB2	1.74	0.86
5:B:822:ASN:HD22	11:J:52:THR:HG21	1.39	0.86
5:B:839:MET:HE2	5:B:990:ILE:HG12	0.89	0.86
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.56	0.86
9:H:2:SER:HB2	9:H:3:ASN:HB2	1.57	0.86
5:B:839:MET:HG3	5:B:989:THR:O	1.75	0.86
4:A:372:LYS:HA	4:A:435:HIS:HD2	1.39	0.86
4:A:367:PRO:HD3	4:A:467:THR:O	1.75	0.86
4:A:466:SER:O	5:B:1103:ILE:HD12	1.75	0.85
5:B:839:MET:HG2	5:B:989:THR:O	1.76	0.85
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.58	0.85
4:A:48:ALA:HA	4:A:49:LYS:CB	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:778:MET:O	5:B:819:ALA:HB1	1.75	0.85
4:A:340:LEU:HD21	5:B:1199:ALA:C	2.02	0.85
5:B:969:ARG:HB3	5:B:969:ARG:HH11	1.42	0.85
4:A:214:ILE:HG22	4:A:215:SER:H	1.41	0.85
4:A:754:SER:H	4:A:757:ASN:ND2	1.74	0.84
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.41	0.84
5:B:976:ILE:CD1	5:B:992:ILE:N	2.34	0.84
5:B:69:LEU:O	5:B:89:GLU:HG2	1.78	0.84
4:A:444:PHE:HE2	4:A:470:LEU:CD2	1.90	0.84
4:A:814:PHE:O	4:A:817:ALA:HB3	1.78	0.83
5:B:879:ARG:HH12	5:B:882:THR:HG22	1.41	0.83
5:B:913:GLY:HA2	5:B:938:SER:OG	1.77	0.83
5:B:1150:ARG:HG3	5:B:1150:ARG:O	1.77	0.83
4:A:117:GLU:H	4:A:118:HIS:HB2	0.69	0.83
5:B:390:LEU:HD13	5:B:392:ARG:HH21	1.44	0.83
4:A:839:ARG:HH11	4:A:839:ARG:CG	1.92	0.82
5:B:263:GLY:HA2	5:B:264:SER:O	1.80	0.82
4:A:79:GLY:O	4:A:243:PRO:HG3	1.79	0.82
4:A:901:LEU:H	4:A:926:GLN:NE2	1.77	0.82
9:H:2:SER:CB	9:H:3:ASN:HB2	2.09	0.82
12:K:37:LYS:HA	12:K:69:ALA:HB1	1.59	0.82
5:B:647:GLY:CA	5:B:648:HIS:CB	2.57	0.82
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.12	0.82
5:B:345:LYS:N	5:B:346:GLU:CA	2.43	0.81
4:A:313:GLN:HG2	4:A:322:VAL:HG22	1.61	0.81
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.63	0.81
4:A:215:SER:HB3	4:A:218:ASP:HB2	1.63	0.81
4:A:14:VAL:H	4:A:1432:GLN:NE2	1.77	0.81
5:B:980:PHE:CE1	5:B:990:ILE:CD1	2.63	0.81
4:A:754:SER:H	4:A:757:ASN:HD22	1.29	0.81
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.14	0.81
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.61	0.81
4:A:353:ILE:HG23	4:A:487:MET:HG3	1.61	0.80
5:B:484:ASN:ND2	5:B:490:SER:OG	2.12	0.80
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.11	0.80
5:B:805:THR:HG21	5:B:815:ARG:HH21	1.46	0.80
4:A:353:ILE:CG2	4:A:487:MET:HG3	2.11	0.80
5:B:1163:CYS:HB3	5:B:1167:GLY:H	1.44	0.80
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.47	0.80
4:A:351:THR:HG21	4:A:466:SER:O	1.81	0.80
5:B:1054:GLY:O	5:B:1055:ILE:C	2.25	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:343:LYS:HZ2	5:B:1156:ASP:CG	1.89	0.80
4:A:407:ARG:HD2	4:A:413:ILE:HD11	1.63	0.80
4:A:336:ILE:HG13	4:A:337:ARG:N	1.95	0.79
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.62	0.79
5:B:448:ILE:HG23	5:B:449:ASN:H	1.47	0.79
4:A:55:ASP:N	4:A:56:PRO:HD2	1.96	0.79
5:B:1122:ARG:CG	5:B:1122:ARG:NH1	2.26	0.79
4:A:336:ILE:HD11	4:A:1405:THR:CG2	1.99	0.79
5:B:655:LYS:O	5:B:658:ILE:HG22	1.82	0.79
5:B:778:MET:CE	5:B:1094:ARG:HH11	1.94	0.79
7:E:130:ALA:HA	7:E:131:THR:OG1	1.83	0.79
5:B:408:LEU:O	5:B:412:LEU:HG	1.83	0.79
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.65	0.79
4:A:1063:MET:SD	4:A:1436:ILE:HG13	2.23	0.79
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.64	0.79
5:B:464:GLY:HA3	5:B:478:GLY:HA2	1.65	0.78
9:H:82:PRO:CB	9:H:83:GLN:HA	2.10	0.78
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.64	0.78
4:A:535:THR:HG21	4:A:617:VAL:H	1.47	0.78
7:E:179:GLN:HB2	7:E:182:ASP:HB2	1.65	0.78
5:B:1072:MET:HE2	5:B:1085:ILE:HB	1.64	0.78
2:T:8:DC:H4'	2:T:9:DA:O5'	1.82	0.78
5:B:167:ILE:O	5:B:167:ILE:CG2	2.30	0.78
11:J:7:CYS:HB2	11:J:49:MET:CG	2.14	0.78
4:A:913:LEU:HD12	4:A:914:GLU:H	1.49	0.78
4:A:500:GLU:OE2	5:B:1145:SER:HB2	1.83	0.77
5:B:807:ARG:HH11	5:B:807:ARG:CG	1.97	0.77
5:B:647:GLY:CA	5:B:648:HIS:HB3	2.13	0.77
5:B:765:PRO:O	5:B:767:ASN:N	2.18	0.77
8:F:103:MET:O	8:F:104:ASN:HB2	1.83	0.77
4:A:341:MET:SD	4:A:1428:VAL:HG11	2.24	0.77
4:A:341:MET:CE	4:A:1428:VAL:HG11	2.14	0.77
4:A:482:PHE:C	4:A:484:GLY:H	1.91	0.77
4:A:543:LEU:HG	4:A:547:LEU:HD11	1.66	0.77
6:C:215:GLU:H	6:C:216:GLY:HA3	1.46	0.77
11:J:48:ARG:HG2	11:J:48:ARG:HH11	1.49	0.77
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.20	0.77
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	1.85	0.77
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.12	0.77
5:B:654:ARG:H	5:B:657:HIS:HD2	1.33	0.77
6:C:123:ASN:ND2	6:C:125:MET:HG3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:48:ALA:CA	4:A:49:LYS:CB	2.60	0.77
4:A:41:MET:HG2	4:A:41:MET:O	1.85	0.77
4:A:341:MET:SD	4:A:1429:ILE:HG13	2.25	0.77
4:A:129:LYS:O	4:A:130:ASP:HB2	1.83	0.76
4:A:341:MET:HE1	4:A:1428:VAL:CG2	2.15	0.76
4:A:760:GLN:HE21	4:A:760:GLN:CA	1.96	0.76
5:B:805:THR:HG21	5:B:815:ARG:NH2	2.00	0.76
4:A:364:VAL:O	4:A:364:VAL:HG13	1.82	0.76
4:A:830:LYS:O	4:A:834:THR:HG23	1.84	0.76
5:B:313:MET:HE2	5:B:390:LEU:HG	1.66	0.76
2:T:27:DT:H2''	2:T:28:DT:O5'	1.85	0.76
4:A:1101:LEU:O	4:A:1105:LEU:HD12	1.84	0.76
5:B:822:ASN:HD22	11:J:52:THR:HG23	1.50	0.76
6:C:33:LEU:HD23	6:C:37:MET:CE	2.15	0.76
4:A:465:TYR:HE1	12:K:67:PHE:CE2	2.03	0.76
5:B:390:LEU:HD13	5:B:392:ARG:NH2	2.00	0.76
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.32	0.76
4:A:311:GLN:HB3	4:A:312:PRO:CD	2.15	0.75
5:B:839:MET:HE1	5:B:990:ILE:HG12	1.67	0.75
5:B:601:ARG:HA	5:B:615:MET:HE1	1.66	0.75
4:A:336:ILE:CG1	4:A:337:ARG:H	1.97	0.75
4:A:1123:GLY:HA3	4:A:1124:HIS:HB2	1.69	0.75
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.68	0.75
7:E:12:LEU:HD11	7:E:58:MET:HE1	1.68	0.75
10:I:65:ASP:OD1	10:I:66:PRO:HD2	1.86	0.75
4:A:343:LYS:NZ	5:B:1156:ASP:CG	2.45	0.75
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.69	0.75
5:B:839:MET:HG3	5:B:990:ILE:HA	1.68	0.75
6:C:73:GLN:HE21	6:C:74:SER:N	1.84	0.75
4:A:1156:PRO:O	4:A:1158:PRO:HD3	1.87	0.74
5:B:483:LEU:O	5:B:484:ASN:HB3	1.87	0.74
5:B:956:THR:HB	13:L:46:VAL:HG21	1.68	0.74
4:A:344:ARG:NH2	5:B:1112:GLN:CD	2.44	0.74
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.70	0.74
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.69	0.74
5:B:486:TYR:HE1	5:B:794:ASN:HB2	1.52	0.74
5:B:840:ILE:HG21	5:B:1011:ILE:HD12	1.68	0.74
5:B:822:ASN:ND2	11:J:52:THR:CG2	2.50	0.74
5:B:986:GLN:NE2	5:B:1022:THR:HG21	2.03	0.74
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.32	0.74
5:B:654:ARG:H	5:B:657:HIS:CD2	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:710:LEU:O	5:B:711:GLU:HB3	1.85	0.74
5:B:841:MET:HE1	5:B:990:ILE:HD11	1.67	0.74
5:B:900:ALA:CB	13:L:61:THR:HG23	2.18	0.74
9:H:123:MET:HE2	9:H:142:LEU:HD13	1.70	0.74
4:A:84:ILE:CD1	4:A:270:LEU:HD12	2.18	0.74
4:A:596:THR:C	4:A:598:LEU:H	1.95	0.74
6:C:167:HIS:CE1	13:L:70:ARG:HA	2.23	0.73
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.69	0.73
11:J:48:ARG:HH11	11:J:48:ARG:CG	2.01	0.73
4:A:214:ILE:HG22	4:A:215:SER:N	2.00	0.73
5:B:515:HIS:HD2	5:B:517:THR:H	1.36	0.73
4:A:116:ASP:HB3	4:A:117:GLU:HB2	1.69	0.73
7:E:55:ARG:HD2	7:E:83:CYS:O	1.88	0.73
6:C:14:SER:O	6:C:240:VAL:HG21	1.88	0.73
4:A:1199:ARG:O	4:A:1203:ASN:ND2	2.20	0.72
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.54	0.72
4:A:598:LEU:HD11	9:H:39:THR:HG21	1.71	0.72
5:B:886:LYS:HB3	5:B:887:HIS:HA	1.68	0.72
5:B:911:ILE:HD11	5:B:941:LEU:HD12	1.70	0.72
4:A:18:GLN:HG2	4:A:1418:LEU:HD12	1.69	0.72
5:B:25:ILE:CD1	5:B:653:VAL:HB	2.20	0.72
5:B:994:TYR:CB	5:B:999:MET:HE3	2.12	0.72
1:R:9:G:H2'	1:R:10:C:C6	2.25	0.72
4:A:106:VAL:HG12	4:A:107:CYS:N	2.03	0.72
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.72	0.72
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.19	0.72
5:B:291:ILE:HD12	5:B:291:ILE:N	2.04	0.72
5:B:880:THR:O	5:B:882:THR:N	2.23	0.72
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.70	0.72
4:A:343:LYS:NZ	5:B:1197:PRO:CB	2.43	0.71
4:A:377:PRO:HB2	4:A:431:LYS:HE3	1.70	0.71
5:B:446:LEU:HG	5:B:447:ALA:N	2.03	0.71
4:A:399:HIS:HD2	4:A:400:PRO:HG3	1.53	0.71
4:A:839:ARG:HH11	4:A:839:ARG:HG2	1.54	0.71
4:A:341:MET:SD	4:A:1428:VAL:CB	2.77	0.71
5:B:459:TYR:C	5:B:459:TYR:CD2	2.66	0.71
5:B:555:ILE:HA	5:B:558:LEU:HD12	1.71	0.71
5:B:822:ASN:ND2	11:J:52:THR:HG23	2.05	0.71
4:A:269:ILE:CG2	4:A:299:HIS:HB2	2.20	0.71
4:A:779:PHE:CZ	5:B:517:THR:HA	2.26	0.71
4:A:1116:LEU:HD13	4:A:1329:THR:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:990:ILE:HG22	5:B:991:GLY:H	1.56	0.71
4:A:482:PHE:O	5:B:989:THR:OG1	2.07	0.71
5:B:807:ARG:HG3	5:B:807:ARG:NH1	1.92	0.71
5:B:976:ILE:HD11	5:B:992:ILE:CA	2.17	0.71
4:A:84:ILE:HD11	4:A:270:LEU:HD12	1.70	0.71
4:A:1206:ASP:HB2	4:A:1274:ARG:HH22	1.55	0.71
8:F:155:LEU:HG	8:F:155:LEU:OXT	1.90	0.71
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.30	0.71
4:A:182:VAL:HG12	4:A:183:GLY:H	1.55	0.71
5:B:1122:ARG:HH11	5:B:1122:ARG:HG3	1.50	0.71
4:A:218:ASP:N	4:A:219:PHE:HB3	2.05	0.71
5:B:1084:GLN:NE2	6:C:191:TYR:HA	2.06	0.71
4:A:308:ILE:HG22	4:A:309:ALA:H	1.56	0.70
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.54	0.70
4:A:353:ILE:HD13	4:A:487:MET:CE	2.20	0.70
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.73	0.70
4:A:351:THR:HG23	5:B:1103:ILE:CD1	2.21	0.70
7:E:168:TYR:O	7:E:169:ARG:HG2	1.91	0.70
4:A:855:THR:CG2	4:A:857:ARG:HE	2.05	0.70
4:A:351:THR:CG2	4:A:352:VAL:N	2.54	0.70
4:A:364:VAL:HG12	4:A:460:VAL:HA	1.72	0.70
4:A:709:THR:HB	4:A:712:GLU:H	1.57	0.70
6:C:186:LEU:HB2	6:C:188:HIS:HD2	1.56	0.70
10:I:10:CYS:SG	10:I:31:THR:HB	2.32	0.70
4:A:260:ASP:OD1	4:A:261:ASP:N	2.23	0.70
6:C:56:THR:HG22	6:C:57:VAL:N	2.07	0.70
7:E:130:ALA:HA	7:E:131:THR:CB	2.21	0.70
8:F:79:ARG:NH1	8:F:145:ASP:O	2.24	0.70
4:A:265:LYS:HE2	4:A:302:THR:HG23	1.74	0.70
4:A:567:LYS:CB	9:H:96:VAL:H	1.98	0.70
5:B:484:ASN:ND2	5:B:484:ASN:O	2.25	0.70
4:A:117:GLU:H	4:A:118:HIS:CA	2.05	0.70
5:B:287:ARG:NH1	5:B:325:GLN:HA	2.06	0.70
5:B:451:LYS:HA	5:B:454:THR:HB	1.74	0.70
4:A:444:PHE:CE2	4:A:470:LEU:HD23	2.26	0.70
4:A:456:MET:HB2	4:A:478:TYR:OH	1.91	0.70
5:B:100:PRO:O	5:B:101:MET:HG3	1.91	0.70
5:B:542:MET:HE1	5:B:743:ILE:HG13	1.74	0.70
4:A:853:ASP:OD1	4:A:855:THR:CG2	2.39	0.69
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.55	0.69
4:A:882:SER:HB2	4:A:953:ASN:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.38	0.69
6:C:29:MET:HE3	12:K:45:LEU:HD11	1.74	0.69
2:T:10:DA:H61	3:N:5:DT:H3	1.40	0.69
4:A:344:ARG:NH2	5:B:1112:GLN:NE2	2.41	0.69
5:B:955:THR:HG22	5:B:956:THR:H	1.56	0.69
4:A:302:THR:HA	4:A:305:ASP:O	1.93	0.69
5:B:815:ARG:HG2	5:B:816:GLU:OE1	1.92	0.69
4:A:290:GLU:C	4:A:292:ALA:H	2.01	0.69
5:B:659:ALA:HA	5:B:662:MET:HE2	1.73	0.69
5:B:879:ARG:O	5:B:882:THR:HB	1.93	0.69
5:B:1058:LEU:O	5:B:1062:HIS:HB2	1.92	0.69
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.25	0.69
4:A:855:THR:HG21	4:A:857:ARG:HE	1.57	0.68
5:B:361:LEU:CD2	5:B:377:PHE:HD2	2.06	0.68
5:B:955:THR:HG22	5:B:956:THR:N	2.08	0.68
4:A:364:VAL:CG1	4:A:460:VAL:HA	2.23	0.68
6:C:56:THR:HG22	6:C:57:VAL:H	1.56	0.68
5:B:346:GLU:HG2	5:B:349:ILE:CD1	2.23	0.68
4:A:672:ASP:HB2	4:A:675:THR:OG1	1.93	0.68
4:A:535:THR:HG21	4:A:617:VAL:N	2.08	0.68
5:B:846:ILE:HG23	5:B:974:PRO:HD2	1.76	0.68
5:B:841:MET:HG2	5:B:842:ASN:H	1.59	0.68
5:B:957:ASN:HB3	5:B:961:LEU:HB2	1.76	0.68
6:C:31:ASN:ND2	6:C:35:ARG:HD2	2.09	0.68
4:A:48:ALA:HA	4:A:49:LYS:HB2	1.76	0.68
4:A:444:PHE:HE2	4:A:470:LEU:HD23	1.58	0.68
5:B:757:PRO:HG3	5:B:983:ARG:CZ	2.24	0.68
1:R:10:C:OP1	5:B:987:LYS:HD2	1.93	0.67
6:C:56:THR:HG21	6:C:145:CYS:SG	2.34	0.67
11:J:36:LEU:HD22	11:J:41:LEU:HD13	1.75	0.67
4:A:332:LYS:H	4:A:337:ARG:HB3	1.59	0.67
4:A:705:LYS:NZ	4:A:716:ASP:OD1	2.26	0.67
4:A:830:LYS:HB2	4:A:830:LYS:NZ	2.09	0.67
4:A:678:GLU:HA	4:A:681:GLU:HG2	1.76	0.67
5:B:487:THR:O	5:B:490:SER:N	2.27	0.67
5:B:1017:ILE:HD12	5:B:1026:LEU:HD21	1.76	0.67
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.75	0.67
5:B:486:TYR:HE2	5:B:1096:ARG:HG2	1.58	0.67
5:B:763:GLN:HG2	5:B:764:SER:N	2.08	0.67
5:B:35:SER:HB3	5:B:39:ARG:HH21	1.60	0.67
5:B:313:MET:CE	5:B:390:LEU:HG	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:117:LYS:HB3	10:I:118:ARG:CA	2.11	0.67
4:A:444:PHE:CE2	4:A:470:LEU:CD2	2.78	0.67
5:B:140:ILE:H	5:B:141:ASP:C	2.02	0.67
5:B:866:TYR:CD1	5:B:867:GLY:HA2	2.30	0.67
5:B:1175:LEU:HD23	5:B:1176:ASN:H	1.58	0.67
4:A:1418:LEU:HD22	5:B:1222:ARG:HH21	1.59	0.67
4:A:496:GLU:HB2	8:F:95:GLY:HA3	1.76	0.67
4:A:956:LEU:HD23	4:A:957:PRO:HD3	1.77	0.66
4:A:715:GLU:O	4:A:719:VAL:HG23	1.95	0.66
5:B:1221:SER:C	5:B:1223:ASP:H	2.03	0.66
4:A:660:ASN:OD1	5:B:1082:MET:HB3	1.96	0.66
6:C:75:MET:HE2	6:C:239:PRO:CD	2.23	0.66
13:L:32:ALA:HB3	13:L:55:ILE:HB	1.77	0.66
4:A:423:ASP:OD2	4:A:424:ILE:N	2.29	0.66
4:A:336:ILE:CD1	4:A:1405:THR:CB	2.72	0.66
4:A:806:ARG:HG2	4:A:806:ARG:HH11	1.59	0.66
6:C:214:ASN:HD22	6:C:215:GLU:HB3	1.61	0.66
4:A:161:LEU:O	4:A:162:VAL:HG23	1.96	0.66
4:A:405:VAL:HG22	4:A:432:VAL:HG22	1.78	0.66
5:B:604:ARG:HD3	5:B:611:PRO:HA	1.76	0.66
5:B:744:HIS:CD2	5:B:746:SER:OG	2.48	0.66
4:A:526:ASP:OD2	5:B:829:CYS:HB3	1.95	0.66
4:A:1446:ASP:HB3	4:A:1448:GLU:N	2.09	0.66
5:B:1006:ILE:HG22	5:B:1007:VAL:N	2.10	0.66
6:C:18:VAL:O	6:C:231:ASN:HA	1.95	0.66
12:K:65:HIS:CD2	12:K:66:PRO:CD	2.78	0.66
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.60	0.66
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.77	0.66
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.77	0.66
4:A:148:CYS:O	4:A:149:GLU:HB2	1.94	0.66
4:A:830:LYS:HB2	4:A:830:LYS:HZ3	1.61	0.66
5:B:190:TYR:CE1	11:J:62:ARG:HG2	2.31	0.66
5:B:841:MET:CE	5:B:990:ILE:CD1	2.73	0.65
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.11	0.65
5:B:465:ASN:HA	5:B:476:ARG:HA	1.78	0.65
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.79	0.65
4:A:756:ILE:O	4:A:760:GLN:HG2	1.95	0.65
5:B:637:LEU:CD1	5:B:740:HIS:HB3	2.27	0.65
5:B:847:ASP:HB3	6:C:167:HIS:NE2	2.10	0.65
6:C:33:LEU:CD2	6:C:37:MET:CE	2.74	0.65
4:A:741:ASN:HD21	4:A:743:VAL:HG23	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:25:ILE:HD12	5:B:653:VAL:HB	1.77	0.65
5:B:1175:LEU:HD23	5:B:1176:ASN:N	2.12	0.65
6:C:123:ASN:HD22	6:C:125:MET:HG3	1.59	0.65
4:A:340:LEU:HD23	5:B:1199:ALA:HB3	1.77	0.65
4:A:1111:MET:HG2	4:A:1114:PRO:HG3	1.78	0.65
7:E:175:LEU:O	7:E:177:ARG:HD2	1.97	0.65
5:B:850:LEU:CD2	5:B:1009:ASP:HB3	2.27	0.65
5:B:877:PRO:HB2	5:B:885:MET:HE1	1.79	0.65
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.31	0.65
5:B:1072:MET:HE3	5:B:1085:ILE:HD13	1.79	0.65
10:I:117:LYS:HD3	10:I:118:ARG:HH21	1.62	0.65
5:B:780:VAL:HB	5:B:817:LEU:HD22	1.77	0.65
5:B:870:ILE:HG22	5:B:870:ILE:O	1.96	0.65
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	1.78	0.64
8:F:97:ARG:HG3	8:F:101:ILE:HD11	1.78	0.64
9:H:77:ARG:NH1	9:H:77:ARG:HB2	2.13	0.64
5:B:805:THR:N	5:B:1042:GLY:O	2.28	0.64
5:B:841:MET:HE3	5:B:990:ILE:CD1	2.27	0.64
4:A:360:GLU:HB2	4:A:363:GLN:OE1	1.98	0.64
4:A:663:SER:OG	5:B:1085:ILE:HG23	1.98	0.64
5:B:879:ARG:HH12	5:B:882:THR:CG2	2.09	0.64
5:B:978:ASP:O	5:B:980:PHE:CD1	2.50	0.64
7:E:147:HIS:HB3	7:E:150:VAL:HG23	1.79	0.64
11:J:9:SER:OG	11:J:45:CYS:HB2	1.98	0.64
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.79	0.64
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.52	0.64
5:B:235:SER:OG	5:B:236:HIS:ND1	2.30	0.64
4:A:503:GLN:HE21	8:F:90:ARG:HH12	1.46	0.64
4:A:806:ARG:HG2	4:A:806:ARG:NH1	2.09	0.64
5:B:899:ILE:HG21	5:B:949:VAL:HG21	1.79	0.64
6:C:235:VAL:HG11	11:J:6:ARG:HH21	1.61	0.64
4:A:399:HIS:CD2	4:A:400:PRO:HG3	2.33	0.64
5:B:839:MET:HE2	5:B:990:ILE:CB	2.28	0.64
12:K:65:HIS:HD2	12:K:67:PHE:H	1.46	0.64
4:A:1101:LEU:HD13	4:A:1355:VAL:HG11	1.78	0.64
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.80	0.64
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.80	0.64
4:A:1446:ASP:HB3	4:A:1448:GLU:H	1.61	0.64
5:B:1033:LYS:O	5:B:1037:LEU:HG	1.97	0.64
4:A:265:LYS:HG2	4:A:303:TYR:HB2	1.79	0.64
4:A:913:LEU:HD12	4:A:914:GLU:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HG2	5:B:1008:PRO:CD	2.27	0.64
5:B:1107:ALA:O	5:B:1108:ARG:HG2	1.98	0.63
6:C:63:ILE:HA	6:C:66:ARG:HG3	1.80	0.63
5:B:448:ILE:CG2	5:B:449:ASN:N	2.60	0.63
6:C:71:PRO:O	6:C:133:ILE:HG12	1.98	0.63
6:C:78:GLU:OE1	6:C:78:GLU:HA	1.96	0.63
4:A:351:THR:CG2	4:A:352:VAL:H	2.08	0.63
4:A:465:TYR:CE1	12:K:67:PHE:CE2	2.86	0.63
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.27	0.63
4:A:146:MET:HE3	4:A:146:MET:H	1.64	0.63
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	1.80	0.63
5:B:346:GLU:O	5:B:348:ARG:N	2.32	0.63
5:B:1168:LEU:HD22	5:B:1208:MET:HE2	1.81	0.63
4:A:508:PRO:O	4:A:510:GLN:N	2.28	0.63
5:B:839:MET:SD	5:B:989:THR:O	2.56	0.63
5:B:886:LYS:HB3	5:B:887:HIS:CA	2.29	0.63
4:A:53:LEU:HD12	4:A:54:ASN:H	1.62	0.63
5:B:100:PRO:C	5:B:101:MET:HG3	2.24	0.63
5:B:530:GLY:O	5:B:531:GLN:C	2.42	0.63
4:A:760:GLN:HA	4:A:760:GLN:NE2	2.07	0.62
4:A:341:MET:SD	4:A:1428:VAL:HB	2.38	0.62
4:A:391:LEU:HD12	4:A:400:PRO:O	2.00	0.62
5:B:65:GLU:CD	5:B:66:ASP:HB3	2.24	0.62
5:B:802:PRO:HA	5:B:822:ASN:HD21	1.65	0.62
7:E:9:ILE:HG12	7:E:53:PRO:HG3	1.80	0.62
7:E:16:PHE:CE2	7:E:20:LYS:HE2	2.33	0.62
4:A:364:VAL:O	4:A:364:VAL:CG1	2.47	0.62
4:A:1144:LYS:HB2	4:A:1268:LEU:O	1.99	0.62
4:A:55:ASP:O	4:A:57:ARG:N	2.32	0.62
6:C:41:ILE:HG22	6:C:250:THR:OG1	1.99	0.62
4:A:401:GLY:C	4:A:435:HIS:HD1	2.08	0.62
6:C:211:ASP:HB3	6:C:212:PRO:HD2	1.81	0.62
7:E:55:ARG:O	7:E:57:MET:N	2.33	0.62
4:A:756:ILE:O	4:A:759:ALA:HB3	1.99	0.62
5:B:997:GLU:HG2	6:C:39:ALA:HB2	1.80	0.62
4:A:726:ARG:HD3	4:A:766:GLY:HA3	1.81	0.62
5:B:346:GLU:HG2	5:B:349:ILE:HD13	1.81	0.62
5:B:839:MET:CE	5:B:990:ILE:CG1	2.46	0.62
6:C:57:VAL:O	6:C:57:VAL:HG12	1.99	0.62
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.64	0.62
4:A:1345:ARG:HD2	4:A:1373:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.45	0.62
5:B:448:ILE:HG23	5:B:449:ASN:N	2.14	0.62
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.35	0.62
10:I:63:GLY:HA3	10:I:104:LEU:HD11	1.82	0.62
4:A:353:ILE:HD11	4:A:480:ALA:HB1	1.81	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.87	0.62
5:B:952:VAL:HG13	5:B:966:VAL:HG22	1.80	0.62
12:K:32:VAL:HG23	12:K:74:ARG:HG3	1.81	0.62
4:A:64:ASN:CB	4:A:66:LYS:HG2	2.30	0.62
4:A:549:MET:SD	4:A:577:ILE:HD13	2.39	0.62
4:A:567:LYS:HB3	9:H:96:VAL:N	1.99	0.62
5:B:276:ILE:CD1	5:B:277:LYS:H	2.12	0.62
5:B:803:LEU:O	5:B:1042:GLY:HA3	1.99	0.62
5:B:1169:MET:HE3	5:B:1208:MET:HE1	1.82	0.62
12:K:61:TYR:HA	12:K:72:LYS:O	2.00	0.62
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.65	0.61
4:A:1064:VAL:O	4:A:1064:VAL:HG12	1.99	0.61
4:A:1110:ASN:HD22	4:A:1110:ASN:H	1.48	0.61
5:B:906:SER:HA	5:B:946:ASN:HB3	1.81	0.61
9:H:42:ILE:HG21	9:H:49:VAL:HG21	1.82	0.61
11:J:44:TYR:CD1	11:J:44:TYR:C	2.77	0.61
4:A:444:PHE:HE2	4:A:470:LEU:HD22	1.63	0.61
5:B:277:LYS:HE2	5:B:335:GLY:H	1.65	0.61
4:A:870:GLU:HG2	7:E:208:TYR:CG	2.36	0.61
5:B:34:ILE:HD13	5:B:747:MET:HE3	1.83	0.61
5:B:229:ALA:O	5:B:261:ARG:NH2	2.33	0.61
7:E:64:PRO:HD3	7:E:76:GLY:HA2	1.80	0.61
4:A:341:MET:O	5:B:1132:GLU:HB3	2.00	0.61
4:A:830:LYS:HE2	4:A:1079:MET:O	1.99	0.61
5:B:765:PRO:O	5:B:766:ARG:C	2.43	0.61
2:T:21:DC:OP1	5:B:1129:ARG:HB3	2.01	0.61
5:B:990:ILE:HG22	5:B:991:GLY:N	2.14	0.61
4:A:313:GLN:HG3	4:A:314:ALA:H	1.64	0.61
4:A:1080:THR:O	4:A:1081:LEU:C	2.43	0.61
6:C:11:ARG:HD3	6:C:21:ILE:HD11	1.81	0.61
13:L:48:CYS:SG	13:L:49:LYS:N	2.74	0.61
4:A:512:VAL:HA	4:A:519:PRO:HA	1.82	0.61
4:A:579:SER:HB3	4:A:611:GLN:HA	1.83	0.61
5:B:474:SER:HA	5:B:476:ARG:HG2	1.82	0.61
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.36	0.61
4:A:1384:VAL:HG23	4:A:1384:VAL:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:37:PHE:O	5:B:38:PHE:HB2	2.01	0.61
6:C:73:GLN:HE21	6:C:74:SER:H	1.49	0.61
5:B:185:THR:O	5:B:188:ASP:HB2	2.01	0.61
5:B:487:THR:O	5:B:490:SER:HB3	2.00	0.61
9:H:82:PRO:HB2	9:H:83:GLN:CA	2.15	0.61
5:B:711:GLU:H	5:B:712:PRO:HD3	1.65	0.60
5:B:826:ALA:HB3	5:B:1011:ILE:HA	1.83	0.60
5:B:863:GLU:CB	5:B:864:LYS:HA	2.30	0.60
4:A:276:LEU:HD11	4:A:292:ALA:CB	2.29	0.60
7:E:55:ARG:C	7:E:57:MET:H	2.10	0.60
6:C:54:ASN:C	6:C:56:THR:H	2.09	0.60
11:J:1:MET:N	11:J:56:LEU:H	2.00	0.60
12:K:37:LYS:O	12:K:38:GLU:HG2	2.01	0.60
5:B:869:SER:O	5:B:870:ILE:HG12	2.01	0.60
5:B:978:ASP:O	5:B:980:PHE:HD1	1.85	0.60
4:A:464:PRO:O	4:A:465:TYR:HB2	2.01	0.60
5:B:976:ILE:O	5:B:976:ILE:CG2	2.44	0.60
6:C:79:GLN:HG3	6:C:127:ARG:HD2	1.83	0.60
4:A:946:VAL:HG22	7:E:201:LYS:HB3	1.84	0.60
5:B:345:LYS:N	5:B:348:ARG:NE	2.50	0.60
5:B:973:ILE:H	5:B:973:ILE:HD12	1.67	0.60
5:B:1039:GLY:HA2	11:J:51:LEU:CD2	2.31	0.60
10:I:77:LYS:HG2	10:I:108:HIS:ND1	2.17	0.60
5:B:1037:LEU:HD12	5:B:1062:HIS:CD2	2.37	0.60
2:T:16:DT:H3'	2:T:17:DA:H8	1.67	0.60
4:A:809:THR:CG2	4:A:810:PRO:HD2	2.30	0.60
5:B:515:HIS:CD2	5:B:517:THR:H	2.18	0.60
5:B:898:LEU:HB2	13:L:58:LYS:HE3	1.83	0.60
4:A:116:ASP:CB	4:A:117:GLU:HB2	2.32	0.60
4:A:116:ASP:C	4:A:118:HIS:HB2	2.23	0.60
4:A:278:THR:O	4:A:282:ASN:HB3	2.02	0.60
4:A:808:LEU:HD13	5:B:760:ASP:O	2.02	0.60
5:B:1156:ASP:HB3	5:B:1198:TYR:H	1.66	0.60
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.42	0.60
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.84	0.59
9:H:47:PHE:HB2	9:H:95:TYR:HD1	1.66	0.59
4:A:134:ARG:CD	4:A:221:SER:O	2.50	0.59
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.02	0.59
5:B:872:GLU:HG2	5:B:916:THR:HB	1.84	0.59
5:B:906:SER:HA	5:B:946:ASN:CB	2.32	0.59
7:E:177:ARG:C	7:E:212:ARG:HD3	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:41:ILE:HD11	6:C:243:VAL:HG13	1.84	0.59
4:A:1134:ILE:O	4:A:1138:ILE:HG13	2.02	0.59
4:A:1219:THR:HG21	4:A:1271:ILE:HD12	1.85	0.59
6:C:33:LEU:HD21	6:C:37:MET:HE1	1.81	0.59
4:A:455:MET:HE2	5:B:1138:MET:SD	2.43	0.59
4:A:482:PHE:C	4:A:484:GLY:N	2.60	0.59
4:A:660:ASN:OD1	5:B:1082:MET:CB	2.50	0.59
4:A:830:LYS:HZ1	4:A:1082:ASN:HB3	1.67	0.59
7:E:36:GLU:O	7:E:38:PRO:HD3	2.02	0.59
7:E:147:HIS:HB3	7:E:150:VAL:CG2	2.32	0.59
12:K:91:CYS:O	12:K:95:ILE:HG13	2.03	0.59
4:A:90:VAL:HB	4:A:297:GLN:HE22	1.68	0.59
4:A:244:PRO:O	4:A:246:VAL:N	2.36	0.59
4:A:350:ARG:HG3	4:A:488:ASN:OD1	2.02	0.59
4:A:723:ASN:O	4:A:724:GLU:C	2.46	0.59
4:A:134:ARG:HD2	4:A:221:SER:O	2.03	0.59
4:A:1383:SER:O	4:A:1388:GLY:HA3	2.02	0.59
5:B:827:ILE:HG23	5:B:1012:ILE:HD12	1.84	0.59
5:B:863:GLU:O	5:B:872:GLU:HB2	2.02	0.59
5:B:889:THR:HG22	5:B:891:ASP:OD2	2.03	0.59
4:A:63:ARG:HA	4:A:74:MET:HG3	1.84	0.59
4:A:112:LYS:HG2	4:A:113:LEU:N	2.16	0.59
4:A:318:SER:O	4:A:320:ARG:NH2	2.36	0.59
4:A:1076:ALA:HA	4:A:1079:MET:HE3	1.84	0.59
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.85	0.59
4:A:782:ARG:NH2	5:B:699:GLU:O	2.35	0.59
5:B:664:THR:HG23	5:B:678:GLU:HB3	1.85	0.59
5:B:899:ILE:HG13	5:B:911:ILE:HG23	1.84	0.59
6:C:63:ILE:O	6:C:66:ARG:HB2	2.03	0.59
4:A:549:MET:SD	4:A:577:ILE:CD1	2.91	0.59
4:A:596:THR:C	4:A:598:LEU:N	2.59	0.59
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.26	0.59
5:B:209:GLU:OE2	5:B:485:ARG:HD3	2.03	0.59
5:B:744:HIS:HD2	5:B:746:SER:H	1.48	0.59
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.85	0.59
6:C:167:HIS:HE1	13:L:70:ARG:HA	1.68	0.59
4:A:74:MET:HE2	4:A:74:MET:HA	1.83	0.58
4:A:106:VAL:HG12	4:A:107:CYS:H	1.67	0.58
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.85	0.58
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.37	0.58
7:E:130:ALA:HB1	7:E:131:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:92:HIS:C	4:A:92:HIS:CD2	2.81	0.58
4:A:583:PRO:O	4:A:610:GLY:HA3	2.03	0.58
4:A:979:SER:OG	4:A:981:LEU:HD12	2.02	0.58
4:A:1364:ASN:ND2	4:A:1366:ARG:H	2.01	0.58
5:B:43:LEU:HD13	5:B:492:LEU:HD21	1.84	0.58
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.68	0.58
5:B:276:ILE:HG23	5:B:277:LYS:N	2.18	0.58
5:B:363:HIS:O	5:B:364:ILE:HB	2.02	0.58
4:A:567:LYS:HB2	9:H:95:TYR:HA	1.83	0.58
5:B:459:TYR:C	5:B:459:TYR:HD2	2.11	0.58
5:B:863:GLU:HB2	5:B:864:LYS:HA	1.83	0.58
5:B:892:LYS:NZ	5:B:904:ARG:O	2.36	0.58
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.84	0.58
1:R:9:G:H2'	1:R:10:C:H6	1.66	0.58
4:A:336:ILE:HD13	4:A:1405:THR:HG21	0.58	0.58
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.37	0.58
4:A:839:ARG:HG2	4:A:839:ARG:NH1	2.16	0.58
4:A:1037:LEU:HD12	4:A:1042:PHE:HA	1.85	0.58
5:B:244:LEU:HD11	5:B:366:GLN:HE22	1.68	0.58
6:C:46:ILE:HG12	6:C:157:CYS:HB3	1.85	0.58
6:C:73:GLN:HA	6:C:133:ILE:HD11	1.86	0.58
4:A:671:ALA:H	4:A:676:MET:HE2	1.69	0.58
4:A:744:LYS:O	4:A:748:MET:HG3	2.03	0.58
5:B:345:LYS:N	5:B:348:ARG:HE	2.00	0.58
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.04	0.58
4:A:296:LEU:O	4:A:296:LEU:HD23	2.03	0.58
4:A:370:ILE:HG12	5:B:1105:ALA:HB2	1.86	0.58
5:B:446:LEU:CG	5:B:447:ALA:H	2.02	0.58
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.39	0.58
4:A:106:VAL:CG1	4:A:107:CYS:N	2.67	0.58
4:A:1206:ASP:O	4:A:1274:ARG:NH2	2.37	0.58
5:B:850:LEU:HD12	11:J:8:PHE:CD1	2.39	0.58
5:B:948:ILE:HD12	5:B:969:ARG:NH1	2.19	0.58
5:B:1002:THR:CG2	5:B:1006:ILE:HB	2.34	0.58
6:C:27:LEU:HA	6:C:228:PHE:CZ	2.38	0.58
4:A:645:LEU:O	4:A:649:ILE:HG13	2.04	0.58
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.22	0.58
4:A:92:HIS:CD2	4:A:92:HIS:O	2.57	0.58
4:A:179:LEU:HD13	4:A:297:GLN:HG3	1.84	0.58
4:A:352:VAL:HB	5:B:1099:VAL:HG12	1.85	0.58
6:C:29:MET:HE2	12:K:98:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:31:ASN:HD22	6:C:35:ARG:HD2	1.69	0.58
4:A:211:PHE:HD1	4:A:231:PRO:HB2	1.69	0.57
4:A:336:ILE:HD11	4:A:1405:THR:CB	2.32	0.57
4:A:979:SER:OG	4:A:981:LEU:CD1	2.52	0.57
5:B:313:MET:HE3	5:B:386:LEU:HD22	1.85	0.57
5:B:656:GLY:O	5:B:657:HIS:C	2.47	0.57
4:A:64:ASN:HB3	4:A:66:LYS:HG2	1.84	0.57
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.86	0.57
5:B:464:GLY:CA	5:B:478:GLY:HA2	2.34	0.57
5:B:913:GLY:HA2	5:B:938:SER:HG	1.69	0.57
5:B:1039:GLY:HA2	11:J:51:LEU:HD21	1.86	0.57
7:E:64:PRO:HG3	7:E:76:GLY:HA2	1.86	0.57
4:A:377:PRO:CB	4:A:431:LYS:HE3	2.34	0.57
5:B:1149:GLU:C	5:B:1151:LEU:H	2.12	0.57
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.87	0.57
4:A:672:ASP:HB3	4:A:674:PRO:HG2	1.86	0.57
4:A:775:ILE:HG12	4:A:797:LYS:O	2.04	0.57
5:B:35:SER:HB3	5:B:39:ARG:NH2	2.18	0.57
5:B:634:TYR:HE1	5:B:692:TYR:CD1	2.22	0.57
5:B:680:THR:O	5:B:683:SER:N	2.34	0.57
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.86	0.57
4:A:37:PHE:HB2	4:A:52:GLY:CA	2.32	0.57
5:B:459:TYR:CD2	5:B:459:TYR:O	2.57	0.57
6:C:244:VAL:HG21	12:K:105:PHE:CE1	2.39	0.57
4:A:1213:GLY:HA3	4:A:1228:TRP:CZ3	2.39	0.57
5:B:658:ILE:O	5:B:661:LEU:HB2	2.05	0.57
5:B:827:ILE:HD11	5:B:1086:PHE:CD2	2.40	0.57
4:A:367:PRO:HG2	4:A:370:ILE:HD12	1.86	0.57
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.15	0.57
4:A:455:MET:O	4:A:456:MET:HG3	2.05	0.57
4:A:547:LEU:HD22	12:K:58:PHE:HD1	1.70	0.57
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.68	0.57
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.86	0.57
5:B:378:LEU:O	5:B:382:ILE:HG12	2.04	0.57
5:B:841:MET:HE1	5:B:990:ILE:CD1	2.35	0.57
6:C:214:ASN:HA	6:C:215:GLU:HB3	1.86	0.57
4:A:92:HIS:O	4:A:94:GLY:N	2.38	0.57
4:A:508:PRO:C	4:A:510:GLN:H	2.12	0.57
4:A:532:ARG:HG3	4:A:618:GLU:HB3	1.85	0.57
4:A:1110:ASN:HD22	4:A:1110:ASN:N	2.03	0.57
5:B:778:MET:HE3	5:B:1094:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:47:GLU:OE1	10:I:50:THR:HG23	2.04	0.57
11:J:18:TRP:CZ2	11:J:22:LEU:HD11	2.40	0.57
4:A:68:GLN:C	4:A:70:CYS:H	2.12	0.57
4:A:577:ILE:O	4:A:580:VAL:HG23	2.05	0.57
5:B:211:VAL:CG2	5:B:483:LEU:HD13	2.35	0.57
5:B:1065:GLN:HG2	5:B:1069:PHE:HB2	1.86	0.57
6:C:163:ILE:O	6:C:166:GLU:HB2	2.05	0.57
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.69	0.57
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.05	0.57
4:A:447:GLN:HE22	4:A:488:ASN:ND2	2.03	0.56
4:A:1005:GLU:N	4:A:1005:GLU:OE1	2.37	0.56
4:A:1313:LEU:C	4:A:1315:GLU:H	2.13	0.56
5:B:406:LEU:HD12	5:B:633:VAL:CG2	2.35	0.56
5:B:1037:LEU:HD12	5:B:1062:HIS:HD2	1.69	0.56
1:R:10:C:O2'	4:A:446:ARG:NH2	2.37	0.56
4:A:116:ASP:CA	4:A:117:GLU:HB2	2.34	0.56
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.04	0.56
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.86	0.56
6:C:46:ILE:O	6:C:169:LYS:NZ	2.38	0.56
4:A:731:ARG:HG3	4:A:755:PHE:CZ	2.41	0.56
5:B:839:MET:HE1	5:B:841:MET:HE3	1.86	0.56
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.86	0.56
9:H:41:ASP:HB3	9:H:121:LEU:HD13	1.87	0.56
11:J:6:ARG:HG2	11:J:11:GLY:O	2.04	0.56
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.45	0.56
4:A:741:ASN:HD22	4:A:741:ASN:C	2.12	0.56
6:C:10:ILE:HG21	12:K:112:GLN:HG3	1.88	0.56
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.70	0.56
5:B:944:THR:HB	5:B:1122:ARG:NH2	2.20	0.56
6:C:54:ASN:O	6:C:56:THR:N	2.38	0.56
6:C:168:ALA:C	6:C:170:TRP:H	2.13	0.56
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.87	0.56
4:A:534:LEU:O	4:A:574:GLY:HA3	2.06	0.56
4:A:537:ARG:HD3	9:H:120:GLY:O	2.06	0.56
4:A:567:LYS:O	4:A:568:PRO:C	2.48	0.56
5:B:314:LEU:C	5:B:316:PRO:HD2	2.30	0.56
5:B:361:LEU:O	5:B:363:HIS:O	2.24	0.56
5:B:680:THR:O	5:B:681:TRP:C	2.48	0.56
12:K:65:HIS:HD2	12:K:66:PRO:HD2	1.68	0.56
4:A:55:ASP:H	4:A:56:PRO:CD	2.05	0.56
4:A:642:CYS:O	4:A:645:LEU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.06	0.56
4:A:1295:THR:OG1	4:A:1297:GLU:OE1	2.24	0.56
4:A:336:ILE:HD11	4:A:1405:THR:OG1	2.06	0.56
4:A:340:LEU:HD23	5:B:1199:ALA:CB	2.36	0.56
4:A:353:ILE:CD1	4:A:480:ALA:HB1	2.36	0.56
5:B:744:HIS:HD2	5:B:746:SER:OG	1.89	0.56
5:B:821:GLN:NE2	11:J:8:PHE:HE1	2.04	0.56
11:J:8:PHE:H	11:J:49:MET:HE3	1.70	0.56
4:A:739:ASP:OD2	9:H:19:ARG:HD3	2.06	0.56
4:A:848:ILE:HD13	4:A:858:ASN:HB3	1.87	0.56
4:A:896:ARG:HH11	4:A:897:TYR:HE1	1.54	0.56
5:B:291:ILE:N	5:B:291:ILE:CD1	2.68	0.56
5:B:988:GLY:C	5:B:989:THR:O	2.48	0.56
5:B:1111:MET:HE2	5:B:1118:PRO:HA	1.87	0.56
5:B:448:ILE:CG2	5:B:449:ASN:H	2.17	0.56
5:B:710:LEU:O	5:B:711:GLU:CB	2.54	0.56
5:B:1006:ILE:CG2	5:B:1007:VAL:N	2.69	0.56
5:B:1120:GLU:HG2	5:B:1121:GLY:N	2.21	0.56
4:A:447:GLN:CB	4:A:448:PRO:HA	2.21	0.55
5:B:60:GLN:HA	5:B:60:GLN:HE21	1.69	0.55
6:C:69:LEU:HD23	11:J:6:ARG:HB2	1.88	0.55
6:C:166:GLU:HG2	12:K:10:PHE:HZ	1.70	0.55
5:B:315:LYS:N	5:B:316:PRO:HD2	2.21	0.55
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.87	0.55
5:B:1016:ALA:O	5:B:1017:ILE:HG12	2.06	0.55
6:C:67:LEU:HD13	6:C:157:CYS:SG	2.47	0.55
4:A:290:GLU:C	4:A:292:ALA:N	2.64	0.55
4:A:679:ILE:O	4:A:682:THR:HB	2.07	0.55
4:A:1392:SER:O	4:A:1399:ARG:HD3	2.07	0.55
5:B:364:ILE:HG22	5:B:365:THR:N	2.21	0.55
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.36	0.55
5:B:705:MET:H	5:B:710:LEU:HD12	1.72	0.55
6:C:10:ILE:HD13	6:C:20:PHE:HB3	1.88	0.55
4:A:91:PHE:HA	4:A:235:ILE:HG22	1.88	0.55
4:A:116:ASP:HA	4:A:117:GLU:CB	2.36	0.55
4:A:365:GLY:O	4:A:468:PHE:HA	2.06	0.55
5:B:850:LEU:O	5:B:851:PHE:HB2	2.06	0.55
4:A:567:LYS:CB	4:A:568:PRO:CD	2.84	0.55
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.39	0.55
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.41	0.55
5:B:597:MET:SD	5:B:624:LEU:HD11	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.88	0.55
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.05	0.55
11:J:18:TRP:CE2	11:J:22:LEU:HD11	2.41	0.55
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.37	0.55
4:A:475:THR:CG2	4:A:476:SER:N	2.70	0.55
4:A:1116:LEU:H	4:A:1308:THR:HG22	1.71	0.55
2:T:24:DG:OP1	5:B:857:ARG:NH2	2.40	0.55
5:B:581:PHE:HB2	5:B:625:LYS:HG3	1.89	0.55
7:E:5:ASN:HD21	7:E:52:ARG:H	1.55	0.55
11:J:3:VAL:HG21	11:J:18:TRP:CD2	2.41	0.55
4:A:374:LEU:C	4:A:436:ILE:HD13	2.31	0.55
4:A:711:ARG:O	4:A:714:PHE:HB3	2.07	0.55
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.41	0.55
11:J:14:VAL:HG21	11:J:49:MET:HG3	1.89	0.55
11:J:44:TYR:CD1	11:J:45:CYS:N	2.75	0.55
4:A:225:ASN:HD22	4:A:227:VAL:H	1.55	0.55
9:H:10:PHE:HB3	9:H:28:ALA:HB1	1.88	0.55
9:H:123:MET:CE	9:H:142:LEU:HD13	2.35	0.55
11:J:24:LEU:CD2	11:J:30:LEU:HD12	2.37	0.55
4:A:447:GLN:HB3	4:A:448:PRO:CA	2.28	0.55
5:B:992:ILE:CD1	12:K:67:PHE:HE2	2.20	0.55
4:A:49:LYS:CD	4:A:55:ASP:OD2	2.48	0.54
4:A:609:ASP:O	4:A:611:GLN:N	2.40	0.54
4:A:663:SER:HA	5:B:827:ILE:O	2.07	0.54
5:B:638:PHE:CE1	5:B:743:ILE:HD13	2.42	0.54
5:B:1106:ARG:CD	5:B:1126:GLY:O	2.50	0.54
2:T:18:DC:H2'	2:T:19:DG:C8	2.42	0.54
4:A:848:ILE:HA	4:A:857:ARG:O	2.07	0.54
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.88	0.54
6:C:67:LEU:HA	6:C:70:ILE:HG13	1.89	0.54
6:C:215:GLU:N	6:C:216:GLY:HA3	2.13	0.54
4:A:806:ARG:HH11	4:A:806:ARG:CG	2.19	0.54
7:E:177:ARG:HG2	7:E:215:MET:SD	2.47	0.54
4:A:106:VAL:CG1	4:A:107:CYS:H	2.21	0.54
4:A:117:GLU:C	4:A:118:HIS:O	2.48	0.54
6:C:102:GLN:HG2	6:C:154:LYS:HG3	1.89	0.54
7:E:124:VAL:HA	7:E:132:ILE:HD11	1.90	0.54
7:E:128:PRO:HB2	7:E:129:PRO:HD3	1.89	0.54
4:A:48:ALA:CB	4:A:49:LYS:HZ3	2.21	0.54
4:A:347:PHE:CE2	5:B:1107:ALA:HB1	2.43	0.54
4:A:376:TYR:C	4:A:376:TYR:CD2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:385:ILE:HG13	4:A:385:ILE:O	2.07	0.54
6:C:6:PRO:HB2	12:K:101:LEU:HD23	1.89	0.54
4:A:200:ARG:HH21	4:A:202:LEU:HA	1.71	0.54
4:A:475:THR:HG22	4:A:476:SER:N	2.23	0.54
4:A:839:ARG:HH11	4:A:839:ARG:HG3	1.71	0.54
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.88	0.54
5:B:769:TYR:O	5:B:770:GLN:C	2.51	0.54
7:E:130:ALA:CA	7:E:131:THR:CB	2.85	0.54
4:A:22:PHE:HB2	5:B:1211:ASN:CG	2.33	0.54
4:A:545:GLN:O	4:A:549:MET:HG3	2.07	0.54
5:B:277:LYS:CE	5:B:335:GLY:H	2.20	0.54
5:B:657:HIS:ND1	5:B:689:LEU:HD11	2.22	0.54
5:B:884:ARG:NH1	5:B:935:ARG:HE	2.06	0.54
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.89	0.54
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.21	0.54
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.43	0.54
5:B:785:TYR:C	5:B:787:VAL:H	2.16	0.54
5:B:1111:MET:HE2	5:B:1118:PRO:N	2.23	0.54
6:C:167:HIS:HD2	6:C:169:LYS:H	1.56	0.54
9:H:2:SER:CA	9:H:3:ASN:HB2	2.38	0.54
9:H:24:CYS:O	9:H:41:ASP:HA	2.07	0.54
9:H:78:SER:OG	9:H:79:TRP:N	2.41	0.54
4:A:352:VAL:HB	5:B:1099:VAL:CG1	2.38	0.54
4:A:494:SER:O	4:A:498:ARG:HG2	2.07	0.54
4:A:1435:PRO:O	4:A:1436:ILE:HD12	2.06	0.54
6:C:244:VAL:CG2	6:C:245:VAL:N	2.70	0.54
2:T:28:DT:H4'	4:A:318:SER:HA	1.90	0.54
4:A:380:VAL:O	4:A:428:TYR:HA	2.07	0.54
5:B:918:ILE:HG13	5:B:935:ARG:HH12	1.73	0.54
7:E:64:PRO:CD	7:E:76:GLY:HA2	2.38	0.54
10:I:116:ASN:HD22	10:I:117:LYS:HG3	1.72	0.54
11:J:44:TYR:C	11:J:44:TYR:HD1	2.16	0.54
4:A:14:VAL:N	4:A:1432:GLN:HE22	1.98	0.53
4:A:665:GLY:O	4:A:668:ASP:HB2	2.09	0.53
4:A:758:ILE:N	4:A:758:ILE:HD13	2.22	0.53
5:B:522:VAL:HG12	5:B:523:CYS:N	2.23	0.53
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.90	0.53
5:B:763:GLN:HG2	5:B:765:PRO:CD	2.38	0.53
4:A:152:VAL:HG22	4:A:163:SER:OG	2.08	0.53
4:A:215:SER:HB3	4:A:218:ASP:CB	2.37	0.53
4:A:387:ARG:O	4:A:391:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:879:GLU:O	4:A:881:GLN:N	2.41	0.53
4:A:1123:GLY:CA	4:A:1124:HIS:HB2	2.38	0.53
5:B:202:TYR:CD2	5:B:202:TYR:N	2.76	0.53
5:B:648:HIS:O	5:B:648:HIS:CG	2.61	0.53
5:B:1099:VAL:O	5:B:1102:LYS:HG2	2.08	0.53
5:B:1106:ARG:NH2	5:B:1111:MET:HE3	2.23	0.53
9:H:47:PHE:CB	9:H:95:TYR:HD1	2.20	0.53
5:B:955:THR:HG23	13:L:54:ARG:O	2.09	0.53
5:B:969:ARG:HB3	5:B:969:ARG:NH1	2.19	0.53
5:B:980:PHE:CZ	5:B:990:ILE:HD11	2.42	0.53
5:B:1156:ASP:HB3	5:B:1198:TYR:N	2.23	0.53
6:C:46:ILE:HA	6:C:159:ALA:HA	1.90	0.53
13:L:61:THR:HB	13:L:63:ARG:H	1.74	0.53
4:A:57:ARG:C	4:A:68:GLN:HG2	2.33	0.53
4:A:253:ASN:HD22	4:A:253:ASN:H	1.56	0.53
4:A:311:GLN:CB	4:A:312:PRO:CD	2.85	0.53
4:A:451:HIS:O	5:B:1137:CYS:HB3	2.07	0.53
5:B:424:LEU:O	5:B:428:ILE:HG12	2.09	0.53
5:B:757:PRO:HG3	5:B:983:ARG:NH2	2.23	0.53
5:B:994:TYR:HB2	5:B:999:MET:HE1	1.83	0.53
4:A:247:ARG:NH1	4:A:263:THR:HG23	2.22	0.53
4:A:1374:VAL:C	4:A:1376:THR:H	2.17	0.53
6:C:244:VAL:HG23	6:C:245:VAL:N	2.23	0.53
5:B:976:ILE:CG1	5:B:991:GLY:C	2.81	0.53
6:C:25:VAL:HG12	6:C:26:ASP:N	2.22	0.53
4:A:303:TYR:CD2	4:A:304:MET:HG3	2.44	0.53
4:A:531:ILE:HG13	4:A:653:VAL:HG21	1.91	0.53
5:B:592:ASN:OD1	5:B:594:ALA:HB3	2.09	0.53
5:B:796:LEU:O	5:B:799:PRO:HD3	2.08	0.53
5:B:558:LEU:C	5:B:560:GLU:H	2.16	0.53
7:E:89:GLY:O	7:E:120:ALA:HB2	2.09	0.53
10:I:53:GLY:HA3	10:I:90:GLN:HG3	1.90	0.53
12:K:24:ASP:CG	12:K:74:ARG:HH11	2.17	0.53
4:A:218:ASP:H	4:A:219:PHE:CB	2.14	0.53
4:A:465:TYR:CD1	12:K:67:PHE:CZ	2.96	0.53
4:A:1342:GLU:HG2	7:E:212:ARG:HH12	1.74	0.53
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.42	0.53
5:B:760:ASP:N	5:B:760:ASP:OD1	2.41	0.53
4:A:826:ASP:HA	4:A:829:VAL:HB	1.91	0.53
4:A:946:VAL:HG12	4:A:947:PHE:N	2.23	0.53
4:A:981:LEU:HD23	4:A:1039:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.09	0.53
5:B:654:ARG:N	5:B:657:HIS:HD2	2.03	0.53
5:B:850:LEU:HD21	5:B:1009:ASP:HB3	1.91	0.53
5:B:1201:LYS:C	5:B:1201:LYS:HD3	2.34	0.53
4:A:276:LEU:CD1	4:A:292:ALA:HB1	2.31	0.52
5:B:822:ASN:ND2	11:J:52:THR:HG21	2.16	0.52
5:B:848:ARG:NH1	11:J:8:PHE:O	2.42	0.52
5:B:863:GLU:HG2	5:B:962:LYS:O	2.10	0.52
5:B:211:VAL:O	5:B:480:SER:HA	2.10	0.52
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.92	0.52
6:C:167:HIS:CD2	6:C:169:LYS:H	2.28	0.52
5:B:836:GLU:O	5:B:838:SER:N	2.40	0.52
5:B:1029:CYS:HB2	5:B:1090:THR:CG2	2.40	0.52
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.42	0.52
6:C:88:CYS:O	6:C:88:CYS:SG	2.67	0.52
1:R:8:G:N2	2:T:22:DT:C2	2.78	0.52
4:A:341:MET:CG	4:A:1429:ILE:HG13	2.38	0.52
4:A:593:GLU:HB3	4:A:601:LYS:HZ2	1.73	0.52
5:B:100:PRO:HG3	5:B:172:ILE:HG13	1.91	0.52
5:B:317:CYS:HA	5:B:320:ASP:HB2	1.90	0.52
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.91	0.52
1:R:2:A:H2'	1:R:3:G:H8	1.74	0.52
5:B:836:GLU:C	5:B:838:SER:H	2.18	0.52
5:B:950:ASP:HB3	5:B:967:ARG:HG3	1.91	0.52
5:B:1029:CYS:HG	5:B:1086:PHE:HE2	1.57	0.52
6:C:12:GLU:H	6:C:19:ASP:HB3	1.75	0.52
9:H:47:PHE:CB	9:H:95:TYR:CD1	2.92	0.52
10:I:52:ILE:HA	10:I:54:GLU:H	1.75	0.52
4:A:72:GLU:HB3	4:A:76:GLU:HG2	1.91	0.52
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.74	0.52
4:A:839:ARG:CG	4:A:839:ARG:NH1	2.61	0.52
4:A:1166:ASP:O	4:A:1167:GLU:HB3	2.10	0.52
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	2.08	0.52
5:B:264:SER:HA	5:B:265:SER:O	2.09	0.52
5:B:779:GLY:HA2	5:B:796:LEU:HB2	1.91	0.52
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.39	0.52
4:A:618:GLU:O	4:A:622:VAL:HG12	2.09	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.09	0.52
5:B:115:GLN:O	5:B:119:LEU:HD12	2.10	0.52
4:A:74:MET:HA	4:A:74:MET:CE	2.40	0.52
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	2.08	0.52
5:B:637:LEU:HD11	5:B:740:HIS:CD2	2.45	0.52
8:F:103:MET:O	8:F:104:ASN:CB	2.56	0.52
8:F:111:LEU:HD12	8:F:111:LEU:H	1.75	0.52
4:A:356:ASP:OD1	5:B:833:TYR:CE2	2.62	0.52
4:A:1080:THR:HG22	4:A:1081:LEU:H	1.75	0.52
4:A:1107:VAL:HG12	4:A:1107:VAL:O	2.08	0.52
5:B:102:VAL:HG21	5:B:112:LEU:HD13	1.92	0.52
5:B:756:ILE:HD11	5:B:770:GLN:HB3	1.92	0.52
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.75	0.52
6:C:142:VAL:HG12	6:C:144:ILE:HD13	1.91	0.52
4:A:148:CYS:HB3	4:A:168:GLY:HA2	1.92	0.51
4:A:364:VAL:HB	4:A:458:HIS:HB3	1.92	0.51
4:A:401:GLY:C	4:A:435:HIS:ND1	2.67	0.51
4:A:629:LEU:HD22	4:A:633:VAL:HG23	1.92	0.51
4:A:858:ASN:O	4:A:861:GLY:N	2.40	0.51
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.25	0.51
5:B:313:MET:HE2	5:B:390:LEU:CG	2.39	0.51
5:B:638:PHE:CD2	5:B:653:VAL:HG21	2.45	0.51
7:E:157:SER:OG	7:E:160:GLU:HG3	2.10	0.51
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.91	0.51
12:K:38:GLU:O	12:K:69:ALA:O	2.27	0.51
12:K:42:LEU:CD2	12:K:46:ILE:HD12	2.41	0.51
4:A:1089:VAL:HB	4:A:1092:LYS:HB2	1.91	0.51
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.10	0.51
5:B:385:LEU:HD23	5:B:386:LEU:N	2.26	0.51
5:B:648:HIS:O	5:B:649:LYS:O	2.27	0.51
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.08	0.51
2:T:18:DC:H2'	2:T:19:DG:H8	1.74	0.51
4:A:816:HIS:O	4:A:817:ALA:C	2.54	0.51
5:B:322:PHE:HZ	10:I:30:ARG:HB2	1.74	0.51
5:B:944:THR:CB	5:B:1122:ARG:HH21	2.23	0.51
5:B:994:TYR:N	5:B:994:TYR:CD2	2.77	0.51
6:C:167:HIS:HB3	6:C:169:LYS:HG2	1.92	0.51
12:K:42:LEU:HD23	12:K:46:ILE:HD12	1.93	0.51
4:A:370:ILE:CG2	4:A:374:LEU:HD11	2.41	0.51
4:A:696:GLU:C	4:A:698:GLN:H	2.19	0.51
5:B:841:MET:HE3	5:B:990:ILE:HG12	1.92	0.51
5:B:1056:SER:O	5:B:1059:LEU:N	2.44	0.51
5:B:1085:ILE:HG22	5:B:1086:PHE:O	2.10	0.51
6:C:66:ARG:NH2	11:J:4:PRO:HA	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:180:TYR:O	6:C:181:ASP:HB3	2.09	0.51
12:K:7:PHE:C	12:K:9:LEU:H	2.18	0.51
13:L:58:LYS:O	13:L:59:ALA:HB3	2.10	0.51
4:A:102:VAL:O	4:A:106:VAL:HG23	2.11	0.51
4:A:367:PRO:CG	4:A:370:ILE:HD12	2.41	0.51
5:B:461:LEU:HD23	5:B:466:TRP:CZ3	2.46	0.51
5:B:485:ARG:NH1	5:B:491:THR:HG21	2.24	0.51
5:B:498:THR:HB	5:B:537:LYS:O	2.10	0.51
5:B:1172:ILE:HD13	5:B:1183:LYS:HG2	1.93	0.51
4:A:726:ARG:O	4:A:726:ARG:HG2	2.07	0.51
5:B:797:TYR:O	11:J:1:MET:HG2	2.11	0.51
5:B:1111:MET:HE2	5:B:1118:PRO:CA	2.40	0.51
4:A:109:HIS:H	4:A:210:ILE:HD12	1.76	0.51
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.91	0.51
5:B:850:LEU:CD1	11:J:8:PHE:CD1	2.93	0.51
4:A:370:ILE:O	4:A:374:LEU:HD12	2.10	0.51
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.46	0.51
5:B:287:ARG:NH1	5:B:324:ILE:O	2.40	0.51
5:B:887:HIS:HB3	5:B:888:GLY:O	2.10	0.51
5:B:915:THR:HB	5:B:934:LYS:HB3	1.93	0.51
5:B:1002:THR:HG22	5:B:1006:ILE:HB	1.91	0.51
5:B:1106:ARG:NH2	5:B:1111:MET:CE	2.74	0.51
7:E:22:MET:HB2	7:E:187:TYR:CE1	2.45	0.51
4:A:588:LEU:HD12	4:A:632:VAL:HG21	1.92	0.51
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.93	0.51
5:B:879:ARG:NH1	5:B:882:THR:CG2	2.58	0.51
11:J:1:MET:HG3	11:J:1:MET:O	2.11	0.51
5:B:956:THR:HB	13:L:46:VAL:CG2	2.40	0.51
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.46	0.51
10:I:28:GLU:HB3	10:I:35:VAL:HG13	1.93	0.51
4:A:55:ASP:N	4:A:56:PRO:CD	2.70	0.50
5:B:263:GLY:HA2	5:B:264:SER:C	2.36	0.50
5:B:653:VAL:HG13	5:B:689:LEU:HD13	1.93	0.50
6:C:101:LEU:HB3	6:C:155:LEU:CD1	2.41	0.50
7:E:99:HIS:CE1	7:E:103:LYS:HE2	2.47	0.50
4:A:14:VAL:O	4:A:15:LYS:HD3	2.11	0.50
4:A:86:LEU:HB2	4:A:237:THR:O	2.11	0.50
4:A:365:GLY:HA3	4:A:469:ARG:HG3	1.92	0.50
6:C:115:SER:C	6:C:117:ASP:H	2.19	0.50
7:E:55:ARG:CZ	7:E:113:GLN:OE1	2.59	0.50
13:L:28:LYS:HB2	13:L:39:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:68:GLN:NE2	4:A:68:GLN:O	2.44	0.50
4:A:68:GLN:O	4:A:70:CYS:N	2.37	0.50
4:A:591:PHE:HD2	4:A:595:THR:HB	1.75	0.50
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.47	0.50
5:B:854:LEU:HD22	5:B:969:ARG:HD3	1.92	0.50
6:C:73:GLN:HB3	6:C:131:HIS:H	1.75	0.50
7:E:164:LEU:HD13	7:E:211:TYR:CE2	2.46	0.50
9:H:98:TYR:C	9:H:118:PHE:HD2	2.19	0.50
4:A:102:VAL:HG11	4:A:211:PHE:HE1	1.76	0.50
4:A:341:MET:SD	4:A:1429:ILE:N	2.84	0.50
4:A:639:PRO:HD2	4:A:640:GLN:H	1.75	0.50
4:A:984:LYS:O	4:A:988:LEU:HB3	2.12	0.50
4:A:1446:ASP:HA	4:A:1447:GLU:HB2	1.93	0.50
5:B:58:THR:O	5:B:62:ILE:HG12	2.11	0.50
5:B:140:ILE:O	5:B:140:ILE:HG22	2.11	0.50
5:B:866:TYR:CB	5:B:867:GLY:HA2	2.42	0.50
7:E:51:GLY:HA2	7:E:52:ARG:C	2.36	0.50
7:E:72:PHE:N	7:E:72:PHE:CD1	2.80	0.50
10:I:117:LYS:HD3	10:I:118:ARG:NH2	2.26	0.50
4:A:378:GLU:OE2	4:A:434:ARG:HD3	2.12	0.50
5:B:879:ARG:HH11	5:B:882:THR:HG22	1.64	0.50
5:B:980:PHE:CE1	5:B:990:ILE:HD12	2.45	0.50
11:J:45:CYS:O	11:J:48:ARG:HG3	2.11	0.50
4:A:12:ARG:O	5:B:1194:ILE:HG22	2.11	0.50
4:A:465:TYR:HD1	12:K:67:PHE:CZ	2.30	0.50
4:A:605:MET:HE3	4:A:614:PHE:O	2.11	0.50
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.94	0.50
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.94	0.50
5:B:976:ILE:HD13	5:B:991:GLY:O	2.03	0.50
4:A:108:MET:O	4:A:109:HIS:HB2	2.10	0.50
4:A:1197:LEU:HD12	4:A:1209:MET:SD	2.52	0.50
8:F:90:ARG:HD2	8:F:155:LEU:HD21	1.94	0.50
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.93	0.50
1:R:9:G:O3'	5:B:979:LYS:NZ	2.45	0.50
4:A:344:ARG:HH21	5:B:1112:GLN:CD	2.20	0.50
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	2.46	0.50
4:A:672:ASP:HB2	4:A:675:THR:CB	2.41	0.50
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
5:B:464:GLY:O	5:B:466:TRP:N	2.45	0.50
5:B:744:HIS:CD2	5:B:746:SER:H	2.28	0.50
5:B:801:LYS:O	11:J:52:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1002:THR:HG23	5:B:1006:ILE:H	1.75	0.50
5:B:1090:THR:O	5:B:1091:TYR:C	2.54	0.50
6:C:180:TYR:O	6:C:180:TYR:CD1	2.65	0.50
7:E:164:LEU:HD23	7:E:165:LEU:N	2.26	0.50
12:K:56:VAL:HA	12:K:77:THR:HG22	1.92	0.50
11:J:48:ARG:HG2	11:J:48:ARG:NH1	2.24	0.50
1:R:1:A:C2	4:A:252:PHE:HB3	2.47	0.49
4:A:280:GLU:C	4:A:282:ASN:H	2.20	0.49
4:A:1135:ARG:HG2	4:A:1282:VAL:HG12	1.94	0.49
4:A:1293:SER:HB2	4:A:1299:VAL:CG2	2.42	0.49
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.76	0.49
13:L:67:PHE:O	13:L:68:GLU:C	2.55	0.49
2:T:13:DA:H2"	2:T:14:DC:C5	2.47	0.49
4:A:303:TYR:HD2	4:A:304:MET:HG3	1.77	0.49
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.94	0.49
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.13	0.49
4:A:758:ILE:HD13	4:A:758:ILE:H	1.77	0.49
4:A:848:ILE:O	4:A:1065:GLY:N	2.44	0.49
4:A:929:LEU:HD21	4:A:1028:THR:HG21	1.93	0.49
5:B:202:TYR:CD1	5:B:209:GLU:HB3	2.47	0.49
5:B:770:GLN:HG2	5:B:983:ARG:O	2.11	0.49
6:C:115:SER:C	6:C:117:ASP:N	2.70	0.49
6:C:241:ASP:HB3	12:K:109:TRP:CZ2	2.46	0.49
7:E:115:ASN:N	7:E:115:ASN:OD1	2.41	0.49
4:A:1042:PHE:CE2	4:A:1046:LEU:HD13	2.47	0.49
4:A:1434:ALA:HB1	4:A:1436:ILE:HD13	1.93	0.49
5:B:276:ILE:HD11	5:B:334:ILE:HG23	1.94	0.49
9:H:96:VAL:HG22	9:H:143:LEU:HG	1.94	0.49
4:A:64:ASN:C	4:A:66:LYS:H	2.20	0.49
4:A:307:ASP:C	4:A:308:ILE:HG13	2.37	0.49
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.47	0.49
4:A:1017:LEU:O	4:A:1020:CYS:HB2	2.13	0.49
4:A:1428:VAL:O	4:A:1431:GLY:N	2.44	0.49
5:B:707:PRO:O	5:B:711:GLU:HG2	2.12	0.49
6:C:57:VAL:HG11	11:J:60:PHE:HB2	1.85	0.49
4:A:185:TRP:HB2	4:A:199:LEU:HG	1.93	0.49
4:A:340:LEU:HD22	5:B:1200:ALA:HB2	1.95	0.49
4:A:370:ILE:HG23	4:A:374:LEU:HD11	1.95	0.49
4:A:440:ASP:O	4:A:460:VAL:HG23	2.11	0.49
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.27	0.49
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:759:PRO:CD	5:B:1046:PRO:HG3	2.43	0.49
5:B:769:TYR:O	5:B:771:SER:N	2.46	0.49
5:B:936:ASP:OD2	5:B:938:SER:HB2	2.12	0.49
7:E:93:MET:O	7:E:94:LYS:HG3	2.12	0.49
5:B:276:ILE:HD13	5:B:277:LYS:H	1.77	0.49
5:B:345:LYS:HB2	5:B:348:ARG:HE	1.78	0.49
5:B:821:GLN:HE22	11:J:8:PHE:HE1	1.61	0.49
5:B:1032:SER:C	5:B:1089:PRO:HG2	2.37	0.49
10:I:52:ILE:HA	10:I:54:GLU:N	2.27	0.49
4:A:405:VAL:HG23	4:A:415:LEU:HD11	1.95	0.49
4:A:464:PRO:HG2	12:K:67:PHE:CE1	2.48	0.49
4:A:1363:VAL:HG12	4:A:1364:ASN:N	2.28	0.49
5:B:850:LEU:HD22	5:B:1009:ASP:HB3	1.94	0.49
5:B:979:LYS:O	5:B:980:PHE:CD1	2.66	0.49
6:C:29:MET:HA	12:K:45:LEU:HD13	1.95	0.49
4:A:519:PRO:O	4:A:624:SER:HB2	2.12	0.49
5:B:834:ASN:HA	5:B:838:SER:HB3	1.95	0.49
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.94	0.49
5:B:1120:GLU:HG2	5:B:1121:GLY:H	1.77	0.49
8:F:93:ILE:HG22	8:F:94:LEU:N	2.28	0.49
1:R:10:C:OP1	5:B:987:LYS:CD	2.60	0.49
4:A:84:ILE:HD12	4:A:270:LEU:HD12	1.93	0.49
4:A:442:VAL:O	4:A:457:ALA:HA	2.12	0.49
4:A:760:GLN:HB3	4:A:804:TYR:HE1	1.78	0.49
4:A:899:VAL:HG12	4:A:929:LEU:HD13	1.95	0.49
5:B:546:SER:HA	5:B:612:GLU:OE2	2.12	0.49
9:H:137:GLN:HB3	9:H:139:ASN:H	1.78	0.49
4:A:548:ASN:OD1	12:K:60:ALA:HB1	2.12	0.49
4:A:941:LYS:CG	4:A:942:PHE:N	2.76	0.49
5:B:782:LEU:C	5:B:784:ASN:H	2.20	0.49
5:B:1084:GLN:NE2	6:C:192:TRP:H	2.07	0.49
11:J:8:PHE:N	11:J:49:MET:HE3	2.27	0.49
4:A:79:GLY:C	4:A:243:PRO:HG3	2.36	0.48
4:A:368:LYS:HD2	4:A:399:HIS:HB2	1.96	0.48
4:A:496:GLU:CB	8:F:95:GLY:HA3	2.43	0.48
4:A:662:PHE:O	5:B:828:ALA:HA	2.12	0.48
5:B:48:LEU:HD23	5:B:173:MET:SD	2.53	0.48
5:B:528:PRO:O	5:B:533:CYS:HB2	2.13	0.48
5:B:944:THR:HG23	5:B:945:GLU:HG3	1.95	0.48
5:B:1095:LEU:C	5:B:1096:ARG:O	2.54	0.48
6:C:147:LEU:HB3	6:C:151:GLN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1148:ILE:HD11	4:A:1198:ASP:HB2	1.94	0.48
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.27	0.48
5:B:484:ASN:ND2	5:B:484:ASN:C	2.70	0.48
5:B:1006:ILE:CG2	5:B:1007:VAL:H	2.26	0.48
5:B:1016:ALA:HB1	5:B:1020:ARG:NH1	2.28	0.48
6:C:142:VAL:N	11:J:16:ASP:HB3	2.13	0.48
4:A:43:GLU:HB3	4:A:50:ILE:HG23	1.94	0.48
4:A:741:ASN:ND2	4:A:743:VAL:H	2.11	0.48
4:A:784:LEU:C	4:A:786:HIS:H	2.22	0.48
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.27	0.48
4:A:1402:PHE:CD2	4:A:1403:GLU:HB2	2.48	0.48
4:A:49:LYS:C	4:A:50:ILE:HG13	2.37	0.48
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.95	0.48
4:A:117:GLU:O	4:A:123:ARG:HG2	2.13	0.48
5:B:278:GLN:CG	5:B:279:ASP:H	2.26	0.48
4:A:313:GLN:HB3	4:A:321:PRO:HA	1.95	0.48
4:A:340:LEU:CD2	5:B:1199:ALA:CB	2.92	0.48
4:A:540:PHE:CE1	9:H:43:ASN:ND2	2.81	0.48
4:A:774:ARG:NH2	4:A:792:TYR:O	2.45	0.48
5:B:523:CYS:SG	5:B:750:GLY:N	2.85	0.48
5:B:841:MET:HE3	5:B:990:ILE:HD13	1.94	0.48
5:B:1077:THR:HG22	6:C:27:LEU:HD21	1.95	0.48
7:E:93:MET:HG3	7:E:120:ALA:HB1	1.94	0.48
11:J:1:MET:H2	11:J:56:LEU:N	2.11	0.48
4:A:125:ALA:O	4:A:128:ILE:HG22	2.12	0.48
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.95	0.48
4:A:669:THR:HG22	4:A:762:SER:HB2	1.95	0.48
4:A:1219:THR:HG21	4:A:1271:ILE:CD1	2.43	0.48
5:B:1037:LEU:HB3	5:B:1062:HIS:NE2	2.27	0.48
5:B:1037:LEU:HB3	5:B:1062:HIS:HE2	1.79	0.48
7:E:204:THR:CG2	7:E:205:SER:N	2.76	0.48
4:A:775:ILE:CG1	4:A:797:LYS:O	2.62	0.48
5:B:174:LEU:HD11	5:B:204:ILE:HG13	1.94	0.48
5:B:213:ILE:HG23	5:B:497:ARG:HB3	1.95	0.48
5:B:1060:ARG:HB2	5:B:1066:SER:HB3	1.96	0.48
6:C:167:HIS:CD2	6:C:168:ALA:N	2.82	0.48
12:K:12:LEU:H	12:K:12:LEU:HD12	1.77	0.48
4:A:381:THR:CG2	4:A:382:PRO:HD2	2.44	0.48
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.49	0.48
4:A:1059:HIS:ND1	8:F:87:LYS:HG2	2.29	0.48
5:B:990:ILE:CG2	5:B:991:GLY:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:161:LYS:O	7:E:162:ARG:C	2.57	0.48
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.43	0.48
4:A:218:ASP:N	4:A:219:PHE:CB	2.74	0.48
4:A:360:GLU:OE1	4:A:360:GLU:HA	2.14	0.48
4:A:404:TYR:HA	4:A:413:ILE:O	2.13	0.48
4:A:541:ILE:HG22	4:A:545:GLN:NE2	2.28	0.48
4:A:1388:GLY:O	4:A:1391:ARG:HG3	2.14	0.48
5:B:26:THR:O	5:B:27:ALA:C	2.56	0.48
5:B:129:PHE:CE2	5:B:166:PHE:HB2	2.49	0.48
5:B:246:LYS:NZ	5:B:246:LYS:HB3	2.29	0.48
6:C:227:THR:C	6:C:228:PHE:CD1	2.92	0.48
7:E:163:GLU:O	7:E:166:LYS:N	2.46	0.48
7:E:167:ARG:C	7:E:169:ARG:H	2.22	0.48
11:J:1:MET:H2	11:J:56:LEU:H	1.60	0.48
4:A:494:SER:HB3	4:A:497:THR:OG1	2.13	0.48
4:A:550:LEU:HD13	4:A:556:TRP:CZ2	2.49	0.48
5:B:785:TYR:O	5:B:787:VAL:N	2.47	0.48
10:I:33:SER:O	10:I:35:VAL:HG23	2.14	0.48
12:K:32:VAL:CG2	12:K:74:ARG:HG3	2.42	0.48
4:A:553:VAL:HG23	4:A:652:VAL:HG22	1.96	0.47
4:A:718:VAL:HG12	4:A:719:VAL:N	2.28	0.47
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.45	0.47
5:B:901:PRO:HB3	5:B:950:ASP:O	2.14	0.47
8:F:116:ASP:HB3	8:F:119:ARG:HG3	1.95	0.47
9:H:137:GLN:HE21	9:H:139:ASN:HB2	1.78	0.47
4:A:619:LYS:O	4:A:623:GLY:HA3	2.14	0.47
5:B:827:ILE:HD11	5:B:1086:PHE:HD2	1.78	0.47
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.36	0.47
6:C:195:GLN:N	6:C:200:GLU:OE2	2.29	0.47
4:A:11:LEU:HB2	5:B:1193:GLN:HG3	1.95	0.47
4:A:75:ASN:O	4:A:76:GLU:HB2	2.13	0.47
4:A:577:ILE:HG13	4:A:578:LEU:N	2.29	0.47
5:B:778:MET:HE1	5:B:1094:ARG:HH12	1.77	0.47
5:B:975:GLN:O	5:B:977:GLY:N	2.44	0.47
5:B:988:GLY:O	5:B:989:THR:O	2.33	0.47
9:H:22:LYS:O	9:H:44:VAL:N	2.47	0.47
4:A:1147:THR:HG22	4:A:1197:LEU:CD2	2.44	0.47
5:B:364:ILE:HG21	5:B:374:LYS:HG2	1.96	0.47
9:H:81:PRO:O	9:H:82:PRO:C	2.57	0.47
12:K:35:PHE:N	12:K:35:PHE:CD1	2.82	0.47
4:A:92:HIS:O	4:A:92:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:336:ILE:CG1	4:A:337:ARG:N	2.58	0.47
4:A:388:LEU:HD22	4:A:432:VAL:HG11	1.95	0.47
4:A:474:VAL:HG22	4:A:478:TYR:CE1	2.50	0.47
4:A:1363:VAL:CG1	4:A:1364:ASN:N	2.77	0.47
5:B:860:MET:SD	5:B:861:ASP:N	2.87	0.47
5:B:942:ARG:HD2	5:B:945:GLU:CD	2.39	0.47
5:B:969:ARG:HE	6:C:59:ALA:HB1	1.78	0.47
12:K:63:VAL:HG23	12:K:63:VAL:O	2.14	0.47
4:A:338:GLY:O	4:A:339:ASN:OD1	2.32	0.47
4:A:590:ARG:HG3	4:A:590:ARG:HH11	1.80	0.47
4:A:612:ILE:O	4:A:612:ILE:HG13	2.14	0.47
4:A:1235:LYS:HB2	4:A:1237:ILE:CD1	2.45	0.47
4:A:1436:ILE:O	4:A:1437:GLY:C	2.56	0.47
5:B:126:SER:HB2	5:B:172:ILE:HD11	1.97	0.47
5:B:475:SER:C	5:B:477:ALA:N	2.72	0.47
7:E:144:ILE:HG13	7:E:145:THR:N	2.30	0.47
7:E:164:LEU:HD13	7:E:211:TYR:CD2	2.50	0.47
4:A:208:LEU:O	4:A:212:LYS:HB2	2.14	0.47
4:A:1235:LYS:HB2	4:A:1237:ILE:HD12	1.96	0.47
5:B:277:LYS:HB2	5:B:277:LYS:HE3	1.44	0.47
5:B:346:GLU:C	5:B:348:ARG:H	2.23	0.47
5:B:424:LEU:O	5:B:427:ASP:HB2	2.13	0.47
6:C:69:LEU:HD23	11:J:6:ARG:HD3	1.97	0.47
6:C:136:ASP:OD1	6:C:139:GLY:N	2.47	0.47
8:F:71:GLU:HA	8:F:72:LYS:HA	1.61	0.47
4:A:134:ARG:HD3	4:A:221:SER:O	2.15	0.47
4:A:344:ARG:NH2	5:B:1112:GLN:OE1	2.48	0.47
4:A:814:PHE:HE1	5:B:514:LEU:HD21	1.78	0.47
5:B:95:ILE:HG23	5:B:95:ILE:O	2.15	0.47
5:B:1037:LEU:HD21	11:J:44:TYR:CD2	2.49	0.47
6:C:242:GLN:HB3	6:C:246:ARG:HE	1.80	0.47
4:A:343:LYS:HZ1	5:B:1197:PRO:CB	2.17	0.47
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.49	0.47
5:B:769:TYR:C	5:B:771:SER:N	2.69	0.47
5:B:801:LYS:O	11:J:52:THR:CG2	2.63	0.47
4:A:121:LEU:HA	4:A:124:GLN:HE22	1.79	0.47
4:A:488:ASN:OD1	5:B:1128:LEU:HD13	2.15	0.47
5:B:276:ILE:HD13	5:B:277:LYS:N	2.30	0.47
5:B:278:GLN:HG2	5:B:279:ASP:H	1.80	0.47
5:B:1171:VAL:HG21	5:B:1191:ILE:HG23	1.96	0.47
5:B:1221:SER:C	5:B:1223:ASP:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:226:ASP:O	6:C:227:THR:HB	2.14	0.47
7:E:55:ARG:HG2	7:E:58:MET:HE2	1.97	0.47
4:A:382:PRO:HD3	4:A:428:TYR:HD2	1.79	0.46
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.97	0.46
4:A:871:ASP:HB3	7:E:204:THR:HG23	1.95	0.46
5:B:663:ALA:O	5:B:667:GLN:HB2	2.15	0.46
6:C:167:HIS:CG	6:C:169:LYS:HG2	2.50	0.46
7:E:89:GLY:HA2	7:E:117:THR:CG2	2.46	0.46
4:A:64:ASN:HB2	4:A:66:LYS:HG2	1.96	0.46
4:A:491:VAL:HA	4:A:492:PRO:HD2	1.78	0.46
4:A:775:ILE:CG1	4:A:798:GLY:HA3	2.45	0.46
4:A:1342:GLU:HG2	7:E:212:ARG:NH1	2.30	0.46
4:A:1344:GLY:O	4:A:1345:ARG:C	2.59	0.46
4:A:1397:LEU:HD22	4:A:1429:ILE:HD13	1.96	0.46
5:B:370:PHE:O	5:B:372:SER:N	2.48	0.46
5:B:649:LYS:O	5:B:650:GLU:HB2	2.15	0.46
5:B:804:GLY:HA2	5:B:1042:GLY:HA3	1.98	0.46
5:B:992:ILE:HD11	12:K:67:PHE:HE2	1.80	0.46
6:C:136:ASP:OD1	6:C:138:GLU:N	2.47	0.46
7:E:156:LEU:HD23	7:E:197:LYS:HB2	1.96	0.46
2:T:15:DT:H2''	2:T:16:DT:O5'	2.14	0.46
4:A:351:THR:HG21	4:A:467:THR:HA	1.98	0.46
4:A:951:GLU:OE1	4:A:951:GLU:HA	2.15	0.46
4:A:1083:THR:HB	4:A:1084:PHE:H	1.50	0.46
4:A:36:ARG:HB2	4:A:36:ARG:NH1	2.30	0.46
4:A:49:LYS:CB	4:A:49:LYS:HZ3	2.28	0.46
4:A:914:GLU:HB2	4:A:979:SER:O	2.15	0.46
5:B:190:TYR:CZ	11:J:62:ARG:HG2	2.50	0.46
5:B:278:GLN:HG2	5:B:279:ASP:N	2.31	0.46
5:B:383:ASN:ND2	5:B:383:ASN:C	2.72	0.46
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.98	0.46
6:C:54:ASN:O	6:C:54:ASN:CG	2.59	0.46
6:C:67:LEU:HA	6:C:70:ILE:CG1	2.46	0.46
7:E:167:ARG:HA	7:E:167:ARG:HD3	1.61	0.46
9:H:94:ASP:HB2	9:H:145:ARG:HA	1.98	0.46
2:T:9:DA:H2'	2:T:9:DA:OP2	2.16	0.46
4:A:64:ASN:HB3	4:A:66:LYS:HE2	1.97	0.46
4:A:403:LYS:C	4:A:404:TYR:CD1	2.93	0.46
5:B:269:ILE:O	5:B:282:ILE:HG23	2.15	0.46
5:B:308:TRP:HA	5:B:311:LEU:HB2	1.98	0.46
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:953:LEU:HD11	13:L:55:ILE:HG22	1.97	0.46
5:B:1170:THR:O	5:B:1171:VAL:C	2.58	0.46
4:A:340:LEU:CD2	5:B:1200:ALA:N	2.78	0.46
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.97	0.46
4:A:394:ASN:HB3	4:A:398:GLU:HB2	1.98	0.46
4:A:441:PRO:HG3	4:A:498:ARG:HB2	1.97	0.46
4:A:446:ARG:HD3	4:A:447:GLN:O	2.16	0.46
4:A:879:GLU:O	4:A:881:GLN:HG3	2.16	0.46
5:B:172:ILE:HD12	5:B:178:ASN:HD22	1.80	0.46
6:C:39:ALA:HA	6:C:164:ALA:CB	2.36	0.46
4:A:88:LYS:HA	4:A:89:PRO:HD2	1.64	0.46
4:A:354:SER:O	4:A:469:ARG:HA	2.16	0.46
4:A:531:ILE:O	4:A:535:THR:HB	2.16	0.46
4:A:567:LYS:HD3	9:H:95:TYR:CG	2.51	0.46
4:A:614:PHE:CD1	4:A:614:PHE:C	2.94	0.46
5:B:410:GLY:O	5:B:413:LEU:N	2.49	0.46
5:B:485:ARG:HH11	5:B:485:ARG:HG3	1.81	0.46
7:E:168:TYR:C	7:E:169:ARG:HG2	2.40	0.46
13:L:31:CYS:HA	13:L:56:LEU:HD23	1.98	0.46
1:R:2:A:H61	2:T:27:DT:H3	1.63	0.46
4:A:466:SER:CB	5:B:1100:ASP:OD1	2.64	0.46
4:A:741:ASN:C	4:A:741:ASN:ND2	2.73	0.46
4:A:1193:LEU:C	4:A:1193:LEU:HD12	2.41	0.46
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.98	0.46
5:B:563:MET:HE1	5:B:587:HIS:HB2	1.98	0.46
5:B:914:LYS:O	5:B:937:ALA:HB3	2.16	0.46
5:B:1002:THR:CG2	5:B:1006:ILE:H	2.29	0.46
6:C:53:THR:O	6:C:153:LEU:HA	2.15	0.46
6:C:186:LEU:CB	6:C:188:HIS:HD2	2.25	0.46
7:E:185:ALA:HA	7:E:190:LEU:HD12	1.98	0.46
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.96	0.46
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.80	0.46
12:K:6:ARG:O	12:K:9:LEU:HD12	2.16	0.46
4:A:34:LYS:HE2	4:A:57:ARG:NH2	2.31	0.46
4:A:92:HIS:HD2	4:A:94:GLY:H	1.64	0.46
4:A:214:ILE:CG2	4:A:215:SER:H	2.12	0.46
4:A:483:ASP:N	5:B:837:ASP:HB2	2.31	0.46
4:A:1407:GLU:HA	4:A:1410:PHE:HB2	1.98	0.46
5:B:350:GLN:O	5:B:353:LYS:N	2.49	0.46
5:B:520:GLY:HA3	5:B:635:ARG:HD2	1.98	0.46
5:B:778:MET:SD	5:B:794:ASN:HB3	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.51	0.46
5:B:843:GLN:HB3	5:B:995:ARG:HG3	1.97	0.46
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.51	0.46
6:C:31:ASN:O	6:C:33:LEU:N	2.49	0.46
6:C:79:GLN:HG3	6:C:127:ARG:CD	2.45	0.46
6:C:258:ILE:HG22	6:C:259:LEU:N	2.30	0.46
7:E:64:PRO:CG	7:E:76:GLY:HA2	2.45	0.46
1:R:8:G:C2	2:T:22:DT:C2	3.04	0.46
4:A:392:VAL:HG11	4:A:424:ILE:HG21	1.97	0.46
5:B:276:ILE:HG23	5:B:277:LYS:H	1.79	0.46
5:B:383:ASN:O	5:B:387:LEU:HB2	2.16	0.46
5:B:546:SER:N	5:B:634:TYR:HE2	2.14	0.46
5:B:681:TRP:O	5:B:684:LEU:N	2.49	0.46
5:B:763:GLN:CG	5:B:764:SER:N	2.76	0.46
8:F:90:ARG:O	8:F:91:ALA:C	2.57	0.46
10:I:115:LYS:HE2	10:I:115:LYS:HA	1.98	0.46
4:A:16:GLU:CD	4:A:1418:LEU:HD11	2.41	0.45
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.56	0.45
5:B:92:PHE:HD2	5:B:132:VAL:HG22	1.82	0.45
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.46	0.45
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.81	0.45
5:B:1162:ILE:HD13	5:B:1162:ILE:HA	1.76	0.45
8:F:85:MET:HE2	8:F:90:ARG:HA	1.98	0.45
9:H:42:ILE:HG21	9:H:49:VAL:CG2	2.45	0.45
4:A:49:LYS:HB2	4:A:49:LYS:NZ	2.31	0.45
4:A:403:LYS:HA	4:A:415:LEU:HB2	1.98	0.45
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	1.98	0.45
5:B:102:VAL:HG23	5:B:112:LEU:HD22	1.98	0.45
5:B:291:ILE:HD12	5:B:291:ILE:H	1.81	0.45
5:B:840:ILE:CG2	5:B:1011:ILE:HD12	2.42	0.45
5:B:1094:ARG:HG3	5:B:1094:ARG:O	2.16	0.45
5:B:1171:VAL:HG11	5:B:1191:ILE:HG21	1.98	0.45
6:C:124:LEU:O	6:C:127:ARG:HG2	2.16	0.45
7:E:89:GLY:O	7:E:120:ALA:CB	2.64	0.45
11:J:1:MET:O	11:J:2:ILE:HB	2.16	0.45
12:K:7:PHE:C	12:K:7:PHE:CD1	2.94	0.45
1:R:2:A:H2'	1:R:3:G:C8	2.52	0.45
4:A:37:PHE:HA	4:A:38:PRO:HD3	1.81	0.45
4:A:1116:LEU:H	4:A:1308:THR:CG2	2.28	0.45
5:B:101:MET:HE3	5:B:101:MET:HB2	1.91	0.45
5:B:782:LEU:HB3	5:B:784:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:130:ALA:CA	7:E:131:THR:HB	2.46	0.45
8:F:93:ILE:O	8:F:94:LEU:C	2.59	0.45
10:I:53:GLY:CA	10:I:90:GLN:HG3	2.46	0.45
11:J:2:ILE:HD12	11:J:3:VAL:H	1.81	0.45
11:J:56:LEU:O	11:J:57:ILE:C	2.57	0.45
13:L:34:CYS:HB3	13:L:51:CYS:SG	2.56	0.45
4:A:116:ASP:HA	4:A:117:GLU:HB2	1.98	0.45
4:A:464:PRO:O	4:A:465:TYR:CB	2.63	0.45
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.97	0.45
4:A:1187:GLN:NE2	4:A:1188:GLN:HG3	2.31	0.45
5:B:620:ARG:NH2	10:I:68:LEU:HD21	2.32	0.45
5:B:681:TRP:HA	5:B:684:LEU:HD12	1.97	0.45
5:B:841:MET:CE	5:B:990:ILE:HD11	2.33	0.45
5:B:841:MET:HE3	5:B:990:ILE:CG1	2.47	0.45
2:T:21:DC:H5''	5:B:1128:LEU:CD2	2.46	0.45
4:A:549:MET:O	4:A:550:LEU:C	2.56	0.45
4:A:693:VAL:HG21	4:A:721:PHE:HE1	1.81	0.45
4:A:1187:GLN:HE22	4:A:1188:GLN:HG3	1.82	0.45
5:B:57:TYR:CD1	5:B:57:TYR:N	2.84	0.45
5:B:871:THR:HG22	5:B:872:GLU:H	1.81	0.45
5:B:979:LYS:HE2	5:B:987:LYS:HG2	1.97	0.45
5:B:1027:ILE:O	5:B:1030:LEU:HB3	2.16	0.45
5:B:1029:CYS:HB2	5:B:1090:THR:HG23	1.98	0.45
13:L:41:SER:O	13:L:43:THR:N	2.45	0.45
1:R:9:G:H2'	1:R:10:C:C5	2.51	0.45
4:A:1115:SER:HB3	4:A:1330:ASN:ND2	2.32	0.45
4:A:1174:PHE:O	4:A:1174:PHE:CG	2.70	0.45
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.99	0.45
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.16	0.45
6:C:34:ARG:NH1	6:C:35:ARG:HG2	2.32	0.45
4:A:1038:THR:O	4:A:1039:LYS:C	2.59	0.45
4:A:1293:SER:HB2	4:A:1299:VAL:HG23	1.98	0.45
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.99	0.45
5:B:999:MET:HB3	5:B:1007:VAL:HG22	1.99	0.45
6:C:69:LEU:O	11:J:6:ARG:NH1	2.49	0.45
4:A:225:ASN:ND2	4:A:227:VAL:H	2.14	0.45
4:A:253:ASN:HD22	4:A:253:ASN:N	2.15	0.45
4:A:322:VAL:O	4:A:322:VAL:HG23	2.17	0.45
4:A:525:GLN:O	4:A:529:CYS:HB3	2.17	0.45
4:A:550:LEU:HD11	4:A:561:PRO:HD2	1.99	0.45
4:A:630:ILE:H	4:A:630:ILE:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:291:ILE:CD1	5:B:291:ILE:H	2.30	0.45
5:B:706:GLN:HB2	5:B:709:ASP:HB2	1.98	0.45
5:B:879:ARG:NE	5:B:879:ARG:CA	2.61	0.45
5:B:990:ILE:CG2	5:B:991:GLY:N	2.78	0.45
6:C:46:ILE:HG13	6:C:72:LEU:HD11	1.99	0.45
4:A:90:VAL:HB	4:A:297:GLN:NE2	2.29	0.45
4:A:453:MET:HE3	4:A:520:CYS:SG	2.57	0.45
4:A:517:ASN:ND2	4:A:1364:ASN:OD1	2.50	0.45
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.52	0.45
4:A:845:LEU:O	4:A:848:ILE:HG12	2.16	0.45
4:A:965:GLN:O	4:A:969:GLN:HB2	2.17	0.45
4:A:1134:ILE:H	4:A:1134:ILE:HD12	1.82	0.45
4:A:1449:SER:HA	4:A:1450:LEU:HA	1.58	0.45
5:B:548:GLY:HA3	5:B:630:ALA:HB2	1.99	0.45
5:B:792:MET:HG3	5:B:855:PHE:HE1	1.82	0.45
5:B:957:ASN:N	5:B:961:LEU:O	2.45	0.45
5:B:1188:LYS:HB2	5:B:1189:ILE:HG13	1.99	0.45
6:C:4:GLU:HG3	6:C:5:GLY:N	2.32	0.45
9:H:77:ARG:HB2	9:H:77:ARG:HH11	1.82	0.45
2:T:20:DC:H2'	2:T:21:DC:O4'	2.17	0.45
4:A:154:SER:HB2	4:A:161:LEU:HD12	1.99	0.45
4:A:718:VAL:O	4:A:721:PHE:N	2.50	0.45
5:B:303:TYR:CD2	5:B:303:TYR:N	2.83	0.45
5:B:361:LEU:CD2	5:B:377:PHE:CD2	2.93	0.45
6:C:31:ASN:C	6:C:33:LEU:N	2.75	0.45
6:C:226:ASP:O	6:C:227:THR:CB	2.65	0.45
1:R:9:G:C6	2:T:21:DC:N3	2.85	0.44
4:A:325:ILE:O	4:A:328:ARG:HB2	2.17	0.44
4:A:413:ILE:O	4:A:413:ILE:HG22	2.17	0.44
4:A:666:ILE:HD11	5:B:1023:VAL:HG12	1.99	0.44
4:A:741:ASN:HD22	4:A:743:VAL:H	1.65	0.44
4:A:1344:GLY:O	4:A:1347:ALA:N	2.49	0.44
5:B:213:ILE:O	5:B:214:ALA:C	2.60	0.44
5:B:557:PHE:C	5:B:557:PHE:CD2	2.96	0.44
5:B:762:ASN:HD22	5:B:762:ASN:HA	1.68	0.44
6:C:231:ASN:C	6:C:231:ASN:HD22	2.25	0.44
9:H:83:GLN:N	9:H:87:ARG:HG3	2.32	0.44
4:A:335:ARG:HH11	5:B:1202:LEU:HD12	1.82	0.44
4:A:391:LEU:HD12	4:A:400:PRO:C	2.41	0.44
4:A:451:HIS:O	5:B:1137:CYS:CB	2.65	0.44
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1155:ASP:HB3	4:A:1241:ARG:NH2	2.32	0.44
5:B:221:ASN:OD1	5:B:242:SER:HA	2.17	0.44
5:B:944:THR:HB	5:B:1122:ARG:HH21	1.81	0.44
5:B:1041:GLU:OE2	5:B:1041:GLU:HA	2.16	0.44
5:B:1078:GLY:O	6:C:180:TYR:HE2	1.99	0.44
5:B:1099:VAL:HB	5:B:1103:ILE:HD11	2.00	0.44
12:K:58:PHE:HE2	12:K:74:ARG:NE	2.06	0.44
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.74	0.44
4:A:1364:ASN:HD22	4:A:1366:ARG:H	1.65	0.44
8:F:79:ARG:HA	8:F:144:GLU:OE2	2.18	0.44
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.44
4:A:1308:THR:CG2	4:A:1309:ASP:N	2.80	0.44
5:B:619:ILE:HG21	10:I:62:ILE:HA	1.99	0.44
5:B:728:ARG:NH1	5:B:760:ASP:OD2	2.43	0.44
5:B:765:PRO:O	5:B:768:THR:N	2.50	0.44
5:B:845:SER:OG	5:B:846:ILE:N	2.50	0.44
5:B:866:TYR:CG	5:B:867:GLY:HA2	2.52	0.44
7:E:122:LYS:HE3	7:E:122:LYS:HA	2.00	0.44
10:I:84:VAL:HG13	10:I:85:PHE:N	2.31	0.44
4:A:225:ASN:HD22	4:A:228:PHE:H	1.64	0.44
4:A:381:THR:HG22	4:A:382:PRO:HD2	2.00	0.44
4:A:474:VAL:O	4:A:478:TYR:HD1	2.00	0.44
4:A:543:LEU:O	4:A:544:ASP:C	2.60	0.44
4:A:673:GLY:N	4:A:674:PRO:HD2	2.32	0.44
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.17	0.44
5:B:1017:ILE:HD12	5:B:1026:LEU:CD2	2.47	0.44
4:A:760:GLN:HB3	4:A:804:TYR:CE1	2.52	0.44
4:A:779:PHE:CE2	5:B:517:THR:HG22	2.52	0.44
4:A:925:LEU:HD22	4:A:983:ILE:HB	2.00	0.44
5:B:49:ASP:C	5:B:51:PHE:N	2.72	0.44
5:B:756:ILE:HA	5:B:757:PRO:HD3	1.46	0.44
5:B:800:GLN:O	5:B:801:LYS:C	2.57	0.44
8:F:97:ARG:HG3	8:F:101:ILE:CD1	2.45	0.44
11:J:7:CYS:CB	11:J:49:MET:HG2	2.30	0.44
2:T:16:DT:H3'	2:T:17:DA:C8	2.51	0.44
4:A:102:VAL:HG11	4:A:211:PHE:CE1	2.53	0.44
4:A:116:ASP:CA	4:A:117:GLU:CB	2.94	0.44
4:A:503:GLN:NE2	8:F:90:ARG:HH12	2.14	0.44
4:A:768:GLN:HB3	4:A:775:ILE:HD11	2.00	0.44
4:A:1121:GLU:O	4:A:1125:ALA:HB2	2.18	0.44
5:B:102:VAL:HG21	5:B:122:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:256:VAL:HG12	5:B:385:LEU:HD13	1.99	0.44
5:B:555:ILE:H	5:B:555:ILE:HG12	1.53	0.44
5:B:1006:ILE:HG22	5:B:1007:VAL:H	1.81	0.44
5:B:1111:MET:CE	5:B:1118:PRO:HD3	2.48	0.44
5:B:1117:GLN:HA	5:B:1118:PRO:HD2	1.70	0.44
5:B:1150:ARG:O	5:B:1150:ARG:CG	2.53	0.44
4:A:96:ILE:CG2	4:A:176:LYS:HE3	2.32	0.44
4:A:244:PRO:C	4:A:246:VAL:H	2.25	0.44
4:A:915:SER:OG	4:A:919:ILE:HD11	2.18	0.44
4:A:1428:VAL:O	4:A:1429:ILE:C	2.59	0.44
5:B:233:PRO:HG2	5:B:234:ILE:HD13	2.00	0.44
5:B:1072:MET:HE2	5:B:1085:ILE:CB	2.42	0.44
6:C:120:ILE:HG22	6:C:121:VAL:H	1.83	0.44
6:C:186:LEU:N	6:C:186:LEU:CD1	2.81	0.44
7:E:130:ALA:CB	7:E:131:THR:HB	2.47	0.44
1:R:3:G:N1	2:T:27:DT:O2	2.51	0.44
4:A:262:LEU:HD21	4:A:325:ILE:HD11	1.99	0.44
4:A:445:ASN:ND2	4:A:455:MET:SD	2.90	0.44
4:A:1198:ASP:OD2	4:A:1200:ALA:HB3	2.18	0.44
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.98	0.44
5:B:381:MET:O	5:B:382:ILE:C	2.60	0.44
5:B:792:MET:N	5:B:792:MET:HE3	2.32	0.44
6:C:168:ALA:C	6:C:170:TRP:N	2.72	0.44
10:I:18:GLU:HG2	10:I:20:LYS:H	1.83	0.44
12:K:60:ALA:O	12:K:73:LEU:HD12	2.18	0.44
4:A:182:VAL:HG12	4:A:183:GLY:N	2.26	0.43
4:A:356:ASP:HA	4:A:357:PRO:HD2	1.66	0.43
4:A:401:GLY:O	4:A:435:HIS:ND1	2.46	0.43
4:A:1206:ASP:HB2	4:A:1274:ARG:NH2	2.30	0.43
5:B:31:TRP:CZ3	5:B:747:MET:HE1	2.53	0.43
5:B:782:LEU:O	5:B:784:ASN:N	2.50	0.43
5:B:839:MET:CE	5:B:841:MET:HE3	2.48	0.43
5:B:839:MET:HE2	5:B:990:ILE:CG2	2.47	0.43
5:B:1158:PHE:CE2	5:B:1160:VAL:HG13	2.53	0.43
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.90	0.43
9:H:15:VAL:O	9:H:15:VAL:HG22	2.17	0.43
4:A:16:GLU:HA	4:A:1419:ASP:O	2.18	0.43
4:A:121:LEU:HA	4:A:124:GLN:NE2	2.34	0.43
4:A:265:LYS:HE2	4:A:302:THR:CG2	2.47	0.43
4:A:480:ALA:HB2	4:A:487:MET:HE2	1.99	0.43
4:A:754:SER:N	4:A:757:ASN:HD22	2.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1444:MET:HE3	4:A:1444:MET:HB2	1.71	0.43
5:B:766:ARG:HA	5:B:766:ARG:HD3	1.82	0.43
6:C:246:ARG:O	6:C:250:THR:OG1	2.34	0.43
7:E:61:GLN:HG3	7:E:105:PHE:CZ	2.52	0.43
9:H:10:PHE:HA	9:H:30:SER:HA	2.00	0.43
11:J:44:TYR:HD1	11:J:45:CYS:N	2.16	0.43
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.53	0.43
4:A:619:LYS:O	4:A:623:GLY:N	2.51	0.43
4:A:635:ARG:HA	4:A:635:ARG:NH1	2.31	0.43
7:E:55:ARG:C	7:E:57:MET:N	2.69	0.43
12:K:40:HIS:H	12:K:40:HIS:CD2	2.35	0.43
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.48	0.43
4:A:567:LYS:HG3	4:A:568:PRO:HG2	2.00	0.43
4:A:920:LEU:HD23	4:A:921:GLY:H	1.82	0.43
5:B:595:ARG:O	5:B:596:LEU:C	2.61	0.43
5:B:657:HIS:CE1	5:B:689:LEU:HD11	2.53	0.43
5:B:979:LYS:C	5:B:980:PHE:CD1	2.96	0.43
5:B:1175:LEU:O	5:B:1176:ASN:HB3	2.18	0.43
9:H:95:TYR:C	9:H:95:TYR:CD2	2.97	0.43
12:K:7:PHE:C	12:K:9:LEU:N	2.75	0.43
4:A:382:PRO:HA	4:A:385:ILE:HG22	2.01	0.43
4:A:397:ASN:HD22	4:A:397:ASN:HA	1.53	0.43
4:A:696:GLU:C	4:A:698:GLN:N	2.77	0.43
4:A:855:THR:O	4:A:855:THR:HG23	2.18	0.43
5:B:498:THR:CG2	5:B:499:ASN:N	2.80	0.43
5:B:578:THR:HG23	5:B:623:GLU:N	2.34	0.43
5:B:656:GLY:C	5:B:658:ILE:N	2.76	0.43
5:B:850:LEU:CD1	11:J:8:PHE:HD1	2.31	0.43
7:E:156:LEU:HD23	7:E:197:LYS:CB	2.48	0.43
7:E:167:ARG:C	7:E:169:ARG:N	2.77	0.43
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.49	0.43
11:J:44:TYR:C	11:J:47:ARG:H	2.27	0.43
4:A:514:PRO:O	4:A:515:GLN:C	2.60	0.43
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.54	0.43
5:B:769:TYR:C	5:B:771:SER:H	2.27	0.43
5:B:842:ASN:O	5:B:845:SER:N	2.49	0.43
9:H:83:GLN:O	9:H:85:GLY:N	2.52	0.43
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.54	0.43
4:A:315:LEU:HB3	4:A:316:GLN:H	1.30	0.43
4:A:673:GLY:O	4:A:677:ARG:HB2	2.19	0.43
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.99	0.43
5:B:581:PHE:HA	5:B:585:VAL:O	2.18	0.43
5:B:762:ASN:OD1	5:B:984:HIS:CD2	2.72	0.43
5:B:858:SER:HA	5:B:967:ARG:HA	2.00	0.43
5:B:916:THR:HA	5:B:917:PRO:HD2	1.91	0.43
5:B:956:THR:HG22	13:L:54:ARG:HD3	2.01	0.43
7:E:156:LEU:CD2	7:E:197:LYS:HB2	2.49	0.43
8:F:99:LEU:O	8:F:99:LEU:HD13	2.17	0.43
4:A:332:LYS:O	4:A:334:GLY:N	2.43	0.43
4:A:336:ILE:C	4:A:338:GLY:H	2.27	0.43
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	2.01	0.43
4:A:1434:ALA:HB3	4:A:1436:ILE:HB	2.00	0.43
5:B:1033:LYS:HG2	5:B:1059:LEU:HD11	2.00	0.43
7:E:196:VAL:HG12	7:E:212:ARG:HB2	2.00	0.43
4:A:71:GLN:O	4:A:73:GLY:N	2.52	0.43
4:A:115:LEU:HD12	4:A:122:MET:HE3	2.00	0.43
4:A:806:ARG:HG3	5:B:728:ARG:HA	2.01	0.43
4:A:1396:ALA:HA	4:A:1399:ARG:NH2	2.34	0.43
5:B:57:TYR:O	5:B:60:GLN:N	2.51	0.43
5:B:190:TYR:CD1	11:J:62:ARG:HG2	2.53	0.43
5:B:549:THR:HG22	5:B:550:ASP:H	1.84	0.43
5:B:1106:ARG:HG3	5:B:1108:ARG:O	2.19	0.43
6:C:186:LEU:HB2	6:C:188:HIS:CD2	2.45	0.43
10:I:19:ASP:O	10:I:21:GLU:N	2.44	0.43
11:J:64:ASN:N	11:J:65:PRO:HD2	2.34	0.43
13:L:32:ALA:CB	13:L:55:ILE:HB	2.46	0.43
4:A:206:GLU:O	4:A:210:ILE:HG12	2.19	0.43
4:A:418:SER:C	4:A:420:ARG:H	2.27	0.43
4:A:535:THR:HG23	4:A:616:VAL:HA	2.00	0.43
4:A:543:LEU:HG	4:A:547:LEU:CD1	2.44	0.43
5:B:65:GLU:OE2	5:B:66:ASP:HB3	2.19	0.43
5:B:514:LEU:HD12	5:B:518:HIS:CD2	2.54	0.43
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	2.00	0.43
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	2.00	0.43
9:H:4:THR:HG22	9:H:5:LEU:N	2.33	0.43
12:K:15:GLY:O	12:K:16:GLU:C	2.62	0.43
4:A:11:LEU:HA	5:B:1193:GLN:O	2.18	0.42
4:A:49:LYS:CB	4:A:49:LYS:NZ	2.81	0.42
4:A:325:ILE:H	4:A:325:ILE:HG12	1.55	0.42
4:A:541:ILE:HG13	4:A:546:VAL:HG22	2.01	0.42
5:B:367:LEU:HB3	5:B:368:GLU:H	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:680:THR:O	5:B:682:SER:N	2.51	0.42
6:C:34:ARG:O	6:C:38:ILE:HG12	2.19	0.42
6:C:84:ARG:HD2	12:K:11:LEU:HD21	2.01	0.42
6:C:254:LYS:HD3	12:K:42:LEU:HD12	2.01	0.42
4:A:417:TYR:O	4:A:418:SER:CB	2.67	0.42
4:A:849:MET:HB3	4:A:1063:MET:SD	2.59	0.42
4:A:1029:ARG:O	4:A:1033:GLN:HB2	2.19	0.42
5:B:557:PHE:O	5:B:560:GLU:HB2	2.19	0.42
5:B:769:TYR:H	5:B:769:TYR:HD2	1.66	0.42
6:C:215:GLU:H	6:C:216:GLY:CA	2.25	0.42
11:J:59:LYS:O	11:J:62:ARG:HB3	2.18	0.42
4:A:464:PRO:CG	12:K:67:PHE:CD1	3.03	0.42
4:A:535:THR:O	4:A:536:LEU:C	2.61	0.42
4:A:553:VAL:HA	4:A:554:PRO:HD3	1.91	0.42
4:A:648:ASN:O	4:A:652:VAL:HG23	2.19	0.42
5:B:471:LYS:O	5:B:476:ARG:HD3	2.19	0.42
6:C:54:ASN:C	6:C:56:THR:N	2.77	0.42
7:E:61:GLN:HG3	7:E:105:PHE:CE2	2.55	0.42
13:L:41:SER:C	13:L:43:THR:H	2.27	0.42
2:T:9:DA:H2"	2:T:10:DA:OP2	2.19	0.42
4:A:639:PRO:HD2	4:A:640:GLN:HG2	2.00	0.42
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	2.94	0.42
4:A:1072:ILE:HD13	4:A:1371:LEU:HD22	2.00	0.42
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.02	0.42
5:B:955:THR:CG2	5:B:956:THR:N	2.77	0.42
6:C:25:VAL:HG12	6:C:26:ASP:H	1.83	0.42
13:L:47:ARG:HG3	13:L:48:CYS:H	1.84	0.42
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.34	0.42
5:B:350:GLN:O	5:B:351:TYR:C	2.62	0.42
5:B:594:ALA:HA	5:B:617:ARG:NH1	2.34	0.42
5:B:781:PHE:HE2	5:B:795:ILE:HD11	1.84	0.42
5:B:832:GLY:O	5:B:835:GLN:HG3	2.18	0.42
5:B:951:GLN:C	5:B:952:VAL:HG23	2.43	0.42
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.52	0.42
10:I:85:PHE:CD1	10:I:85:PHE:C	2.98	0.42
12:K:62:LYS:O	12:K:62:LYS:HG3	2.20	0.42
4:A:821:ARG:O	4:A:822:GLU:C	2.62	0.42
4:A:900:ASP:HA	4:A:926:GLN:HE22	1.85	0.42
4:A:908:LEU:O	4:A:909:ASP:C	2.62	0.42
10:I:79:HIS:O	10:I:80:SER:C	2.63	0.42
10:I:96:SER:HB2	10:I:98:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:65:HIS:CD2	12:K:67:PHE:H	2.30	0.42
12:K:105:PHE:CD2	12:K:105:PHE:C	2.98	0.42
13:L:61:THR:HG21	13:L:63:ARG:HG3	2.01	0.42
4:A:299:HIS:O	4:A:300:VAL:C	2.62	0.42
4:A:778:GLY:HA3	5:B:516:ASN:CG	2.45	0.42
4:A:826:ASP:HB2	4:A:1082:ASN:HD21	1.84	0.42
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	2.02	0.42
5:B:380:TYR:CD2	5:B:380:TYR:C	2.97	0.42
5:B:544:CYS:C	5:B:545:ILE:HD12	2.44	0.42
5:B:1084:GLN:NE2	6:C:191:TYR:HD2	2.17	0.42
5:B:1099:VAL:O	5:B:1103:ILE:HG12	2.19	0.42
6:C:145:CYS:SG	6:C:146:LYS:N	2.93	0.42
8:F:93:ILE:HD11	8:F:134:ILE:CD1	2.49	0.42
9:H:139:ASN:HB3	9:H:140:ALA:H	1.53	0.42
2:T:26:DC:H2''	2:T:27:DT:C5'	2.50	0.42
4:A:366:VAL:HA	4:A:367:PRO:HD2	1.72	0.42
4:A:589:GLN:HG3	4:A:606:LEU:HD13	2.01	0.42
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.19	0.42
5:B:60:GLN:HE21	5:B:60:GLN:CA	2.32	0.42
5:B:240:ILE:O	5:B:240:ILE:HG23	2.19	0.42
5:B:596:LEU:HD12	5:B:596:LEU:O	2.20	0.42
5:B:805:THR:HA	5:B:809:MET:CE	2.49	0.42
5:B:970:THR:HG22	5:B:971:THR:N	2.35	0.42
6:C:186:LEU:CB	6:C:188:HIS:CD2	3.03	0.42
7:E:92:THR:C	7:E:94:LYS:H	2.27	0.42
8:F:81:THR:HG23	8:F:144:GLU:OE1	2.20	0.42
10:I:89:GLN:O	10:I:91:ARG:N	2.53	0.42
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.55	0.42
5:B:54:PHE:HA	5:B:58:THR:HB	2.01	0.42
5:B:332:ASP:O	5:B:333:PHE:C	2.63	0.42
5:B:637:LEU:HD11	5:B:740:HIS:HD2	1.82	0.42
5:B:653:VAL:H	5:B:653:VAL:HG23	1.58	0.42
5:B:656:GLY:O	5:B:658:ILE:N	2.52	0.42
5:B:1155:SER:HB3	5:B:1156:ASP:H	1.46	0.42
6:C:11:ARG:NH1	6:C:209:TYR:CE1	2.88	0.42
6:C:167:HIS:HD2	6:C:168:ALA:N	2.18	0.42
6:C:254:LYS:CD	12:K:42:LEU:HD12	2.50	0.42
4:A:99:ILE:CD1	4:A:234:MET:HB3	2.50	0.42
4:A:211:PHE:O	4:A:214:ILE:HG12	2.19	0.42
4:A:211:PHE:CD1	4:A:231:PRO:HB2	2.51	0.42
4:A:353:ILE:HD12	4:A:482:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:482:PHE:HD1	5:B:836:GLU:O	2.03	0.42
4:A:697:ALA:HA	4:A:702:LEU:HB2	2.01	0.42
4:A:1072:ILE:O	4:A:1075:PRO:HD2	2.19	0.42
4:A:1220:PHE:N	4:A:1220:PHE:CD1	2.88	0.42
4:A:1337:GLU:O	7:E:183:PRO:HG3	2.20	0.42
5:B:261:ARG:HB3	5:B:262:GLU:H	1.67	0.42
5:B:287:ARG:C	5:B:289:LEU:N	2.78	0.42
5:B:386:LEU:C	5:B:388:CYS:N	2.78	0.42
5:B:448:ILE:HD13	5:B:448:ILE:HA	1.63	0.42
5:B:901:PRO:HG3	5:B:952:VAL:HG23	2.02	0.42
5:B:973:ILE:HD12	5:B:973:ILE:N	2.32	0.42
7:E:180:ARG:HB2	7:E:215:MET:OXT	2.20	0.42
9:H:77:ARG:HB2	9:H:77:ARG:CZ	2.49	0.42
12:K:58:PHE:CE2	12:K:74:ARG:NE	2.74	0.42
4:A:465:TYR:CE1	12:K:67:PHE:CZ	3.08	0.41
4:A:541:ILE:H	4:A:541:ILE:HG12	1.81	0.41
4:A:921:GLY:O	4:A:922:ASP:HB3	2.20	0.41
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.35	0.41
5:B:280:ILE:HB	5:B:285:ILE:HD11	2.01	0.41
5:B:435:THR:C	5:B:437:GLU:N	2.77	0.41
5:B:475:SER:C	5:B:477:ALA:H	2.27	0.41
5:B:641:GLU:HG3	5:B:642:ASP:H	1.85	0.41
5:B:778:MET:O	5:B:819:ALA:CB	2.58	0.41
5:B:785:TYR:C	5:B:787:VAL:N	2.75	0.41
6:C:57:VAL:CG1	6:C:57:VAL:O	2.68	0.41
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.80	0.41
4:A:260:ASP:OD1	4:A:262:LEU:N	2.51	0.41
4:A:344:ARG:NE	5:B:1118:PRO:O	2.37	0.41
4:A:356:ASP:OD2	12:K:65:HIS:HE1	2.03	0.41
4:A:877:HIS:CD2	4:A:877:HIS:N	2.88	0.41
4:A:1363:VAL:HB	4:A:1368:MET:HE2	2.03	0.41
5:B:417:PHE:O	5:B:418:LYS:C	2.62	0.41
5:B:757:PRO:HG3	5:B:983:ARG:NH1	2.35	0.41
6:C:31:ASN:O	6:C:35:ARG:HG3	2.20	0.41
9:H:47:PHE:HA	9:H:48:PRO:HD2	1.94	0.41
2:T:13:DA:N3	3:N:3:DA:N1	2.69	0.41
4:A:613:ILE:HG21	9:H:102:TYR:CG	2.55	0.41
4:A:658:LEU:HD23	4:A:659:HIS:NE2	2.34	0.41
4:A:818:MET:HE2	4:A:818:MET:HB3	1.85	0.41
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.55	0.41
4:A:837:ILE:HD13	4:A:837:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:886:ILE:HD11	4:A:943:LEU:HB2	1.99	0.41
4:A:1376:THR:HG23	7:E:212:ARG:NH2	2.35	0.41
5:B:839:MET:HE2	5:B:990:ILE:HG23	2.02	0.41
5:B:1059:LEU:HA	5:B:1059:LEU:HD12	1.81	0.41
5:B:1188:LYS:HE3	5:B:1189:ILE:HD11	2.02	0.41
5:B:1200:ALA:HA	5:B:1203:LEU:HB3	2.01	0.41
7:E:85:GLU:C	7:E:113:GLN:HE21	2.27	0.41
9:H:23:VAL:CG1	9:H:24:CYS:N	2.83	0.41
12:K:73:LEU:HD12	12:K:73:LEU:HA	1.83	0.41
1:R:3:G:C4	1:R:4:A:C8	3.08	0.41
4:A:423:ASP:CG	4:A:424:ILE:N	2.78	0.41
4:A:513:SER:O	4:A:514:PRO:C	2.63	0.41
4:A:1266:THR:O	4:A:1270:ASN:HB2	2.20	0.41
4:A:1313:LEU:O	4:A:1315:GLU:N	2.53	0.41
5:B:486:TYR:C	5:B:486:TYR:CD1	2.97	0.41
5:B:773:MET:C	5:B:775:LYS:N	2.77	0.41
5:B:984:HIS:ND1	5:B:1025:HIS:HB2	2.36	0.41
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.52	0.41
7:E:204:THR:HG23	7:E:205:SER:HB3	2.02	0.41
1:R:6:C:H2'	1:R:7:A:H8	1.85	0.41
4:A:344:ARG:O	5:B:1118:PRO:HG2	2.20	0.41
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.56	0.41
4:A:949:ASP:OD1	4:A:949:ASP:N	2.48	0.41
4:A:1389:PHE:O	4:A:1392:SER:HB3	2.21	0.41
5:B:416:LEU:HD22	5:B:420:LEU:CD1	2.50	0.41
5:B:905:VAL:O	5:B:946:ASN:HB2	2.20	0.41
5:B:1109:GLY:HA3	5:B:1110:PRO:HD2	1.91	0.41
5:B:1178:ASN:HD22	5:B:1178:ASN:HA	1.66	0.41
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.56	0.41
10:I:98:VAL:CG1	10:I:113:ASP:HB2	2.50	0.41
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.50	0.41
5:B:404:LYS:O	5:B:405:ARG:HD3	2.20	0.41
5:B:473:MET:HE3	5:B:473:MET:HB2	1.87	0.41
5:B:897:GLY:C	5:B:898:LEU:HD23	2.46	0.41
5:B:978:ASP:O	5:B:980:PHE:CE1	2.72	0.41
6:C:101:LEU:HB3	6:C:155:LEU:HD12	2.01	0.41
6:C:265:MET:HE3	6:C:265:MET:HB2	2.00	0.41
10:I:71:SER:HG	10:I:83:ASN:HD21	1.65	0.41
4:A:243:PRO:HB2	4:A:244:PRO:CD	2.51	0.41
4:A:845:LEU:O	4:A:847:ASP:N	2.54	0.41
4:A:1175:SER:HA	4:A:1176:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:7:CYS:HA	11:J:49:MET:CG	2.51	0.41
12:K:65:HIS:HD2	12:K:66:PRO:CD	2.26	0.41
4:A:455:MET:HB3	5:B:1141:HIS:HE1	1.86	0.41
4:A:508:PRO:C	4:A:510:GLN:N	2.73	0.41
4:A:811:GLN:HE21	4:A:811:GLN:HB2	1.42	0.41
4:A:1030:ARG:HG2	4:A:1034:GLU:OE2	2.21	0.41
4:A:1141:THR:CG2	4:A:1205:LYS:HD3	2.51	0.41
4:A:1205:LYS:HB3	4:A:1274:ARG:NH1	2.35	0.41
5:B:817:LEU:HD23	5:B:817:LEU:HA	1.86	0.41
5:B:880:THR:C	5:B:882:THR:N	2.78	0.41
5:B:956:THR:CB	13:L:46:VAL:HG21	2.43	0.41
5:B:978:ASP:CB	5:B:980:PHE:HE1	2.34	0.41
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.55	0.41
6:C:82:TYR:O	6:C:83:SER:C	2.64	0.41
6:C:241:ASP:CB	12:K:109:TRP:CE2	3.04	0.41
9:H:10:PHE:HE2	9:H:36:CYS:SG	2.43	0.41
4:A:272:ALA:C	4:A:296:LEU:HD12	2.46	0.41
4:A:434:ARG:NH2	4:A:440:ASP:OD1	2.46	0.41
4:A:447:GLN:HA	4:A:448:PRO:C	2.44	0.41
4:A:497:THR:HG23	5:B:1146:PHE:HA	2.02	0.41
4:A:608:ILE:O	4:A:609:ASP:O	2.38	0.41
4:A:639:PRO:CD	4:A:640:GLN:H	2.34	0.41
4:A:896:ARG:HB3	4:A:897:TYR:HD1	1.86	0.41
4:A:896:ARG:NH1	4:A:897:TYR:HE1	2.18	0.41
4:A:1242:VAL:CG1	4:A:1243:VAL:N	2.84	0.41
4:A:1266:THR:O	4:A:1267:MET:C	2.64	0.41
5:B:164:LYS:O	5:B:165:VAL:HB	2.20	0.41
5:B:173:MET:HE3	5:B:173:MET:HB2	1.99	0.41
5:B:244:LEU:CD1	5:B:366:GLN:HE22	2.34	0.41
5:B:264:SER:HA	5:B:265:SER:HB2	2.03	0.41
5:B:346:GLU:C	5:B:348:ARG:N	2.79	0.41
5:B:778:MET:HG2	5:B:794:ASN:HB3	2.02	0.41
5:B:830:TYR:HB3	5:B:831:SER:H	1.56	0.41
7:E:88:VAL:HB	7:E:116:ILE:HD13	2.02	0.41
8:F:89:GLU:HG2	8:F:134:ILE:HD12	2.03	0.41
10:I:61:ASP:OD2	10:I:61:ASP:N	2.54	0.41
4:A:92:HIS:C	4:A:92:HIS:HD2	2.29	0.41
4:A:465:TYR:N	12:K:2:ASN:O	2.29	0.41
4:A:705:LYS:HD2	4:A:713:SER:HB2	2.03	0.41
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	3.03	0.41
5:B:244:LEU:HD21	5:B:366:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:617:ARG:CG	5:B:618:ASP:N	2.83	0.41
5:B:842:ASN:O	5:B:843:GLN:C	2.62	0.41
5:B:848:ARG:HH22	5:B:996:ARG:NH1	2.18	0.41
5:B:951:GLN:C	5:B:952:VAL:CG2	2.94	0.41
5:B:951:GLN:O	5:B:952:VAL:CG2	2.69	0.41
6:C:134:ILE:HG23	6:C:141:GLY:H	1.85	0.41
8:F:85:MET:O	8:F:155:LEU:HD22	2.21	0.41
4:A:482:PHE:CD1	4:A:482:PHE:N	2.88	0.40
5:B:40:GLU:CD	5:B:681:TRP:HB3	2.45	0.40
5:B:49:ASP:O	5:B:50:SER:C	2.64	0.40
5:B:275:TYR:HB3	5:B:355:ILE:HD11	2.03	0.40
5:B:287:ARG:C	5:B:289:LEU:H	2.28	0.40
5:B:299:GLU:OE2	5:B:572:HIS:HB3	2.21	0.40
5:B:557:PHE:CZ	5:B:561:TRP:CD1	3.09	0.40
5:B:1013:ASN:HA	5:B:1014:PRO:HD2	1.70	0.40
5:B:1090:THR:O	5:B:1092:TYR:HD1	2.04	0.40
7:E:89:GLY:HA2	7:E:117:THR:HG23	2.03	0.40
9:H:4:THR:HG22	9:H:5:LEU:H	1.84	0.40
9:H:45:GLU:HG2	9:H:45:GLU:O	2.20	0.40
11:J:3:VAL:HA	11:J:4:PRO:HD2	1.94	0.40
13:L:34:CYS:O	13:L:35:SER:HB2	2.20	0.40
1:R:4:A:C4	1:R:5:C:C5	3.10	0.40
4:A:315:LEU:HD23	4:A:320:ARG:NH2	2.36	0.40
4:A:376:TYR:HA	4:A:377:PRO:HD3	1.81	0.40
4:A:709:THR:HG22	4:A:710:LEU:N	2.36	0.40
4:A:821:ARG:O	4:A:825:ILE:HG12	2.21	0.40
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.36	0.40
4:A:1123:GLY:C	4:A:1125:ALA:H	2.29	0.40
5:B:37:PHE:HD1	5:B:681:TRP:CZ2	2.39	0.40
5:B:57:TYR:O	5:B:59:LEU:N	2.54	0.40
5:B:264:SER:HA	5:B:265:SER:C	2.45	0.40
5:B:370:PHE:HD2	5:B:373:ARG:HD2	1.87	0.40
5:B:383:ASN:C	5:B:383:ASN:HD22	2.29	0.40
5:B:526:GLU:OE1	5:B:752:ALA:HB3	2.21	0.40
6:C:148:ARG:H	6:C:151:GLN:HG3	1.87	0.40
6:C:202:PRO:O	6:C:203:GLN:C	2.64	0.40
9:H:139:ASN:HD22	9:H:139:ASN:HA	1.70	0.40
10:I:86:PHE:CD2	10:I:86:PHE:N	2.88	0.40
13:L:46:VAL:HG12	13:L:47:ARG:N	2.35	0.40
4:A:756:ILE:HD13	4:A:756:ILE:N	2.36	0.40
4:A:1152:ILE:HB	10:I:44:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:46:GLN:H	5:B:46:GLN:HG3	1.63	0.40
5:B:1057:LYS:O	5:B:1061:GLU:HG2	2.21	0.40
9:H:47:PHE:HB2	9:H:95:TYR:CD1	2.50	0.40
4:A:108:MET:O	4:A:109:HIS:CB	2.69	0.40
4:A:146:MET:H	4:A:146:MET:CE	2.32	0.40
4:A:299:HIS:O	4:A:301:ALA:N	2.54	0.40
4:A:471:ASN:O	4:A:474:VAL:HG12	2.22	0.40
5:B:658:ILE:HA	5:B:658:ILE:HD12	1.93	0.40
5:B:911:ILE:HD11	5:B:941:LEU:CD1	2.45	0.40
5:B:1207:LEU:HD23	5:B:1207:LEU:HA	1.79	0.40
6:C:148:ARG:HB3	6:C:151:GLN:HG3	2.03	0.40
7:E:16:PHE:CZ	7:E:20:LYS:HE2	2.56	0.40
4:A:219:PHE:HZ	4:A:230:ARG:HD3	1.87	0.40
4:A:1075:PRO:O	4:A:1078:GLN:N	2.47	0.40
4:A:1407:GLU:O	4:A:1411:GLU:HG2	2.21	0.40
5:B:287:ARG:HA	5:B:291:ILE:O	2.22	0.40
5:B:402:GLY:HA3	5:B:695:ALA:HB3	2.04	0.40
5:B:638:PHE:HD2	5:B:653:VAL:HG21	1.86	0.40
5:B:745:PRO:O	5:B:748:ILE:HG12	2.21	0.40
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.57	0.40
5:B:825:VAL:N	5:B:1088:GLY:O	2.48	0.40
9:H:118:PHE:HB2	9:H:121:LEU:HB2	2.03	0.40
12:K:47:ARG:HD2	12:K:60:ALA:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:418:SER:OG	6:C:87:PHE:O[2_555]	1.88	0.32

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	1401/1733 (81%)	1073 (77%)	223 (16%)	105 (8%)	1	5
5	B	1096/1224 (90%)	823 (75%)	190 (17%)	83 (8%)	1	5
6	C	265/318 (83%)	211 (80%)	38 (14%)	16 (6%)	1	7
7	E	212/215 (99%)	178 (84%)	25 (12%)	9 (4%)	2	13
8	F	83/155 (54%)	65 (78%)	14 (17%)	4 (5%)	2	11
9	H	129/146 (88%)	90 (70%)	25 (19%)	14 (11%)	0	2
10	I	117/122 (96%)	86 (74%)	24 (20%)	7 (6%)	1	7
11	J	63/70 (90%)	53 (84%)	6 (10%)	4 (6%)	1	7
12	K	112/120 (93%)	94 (84%)	16 (14%)	2 (2%)	6	26
13	L	44/70 (63%)	26 (59%)	12 (27%)	6 (14%)	0	0
All	All	3522/4173 (84%)	2699 (77%)	573 (16%)	250 (7%)	1	5

All (250) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	50	ILE
4	A	56	PRO
4	A	68	GLN
4	A	69	THR
4	A	72	GLU
4	A	76	GLU
4	A	89	PRO
4	A	93	VAL
4	A	109	HIS
4	A	118	HIS
4	A	130	ASP
4	A	182	VAL
4	A	255	SER
4	A	282	ASN
4	A	312	PRO
4	A	315	LEU
4	A	423	ASP
4	A	426	LEU
4	A	485	ASP
4	A	567	LYS
4	A	610	GLY
4	A	760	GLN
4	A	793	SER
4	A	801	GLU

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Mol	Chain	Res	Type
4	A	880	LYS
4	A	916	GLY
4	A	1221	LYS
5	B	25	ILE
5	B	27	ALA
5	B	66	ASP
5	B	67	SER
5	B	264	SER
5	B	266	ALA
5	B	347	LYS
5	B	469	GLN
5	B	476	ARG
5	B	648	HIS
5	B	649	LYS
5	B	681	TRP
5	B	711	GLU
5	B	731	VAL
5	B	766	ARG
5	B	783	THR
5	B	837	ASP
5	B	863	GLU
5	B	870	ILE
5	B	881	ASN
5	B	989	THR
5	B	1055	ILE
5	B	1096	ARG
5	B	1157	ALA
5	B	1171	VAL
5	B	1181	GLU
6	C	55	THR
6	C	142	VAL
7	E	131	THR
7	E	163	GLU
9	H	77	ARG
9	H	109	LYS
9	H	136	LYS
10	I	51	ASN
10	I	54	GLU
10	I	69	PRO
12	K	70	ARG
13	L	42	ARG
13	L	64	LEU

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Mol	Chain	Res	Type
4	A	40	THR
4	A	46	THR
4	A	49	LYS
4	A	65	LEU
4	A	74	MET
4	A	149	GLU
4	A	168	GLY
4	A	219	PHE
4	A	250	ILE
4	A	254	GLU
4	A	283	GLY
4	A	291	GLU
4	A	364	VAL
4	A	404	TYR
4	A	410	GLY
4	A	419	LYS
4	A	466	SER
4	A	536	LEU
4	A	609	ASP
4	A	759	ALA
4	A	846	GLU
4	A	1081	LEU
4	A	1083	THR
4	A	1234	GLU
4	A	1314	SER
4	A	1375	MET
4	A	1394	THR
4	A	1416	ALA
4	A	1447	GLU
5	B	38	PHE
5	B	58	THR
5	B	68	THR
5	B	137	TYR
5	B	165	VAL
5	B	364	ILE
5	B	369	GLY
5	B	371	GLU
5	B	411	PRO
5	B	465	ASN
5	B	480	SER
5	B	516	ASN
5	B	765	PRO

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Mol	Chain	Res	Type
5	B	880	THR
5	B	1046	PRO
5	B	1054	GLY
5	B	1150	ARG
5	B	1221	SER
6	C	32	SER
6	C	196	ASP
6	C	225	ALA
7	E	56	LYS
7	E	162	ARG
7	E	168	TYR
8	F	110	ASP
9	H	18	GLY
9	H	34	ASP
9	H	61	SER
9	H	62	SER
9	H	82	PRO
9	H	84	ALA
9	H	111	LEU
9	H	131	ASN
10	I	47	GLU
11	J	2	ILE
11	J	6	ARG
12	K	10	PHE
13	L	46	VAL
13	L	55	ILE
4	A	55	ASP
4	A	117	GLU
4	A	119	ASN
4	A	245	PRO
4	A	285	PRO
4	A	297	GLN
4	A	316	GLN
4	A	483	ASP
4	A	486	GLU
4	A	509	LEU
4	A	1166	ASP
4	A	1438	THR
5	B	111	ALA
5	B	139	ALA
5	B	261	ARG
5	B	650	GLU

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Mol	Chain	Res	Type
5	B	733	HIS
5	B	786	ASN
5	B	865	LYS
5	B	879	ARG
5	B	977	GLY
5	B	978	ASP
5	B	1017	ILE
5	B	1118	PRO
5	B	1155	SER
5	B	1211	ASN
6	C	214	ASN
6	C	227	THR
7	E	76	GLY
8	F	73	ALA
8	F	104	ASN
8	F	154	ASP
9	H	3	ASN
9	H	132	LEU
10	I	90	GLN
10	I	91	ARG
11	J	58	GLU
13	L	45	ALA
13	L	59	ALA
4	A	44	THR
4	A	54	ASN
4	A	318	SER
4	A	332	LYS
4	A	335	ARG
4	A	336	ILE
4	A	597	LEU
5	B	231	PRO
5	B	278	GLN
5	B	467	GLY
5	B	531	GLN
5	B	559	SER
5	B	792	MET
5	B	976	ILE
5	B	1086	PHE
5	B	1102	LYS
6	C	90	ASP
6	C	121	VAL
6	C	181	ASP

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Mol	Chain	Res	Type
7	E	3	GLN
10	I	3	THR
4	A	35	ILE
4	A	120	GLU
4	A	214	ILE
4	A	248	PRO
4	A	418	SER
4	A	424	ILE
4	A	592	ASP
4	A	634	THR
4	A	677	ARG
4	A	1218	GLN
5	B	276	ILE
5	B	288	ALA
5	B	563	MET
5	B	646	LEU
6	C	206	ASN
6	C	213	PRO
6	C	231	ASN
9	H	19	ARG
11	J	19	GLU
4	A	325	ILE
4	A	395	GLY
4	A	465	TYR
4	A	568	PRO
4	A	569	LYS
4	A	599	SER
4	A	724	GLU
5	B	292	ILE
5	B	471	LYS
5	B	484	ASN
6	C	60	ASP
6	C	129	ILE
7	E	93	MET
4	A	183	GLY
4	A	785	PRO
4	A	848	ILE
4	A	986	ILE
5	B	725	PRO
5	B	1172	ILE
5	B	1184	GLY
7	E	183	PRO

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Mol	Chain	Res	Type
4	A	399	HIS
4	A	632	VAL
4	A	958	VAL
4	A	1437	GLY
5	B	260	GLY
5	B	263	GLY
5	B	750	GLY
5	B	991	GLY
4	A	583	PRO
4	A	1107	VAL
5	B	410	GLY
4	A	27	VAL
4	A	308	ILE
4	A	639	PRO
5	B	290	GLY
6	C	202	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1231/1520 (81%)	986 (80%)	245 (20%)	1	5
5	B	967/1061 (91%)	760 (79%)	207 (21%)	1	3
6	C	235/274 (86%)	206 (88%)	29 (12%)	4	18
7	E	196/197 (100%)	164 (84%)	32 (16%)	2	10
8	F	75/137 (55%)	67 (89%)	8 (11%)	6	23
9	H	117/128 (91%)	86 (74%)	31 (26%)	0	1
10	I	113/116 (97%)	95 (84%)	18 (16%)	2	10
11	J	60/65 (92%)	46 (77%)	14 (23%)	1	2
12	K	99/102 (97%)	84 (85%)	15 (15%)	3	11
13	L	40/57 (70%)	31 (78%)	9 (22%)	1	3
All	All	3133/3657 (86%)	2525 (81%)	608 (19%)	1	5

All (608) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	5	GLN
4	A	11	LEU
4	A	14	VAL
4	A	28	ARG
4	A	30	ILE
4	A	32	VAL
4	A	41	MET
4	A	43	GLU
4	A	49	LYS
4	A	50	ILE
4	A	54	ASN
4	A	58	LEU
4	A	61	ILE
4	A	68	GLN
4	A	69	THR
4	A	70	CYS
4	A	74	MET
4	A	86	LEU
4	A	93	VAL
4	A	99	ILE
4	A	119	ASN
4	A	121	LEU
4	A	124	GLN
4	A	126	LEU
4	A	140	THR
4	A	143	LYS
4	A	146	MET
4	A	173	THR
4	A	179	LEU
4	A	186	LYS
4	A	201	VAL
4	A	208	LEU
4	A	209	ASN
4	A	218	ASP
4	A	221	SER
4	A	222	LEU
4	A	227	VAL
4	A	235	ILE
4	A	249	SER
4	A	252	PHE
4	A	253	ASN

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Mol	Chain	Res	Type
4	A	262	LEU
4	A	266	LEU
4	A	271	LYS
4	A	274	ILE
4	A	278	THR
4	A	295	LEU
4	A	298	PHE
4	A	302	THR
4	A	315	LEU
4	A	320	ARG
4	A	323	LYS
4	A	325	ILE
4	A	330	LYS
4	A	335	ARG
4	A	350	ARG
4	A	370	ILE
4	A	374	LEU
4	A	375	THR
4	A	379	VAL
4	A	383	TYR
4	A	385	ILE
4	A	403	LYS
4	A	404	TYR
4	A	409	SER
4	A	416	ARG
4	A	424	ILE
4	A	427	GLN
4	A	428	TYR
4	A	438	ASP
4	A	440	ASP
4	A	443	LEU
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	463	ILE
4	A	466	SER
4	A	467	THR
4	A	469	ARG
4	A	470	LEU
4	A	472	LEU
4	A	475	THR

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Mol	Chain	Res	Type
4	A	482	PHE
4	A	485	ASP
4	A	495	GLU
4	A	496	GLU
4	A	501	LEU
4	A	505	CYS
4	A	513	SER
4	A	518	LYS
4	A	529	CYS
4	A	535	THR
4	A	541	ILE
4	A	544	ASP
4	A	560	ILE
4	A	571	LEU
4	A	597	LEU
4	A	598	LEU
4	A	612	ILE
4	A	618	GLU
4	A	629	LEU
4	A	635	ARG
4	A	645	LEU
4	A	663	SER
4	A	666	ILE
4	A	669	THR
4	A	679	ILE
4	A	683	ILE
4	A	688	LYS
4	A	695	LYS
4	A	702	LEU
4	A	708	MET
4	A	709	THR
4	A	710	LEU
4	A	716	ASP
4	A	719	VAL
4	A	720	ARG
4	A	722	LEU
4	A	740	LEU
4	A	741	ASN
4	A	743	VAL
4	A	756	ILE
4	A	758	ILE
4	A	760	GLN

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Mol	Chain	Res	Type
4	A	764	CYS
4	A	770	VAL
4	A	771	GLU
4	A	774	ARG
4	A	803	SER
4	A	805	LEU
4	A	806	ARG
4	A	809	THR
4	A	811	GLN
4	A	821	ARG
4	A	826	ASP
4	A	830	LYS
4	A	834	THR
4	A	839	ARG
4	A	854	ASN
4	A	859	SER
4	A	864	ILE
4	A	878	ILE
4	A	879	GLU
4	A	882	SER
4	A	895	LYS
4	A	896	ARG
4	A	913	LEU
4	A	914	GLU
4	A	919	ILE
4	A	920	LEU
4	A	927	VAL
4	A	935	GLN
4	A	938	LYS
4	A	941	LYS
4	A	946	VAL
4	A	948	VAL
4	A	960	ILE
4	A	964	ILE
4	A	969	GLN
4	A	974	ASP
4	A	976	THR
4	A	981	LEU
4	A	982	THR
4	A	985	ASP
4	A	988	LEU
4	A	990	VAL

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Mol	Chain	Res	Type
4	A	1000	LEU
4	A	1022	LEU
4	A	1029	ARG
4	A	1037	LEU
4	A	1047	SER
4	A	1048	ASN
4	A	1067	LEU
4	A	1080	THR
4	A	1083	THR
4	A	1084	PHE
4	A	1094	VAL
4	A	1095	THR
4	A	1109	LYS
4	A	1110	ASN
4	A	1111	MET
4	A	1113	THR
4	A	1116	LEU
4	A	1121	GLU
4	A	1129	GLU
4	A	1135	ARG
4	A	1138	ILE
4	A	1141	THR
4	A	1146	VAL
4	A	1159	ARG
4	A	1161	THR
4	A	1163	ILE
4	A	1169	ILE
4	A	1170	ILE
4	A	1172	LEU
4	A	1193	LEU
4	A	1199	ARG
4	A	1215	ARG
4	A	1219	THR
4	A	1220	PHE
4	A	1221	LYS
4	A	1237	ILE
4	A	1240	CYS
4	A	1243	VAL
4	A	1255	GLU
4	A	1256	GLU
4	A	1259	MET
4	A	1264	GLU

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Mol	Chain	Res	Type
4	A	1266	THR
4	A	1269	GLU
4	A	1270	ASN
4	A	1274	ARG
4	A	1277	GLU
4	A	1280	GLU
4	A	1283	VAL
4	A	1297	GLU
4	A	1308	THR
4	A	1322	ILE
4	A	1325	THR
4	A	1333	ILE
4	A	1334	ASP
4	A	1335	ILE
4	A	1336	MET
4	A	1354	ASN
4	A	1355	VAL
4	A	1359	ASP
4	A	1361	SER
4	A	1372	VAL
4	A	1376	THR
4	A	1382	THR
4	A	1385	THR
4	A	1392	SER
4	A	1393	ASN
4	A	1394	THR
4	A	1398	MET
4	A	1400	CYS
4	A	1403	GLU
4	A	1406	VAL
4	A	1426	GLU
4	A	1438	THR
4	A	1444	MET
4	A	1447	GLU
4	A	1449	SER
5	B	22	SER
5	B	43	LEU
5	B	46	GLN
5	B	60	GLN
5	B	63	ILE
5	B	66	ASP
5	B	89	GLU

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Mol	Chain	Res	Type
5	B	98	THR
5	B	105	SER
5	B	108	VAL
5	B	109	THR
5	B	112	LEU
5	B	138	GLU
5	B	164	LYS
5	B	175	ARG
5	B	181	LEU
5	B	183	GLU
5	B	191	LYS
5	B	202	TYR
5	B	213	ILE
5	B	217	ARG
5	B	223	VAL
5	B	225	VAL
5	B	232	SER
5	B	234	ILE
5	B	244	LEU
5	B	246	LYS
5	B	248	SER
5	B	249	ARG
5	B	261	ARG
5	B	268	THR
5	B	275	TYR
5	B	276	ILE
5	B	284	ILE
5	B	291	ILE
5	B	296	GLU
5	B	305	VAL
5	B	311	LEU
5	B	319	GLU
5	B	346	GLU
5	B	355	ILE
5	B	366	GLN
5	B	378	LEU
5	B	383	ASN
5	B	391	ASP
5	B	398	ARG
5	B	408	LEU
5	B	416	LEU
5	B	429	PHE

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Mol	Chain	Res	Type
5	B	437	GLU
5	B	448	ILE
5	B	451	LYS
5	B	453	ILE
5	B	463	THR
5	B	468	GLU
5	B	469	GLN
5	B	474	SER
5	B	480	SER
5	B	484	ASN
5	B	485	ARG
5	B	489	SER
5	B	498	THR
5	B	500	THR
5	B	527	THR
5	B	533	CYS
5	B	539	LEU
5	B	547	VAL
5	B	549	THR
5	B	552	MET
5	B	555	ILE
5	B	556	THR
5	B	564	GLU
5	B	579	ARG
5	B	581	PHE
5	B	591	ARG
5	B	602	THR
5	B	604	ARG
5	B	612	GLU
5	B	613	VAL
5	B	619	ILE
5	B	620	ARG
5	B	623	GLU
5	B	625	LYS
5	B	626	ILE
5	B	628	THR
5	B	637	LEU
5	B	646	LEU
5	B	649	LYS
5	B	651	LEU
5	B	653	VAL
5	B	655	LYS

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Mol	Chain	Res	Type
5	B	667	GLN
5	B	668	ASP
5	B	706	GLN
5	B	708	GLU
5	B	723	VAL
5	B	731	VAL
5	B	732	SER
5	B	751	VAL
5	B	755	ILE
5	B	762	ASN
5	B	769	TYR
5	B	780	VAL
5	B	782	LEU
5	B	783	THR
5	B	786	ASN
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	795	ILE
5	B	796	LEU
5	B	801	LYS
5	B	807	ARG
5	B	812	LEU
5	B	815	ARG
5	B	825	VAL
5	B	827	ILE
5	B	829	CYS
5	B	831	SER
5	B	838	SER
5	B	843	GLN
5	B	844	SER
5	B	871	THR
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	881	ASN
5	B	882	THR
5	B	883	LEU
5	B	885	MET
5	B	889	THR
5	B	894	ASP
5	B	899	ILE

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Mol	Chain	Res	Type
5	B	904	ARG
5	B	905	VAL
5	B	909	ASP
5	B	916	THR
5	B	918	ILE
5	B	934	LYS
5	B	938	SER
5	B	941	LEU
5	B	944	THR
5	B	948	ILE
5	B	956	THR
5	B	962	LYS
5	B	963	PHE
5	B	964	VAL
5	B	967	ARG
5	B	969	ARG
5	B	972	LYS
5	B	973	ILE
5	B	987	LYS
5	B	989	THR
5	B	995	ARG
5	B	996	ARG
5	B	997	GLU
5	B	999	MET
5	B	1007	VAL
5	B	1010	LEU
5	B	1022	THR
5	B	1026	LEU
5	B	1034	VAL
5	B	1037	LEU
5	B	1050	ILE
5	B	1052	VAL
5	B	1057	LYS
5	B	1060	ARG
5	B	1065	GLN
5	B	1071	VAL
5	B	1090	THR
5	B	1094	ARG
5	B	1095	LEU
5	B	1096	ARG
5	B	1097	HIS
5	B	1099	VAL

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Mol	Chain	Res	Type
5	B	1101	ASP
5	B	1102	LYS
5	B	1111	MET
5	B	1113	VAL
5	B	1122	ARG
5	B	1123	SER
5	B	1125	ASP
5	B	1134	GLU
5	B	1137	CYS
5	B	1138	MET
5	B	1147	LEU
5	B	1148	LYS
5	B	1150	ARG
5	B	1155	SER
5	B	1159	ARG
5	B	1160	VAL
5	B	1162	ILE
5	B	1176	ASN
5	B	1178	ASN
5	B	1187	ASN
5	B	1188	LYS
5	B	1189	ILE
5	B	1191	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1203	LEU
5	B	1210	MET
5	B	1220	ARG
5	B	1221	SER
5	B	1222	ARG
5	B	1223	ASP
6	C	15	LYS
6	C	16	ASP
6	C	18	VAL
6	C	33	LEU
6	C	66	ARG
6	C	77	ILE
6	C	78	GLU
6	C	79	GLN
6	C	86	CYS
6	C	93	ASP

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Mol	Chain	Res	Type
6	C	106	GLU
6	C	109	SER
6	C	119	VAL
6	C	133	ILE
6	C	137	LYS
6	C	143	LEU
6	C	145	CYS
6	C	149	LYS
6	C	163	ILE
6	C	186	LEU
6	C	199	LYS
6	C	221	TYR
6	C	231	ASN
6	C	240	VAL
6	C	244	VAL
6	C	250	THR
6	C	251	LEU
6	C	254	LYS
6	C	258	ILE
7	E	3	GLN
7	E	20	LYS
7	E	31	THR
7	E	45	LYS
7	E	48	ASP
7	E	54	GLN
7	E	72	PHE
7	E	80	VAL
7	E	83	CYS
7	E	87	SER
7	E	92	THR
7	E	95	THR
7	E	98	ILE
7	E	100	ILE
7	E	101	GLN
7	E	106	GLN
7	E	107	THR
7	E	119	SER
7	E	122	LYS
7	E	123	LEU
7	E	127	ILE
7	E	131	THR
7	E	137	GLU

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Mol	Chain	Res	Type
7	E	142	VAL
7	E	150	VAL
7	E	162	ARG
7	E	164	LEU
7	E	165	LEU
7	E	166	LYS
7	E	171	LYS
7	E	177	ARG
7	E	204	THR
8	F	74	ILE
8	F	82	THR
8	F	87	LYS
8	F	111	LEU
8	F	118	LEU
8	F	133	VAL
8	F	153	VAL
8	F	155	LEU
9	H	2	SER
9	H	3	ASN
9	H	11	GLN
9	H	15	VAL
9	H	22	LYS
9	H	24	CYS
9	H	31	THR
9	H	35	GLN
9	H	39	THR
9	H	52	GLN
9	H	76	THR
9	H	77	ARG
9	H	83	GLN
9	H	86	ASP
9	H	91	ASP
9	H	92	ASP
9	H	95	TYR
9	H	100	THR
9	H	109	LYS
9	H	110	ASP
9	H	114	VAL
9	H	121	LEU
9	H	123	MET
9	H	130	ARG
9	H	132	LEU

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Mol	Chain	Res	Type
9	H	136	LYS
9	H	137	GLN
9	H	138	GLU
9	H	139	ASN
9	H	144	ILE
9	H	146	ARG
10	I	3	THR
10	I	17	ARG
10	I	20	LYS
10	I	29	CYS
10	I	31	THR
10	I	47	GLU
10	I	55	THR
10	I	70	ARG
10	I	71	SER
10	I	75	CYS
10	I	78	CYS
10	I	84	VAL
10	I	90	GLN
10	I	95	THR
10	I	104	LEU
10	I	115	LYS
10	I	118	ARG
10	I	119	THR
11	J	2	ILE
11	J	5	VAL
11	J	7	CYS
11	J	9	SER
11	J	13	VAL
11	J	14	VAL
11	J	19	GLU
11	J	20	SER
11	J	24	LEU
11	J	41	LEU
11	J	43	ARG
11	J	48	ARG
11	J	49	MET
11	J	52	THR
12	K	5	ASP
12	K	6	ARG
12	K	12	LEU
12	K	18	LYS

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Mol	Chain	Res	Type
12	K	20	LYS
12	K	32	VAL
12	K	40	HIS
12	K	47	ARG
12	K	51	LEU
12	K	56	VAL
12	K	78	THR
12	K	91	CYS
12	K	103	THR
12	K	107	THR
12	K	114	LEU
13	L	27	LEU
13	L	33	GLU
13	L	42	ARG
13	L	43	THR
13	L	47	ARG
13	L	50	ASP
13	L	55	ILE
13	L	56	LEU
13	L	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	68	GLN
4	A	75	ASN
4	A	92	HIS
4	A	225	ASN
4	A	253	ASN
4	A	273	ASN
4	A	282	ASN
4	A	306	ASN
4	A	397	ASN
4	A	399	HIS
4	A	445	ASN
4	A	447	GLN
4	A	503	GLN
4	A	517	ASN
4	A	545	GLN
4	A	631	HIS
4	A	741	ASN

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Mol	Chain	Res	Type
4	A	742	ASN
4	A	757	ASN
4	A	760	GLN
4	A	767	GLN
4	A	811	GLN
4	A	877	HIS
4	A	926	GLN
4	A	965	GLN
4	A	968	GLN
4	A	969	GLN
4	A	1004	ASN
4	A	1078	GLN
4	A	1082	ASN
4	A	1085	HIS
4	A	1110	ASN
4	A	1140	HIS
4	A	1187	GLN
4	A	1265	ASN
4	A	1278	ASN
4	A	1330	ASN
4	A	1364	ASN
4	A	1390	ASN
4	A	1432	GLN
5	B	110	HIS
5	B	115	GLN
5	B	178	ASN
5	B	206	ASN
5	B	215	GLN
5	B	255	GLN
5	B	366	GLN
5	B	383	ASN
5	B	484	ASN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	657	HIS
5	B	686	ASN
5	B	706	GLN
5	B	744	HIS
5	B	770	GLN
5	B	794	ASN
5	B	822	ASN

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Mol	Chain	Res	Type
5	B	842	ASN
5	B	862	GLN
5	B	881	ASN
5	B	984	HIS
5	B	1015	HIS
5	B	1025	HIS
5	B	1040	ASN
5	B	1062	HIS
5	B	1084	GLN
5	B	1177	HIS
5	B	1178	ASN
6	C	17	ASN
6	C	65	HIS
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN
6	C	131	HIS
6	C	167	HIS
6	C	188	HIS
6	C	214	ASN
6	C	231	ASN
6	C	242	GLN
7	E	3	GLN
7	E	5	ASN
7	E	8	ASN
7	E	61	GLN
7	E	99	HIS
7	E	104	ASN
7	E	146	HIS
7	E	147	HIS
7	E	174	GLN
9	H	33	GLN
9	H	43	ASN
9	H	52	GLN
9	H	131	ASN
9	H	137	GLN
9	H	139	ASN
10	I	60	GLN
10	I	90	GLN
10	I	114	GLN
10	I	116	ASN
10	I	120	GLN

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Mol	Chain	Res	Type
11	J	23	ASN
12	K	65	HIS
12	K	89	ASN
12	K	96	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	3 (30%)	1 (10%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	A
1	R	3	G
1	R	8	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
14	G2P	T	3000	-	30,34,34	1.33	4 (13%)	46,54,54	2.03	12 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	G2P	T	3000	-	-	4/19/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	G2P	PB-O3B	4.08	1.62	1.58
14	T	3000	G2P	C2-N3	2.66	1.39	1.33
14	T	3000	G2P	PA-O1A	-2.23	1.51	1.56
14	T	3000	G2P	C5-N7	-2.16	1.34	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	C5-C4-N3	-6.51	118.03	128.39
14	T	3000	G2P	C2-N3-C4	5.13	121.14	112.30
14	T	3000	G2P	N9-C4-N3	4.36	134.67	125.95
14	T	3000	G2P	C2-N1-C6	-3.48	118.80	125.11
14	T	3000	G2P	PB-O3B-PG	-3.37	120.37	132.45
14	T	3000	G2P	O4'-C4'-C5'	3.22	119.65	109.33
14	T	3000	G2P	C5-C6-N1	2.65	120.01	113.25
14	T	3000	G2P	C2'-C1'-N9	-2.55	106.17	113.25
14	T	3000	G2P	C8-N7-C5	2.50	108.70	104.26
14	T	3000	G2P	O5'-C5'-C4'	2.44	117.32	108.99
14	T	3000	G2P	O6-C6-C5	-2.27	120.54	126.53
14	T	3000	G2P	N9-C8-N7	-2.21	109.31	113.40

There are no chirality outliers.

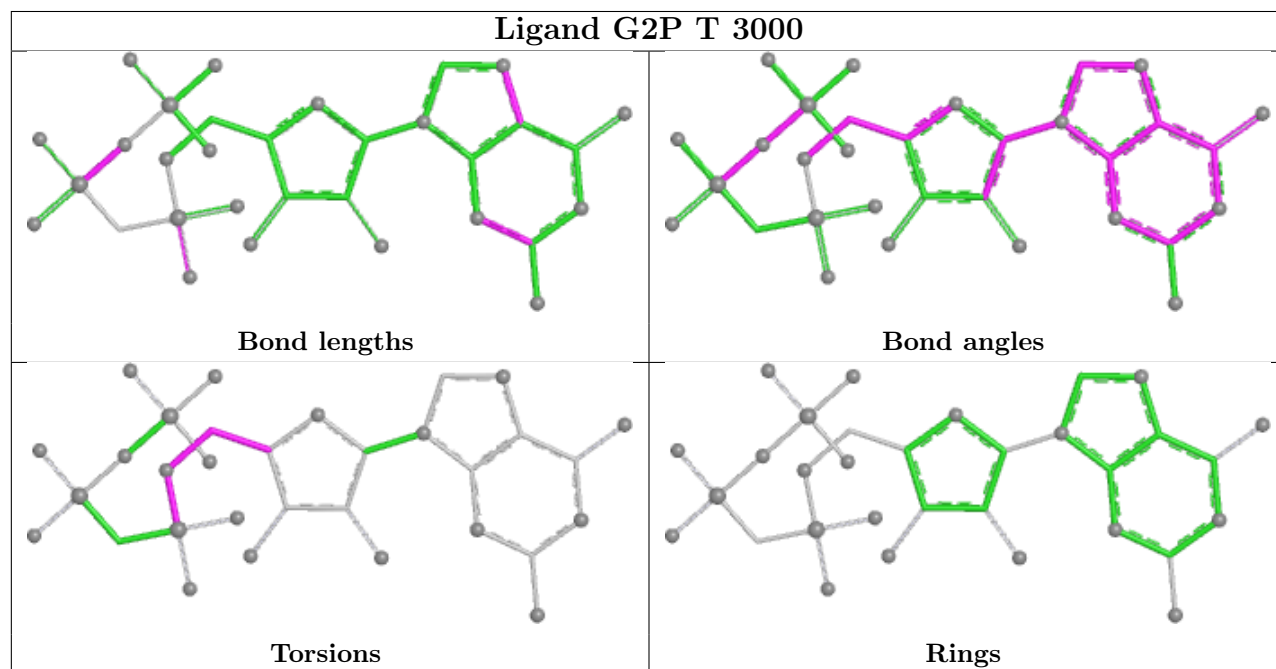
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	3000	G2P	O4'-C4'-C5'-O5'
14	T	3000	G2P	C3'-C4'-C5'-O5'
14	T	3000	G2P	C4'-C5'-O5'-PA
14	T	3000	G2P	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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%)	-0.31	0 100 100	76, 118, 173, 179	0
2	T	21/21 (100%)	0.27	0 100 100	100, 128, 234, 236	0
3	N	7/7 (100%)	0.85	0 100 100	225, 230, 244, 248	0
4	A	1411/1733 (81%)	0.29	43 (3%) 52 38	83, 119, 142, 195	0
5	B	1114/1224 (91%)	0.43	34 (3%) 51 38	76, 121, 146, 177	0
6	C	267/318 (83%)	0.14	1 (0%) 88 81	104, 119, 141, 159	0
7	E	214/215 (99%)	0.19	3 (1%) 73 59	100, 124, 146, 151	0
8	F	85/155 (54%)	0.01	1 (1%) 76 63	107, 126, 146, 152	0
9	H	133/146 (91%)	0.48	5 (3%) 44 31	115, 134, 153, 156	0
10	I	119/122 (97%)	0.33	5 (4%) 40 28	101, 122, 146, 158	0
11	J	65/70 (92%)	0.14	0 100 100	94, 118, 138, 145	0
12	K	114/120 (95%)	0.28	2 (1%) 67 51	114, 123, 134, 140	0
13	L	46/70 (65%)	0.98	4 (8%) 16 14	131, 170, 177, 179	0
All	All	3606/4211 (85%)	0.32	98 (2%) 56 41	76, 121, 147, 248	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	L	27	LEU	6.1
4	A	341	MET	5.4
9	H	63	LEU	4.7
5	B	990	ILE	4.3
5	B	883	LEU	4.2
4	A	1089	VAL	4.1
4	A	141	LEU	3.9
4	A	1176	LEU	3.6
4	A	252	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
4	A	831	THR	3.5
5	B	731	VAL	3.5
4	A	175	ARG	3.4
4	A	932	GLU	3.4
4	A	486	GLU	3.3
4	A	465	TYR	3.2
10	I	2	THR	3.2
4	A	69	THR	3.2
13	L	30	ILE	3.2
5	B	746	SER	3.0
4	A	664	THR	3.0
4	A	76	GLU	3.0
5	B	529	GLU	2.9
4	A	146	MET	2.9
4	A	339	ASN	2.9
7	E	209	ALA	2.9
5	B	43	LEU	2.9
4	A	852	TYR	2.9
5	B	611	PRO	2.9
4	A	1081	LEU	2.9
5	B	989	THR	2.8
9	H	114	VAL	2.7
10	I	52	ILE	2.7
4	A	1451	VAL	2.7
5	B	140	ILE	2.7
5	B	1103	ILE	2.7
4	A	176	LYS	2.7
5	B	798	TYR	2.7
5	B	734	HIS	2.7
5	B	646	LEU	2.6
12	K	114	LEU	2.6
4	A	1086	PHE	2.6
5	B	394	ASP	2.6
5	B	167	ILE	2.5
4	A	1401	SER	2.5
5	B	839	MET	2.5
5	B	480	SER	2.5
12	K	1	MET	2.5
4	A	151	ASP	2.5
4	A	336	ILE	2.5
6	C	16	ASP	2.5
4	A	170	THR	2.5

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Mol	Chain	Res	Type	RSRZ
10	I	55	THR	2.5
5	B	393	LYS	2.5
13	L	28	LYS	2.5
5	B	245	GLU	2.4
5	B	710	LEU	2.4
4	A	147	VAL	2.4
5	B	709	ASP	2.4
4	A	622	VAL	2.4
4	A	1108	ALA	2.4
9	H	90	ALA	2.4
5	B	821	GLN	2.4
4	A	149	GLU	2.4
4	A	344	ARG	2.4
4	A	168	GLY	2.3
5	B	531	GLN	2.3
4	A	467	THR	2.3
4	A	355	GLY	2.3
5	B	509	ALA	2.3
5	B	645	SER	2.3
4	A	1332	PHE	2.3
10	I	49	ILE	2.3
5	B	252	SER	2.3
4	A	1094	VAL	2.3
4	A	108	MET	2.2
4	A	1090	ALA	2.2
13	L	32	ALA	2.2
5	B	484	ASN	2.2
5	B	502	ILE	2.2
7	E	121	MET	2.2
5	B	429	PHE	2.2
4	A	1175	SER	2.2
5	B	92	PHE	2.2
5	B	487	THR	2.2
4	A	568	PRO	2.2
5	B	754	SER	2.2
5	B	777	ALA	2.2
4	A	1088	GLY	2.2
4	A	1077	THR	2.1
10	I	13	MET	2.1
5	B	212	LEU	2.1
7	E	93	MET	2.1
9	H	141	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
8	F	91	ALA	2.1
4	A	250	ILE	2.1
9	H	111	LEU	2.0
4	A	258	GLY	2.0
4	A	450	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

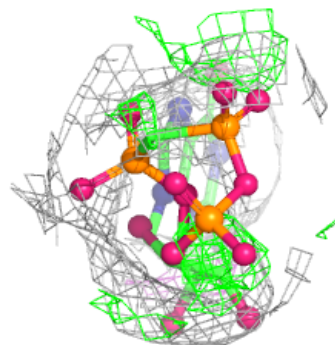
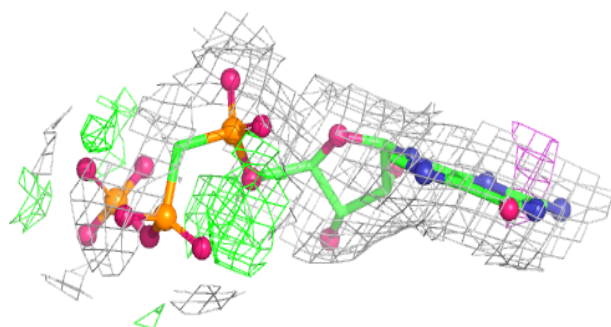
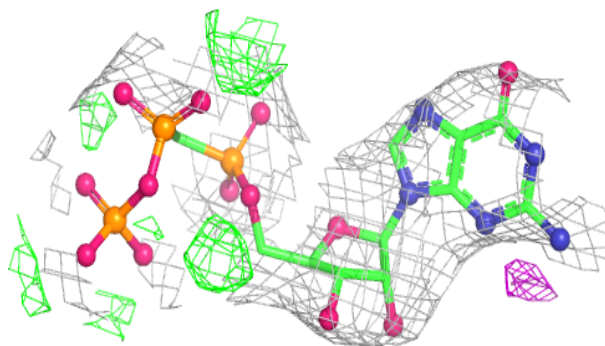
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	G2P	T	3000	32/32	0.88	0.12	120,126,149,149	0
16	MG	A	2002	1/1	0.91	0.19	79,79,79,79	0
15	ZN	A	1734	1/1	0.96	0.13	141,141,141,141	0
15	ZN	L	105	1/1	0.97	0.05	170,170,170,170	0
15	ZN	B	1307	1/1	0.97	0.04	134,134,134,134	0
15	ZN	I	204	1/1	0.98	0.04	128,128,128,128	0
15	ZN	J	101	1/1	0.99	0.02	107,107,107,107	0
15	ZN	I	203	1/1	0.99	0.03	114,114,114,114	0
15	ZN	A	1735	1/1	0.99	0.03	141,141,141,141	0
16	MG	A	2003	1/1	0.99	0.03	50,50,50,50	0
15	ZN	C	319	1/1	1.00	0.02	120,120,120,120	0

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

Electron density around G2P T 3000:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.