



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:12 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

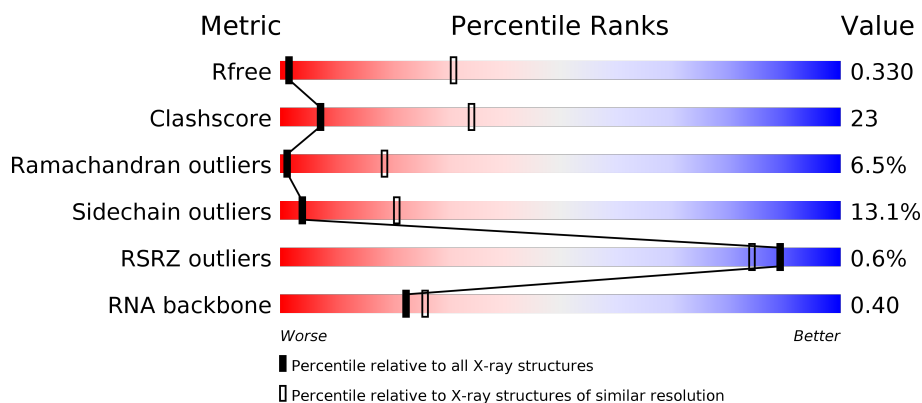
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




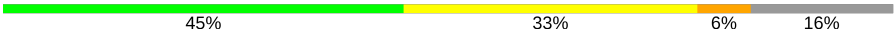
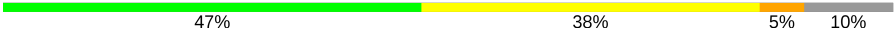



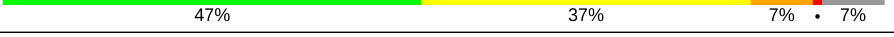

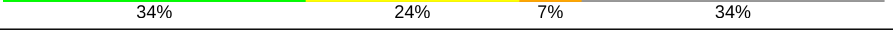
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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 on 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	<div> <div>50%</div> <div>50%</div> </div>
2	T	28	<div> <div>29%</div> <div>39%</div> <div>39%</div> <div>21%</div> </div>
3	N	14	<div> <div>50%</div> <div>79%</div> <div>21%</div> </div>
4	A	1733	<div> <div>42%</div> <div>31%</div> <div>6%</div> <div>19%</div> </div>

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

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

tide.

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

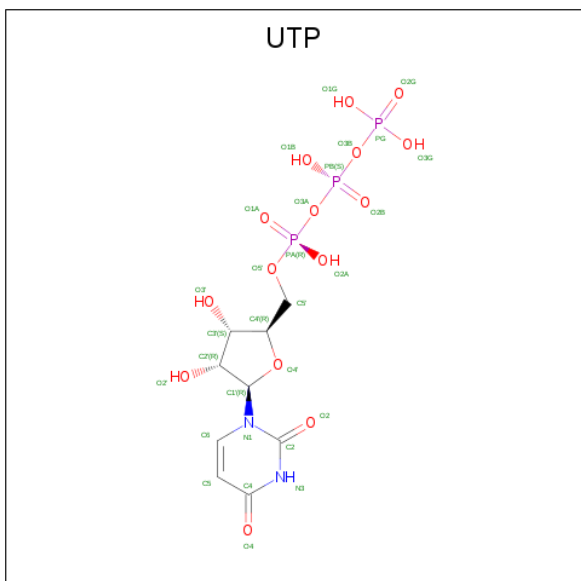
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



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

3 Residue-property plots

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

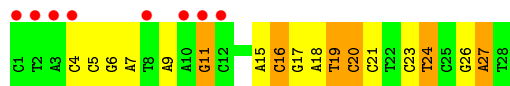
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R: 




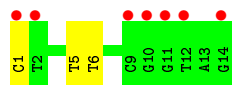
- Molecule 2: 28-MER DNA template strand

Chain T: 



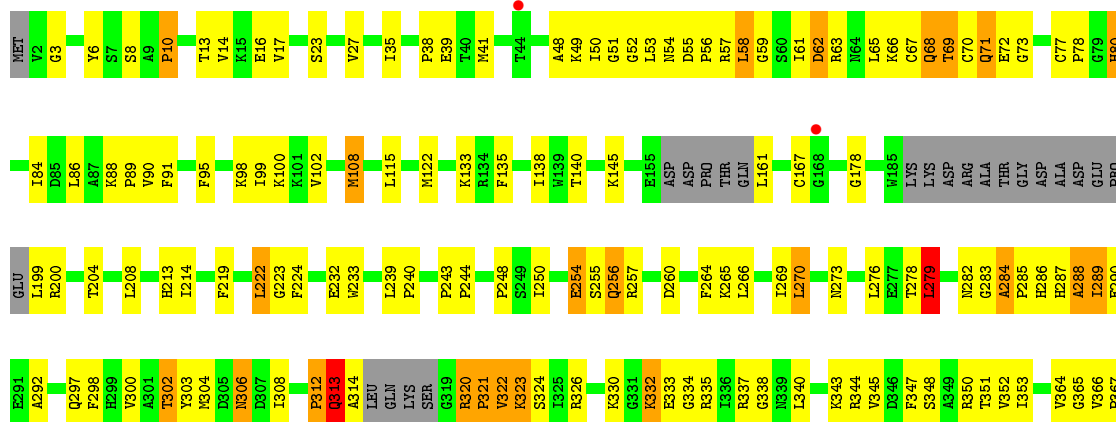
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

Chain N: 



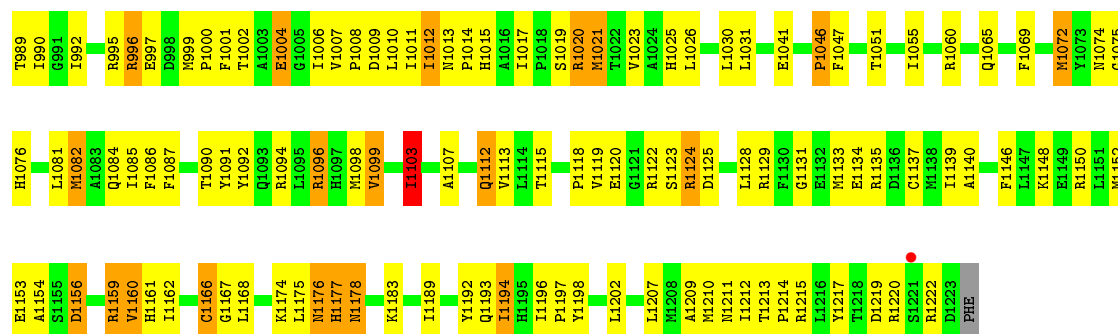
- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

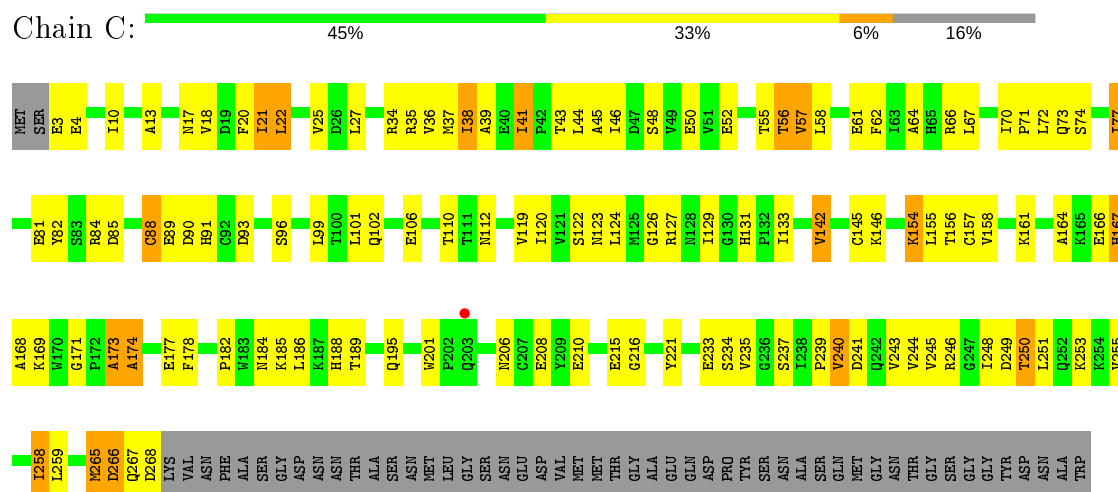


SER	ALA	MET	V1374	M1267	ASP	L1105	C1019	L928	L848	G766	P674	Q589	Q510	L443	I370
PRO	ASP	PRO	M1375	L1268	Q1187	M1106	R1025	L929	M849	Q767	T675	R590	Q513	F444	I370
TYR	TYR	GLN	T1376	E1269	Q1188	V1107	R1025	D930	D863	Q768	T680	F591	S513	N445	T373
SER	GLU	LYS	V1384	I1271	S1189	T1113	T1028	E932	M854	R774	B631	T896	Q515	Q447	L374
PRO	ALA	ILE	T1385	I1271	P1190	P1114	R1028	E933	T855	T775	T682	L587	S516	P448	T375
SER	THR	THR	G1388	E1277	V1191	S1115	R1030	L936	T856	A776	I633	L598	N517	S449	E378
PRO	SER	ILE	F1389	E1277	L1193	L1116	E1034	L941	M858	R782	K687	L606	M521	R461	V379
PRO	PRO	ILE	T1390	R1281	R1194	T1117	R1036	K941	R860	R783	D692	G610	G522	K452	V380
SER	THR	GLU	M1390	V1282	L1195	V1118	R1036	E942	L860	T792	Q698	Q611	I523	T381	T381
TYR	ASP	ASP	R1391	V1283	E1196	V1119	R1036	R943	L864	R783	A699	Q612	I524	P382	P382
SER	ALA	GLY	S1392	M1284	L1197	L1120	E1050	R944	L864	S788	N700	I611	W524	S454	S454
PRO	TYR	GLN	M1393	D1198	D1198	L1120	E1050	R944	L864	K789	K695	I613	Q525	M455	Y383
THR	GLY	ASP	T1394	R1199	D1127	D1127	E1050	E945	L864	S788	K695	I613	Q525	M456	Y383
SER	GLU	GLY	V1398	Y1287	Q1128	Q1128	L1054	E945	L864	K789	K695	I613	Q525	M456	Y383
PRO	ALA	GLY	M1398	T1295	A1131	A1131	L1054	E945	L864	K789	K695	I613	Q525	M456	Y383
SER	PRO	VAL	F1402	T1295	M1202	M1202	L1054	E945	L864	K789	K695	I613	Q525	M456	Y383
TYR	THR	THR	Y1402	T1295	M1202	M1202	L1054	E945	L864	K789	K695	I613	Q525	M456	Y383
SER	SER	PRO	V1406	W1304	D1206	I1134	V1058	P957	D871	E795	L701	K619	L534	K461	L391
PRO	PRO	TYR	V1406	W1304	D1206	I1134	V1058	P957	D871	E795	L701	K619	L534	K461	L391
THR	GLY	SER	L1409	V1306	G1213	T1141	V1064	P958	K872	S796	L702	V622	T535	V462	V462
SER	THR	ASN	E1307	L1306	E1307	T1142	V1064	P958	K872	S796	L702	V622	T535	V462	V462
PRO	GLY	GLU	F1410	T1308	E1214	L1143	V1066	P959	K872	S796	L702	V622	T535	V462	V462
SER	VAL	SER	E1411	T1308	E1214	L1143	V1066	P959	K872	S796	L702	V622	T535	V462	V462
TYR	SER	GLY	A1414	V1311	R1215	S1150	L1067	R961	K880	V800	G707	S625	D538	Y465	P400
SER	SER	LEU	A1414	N1312	I1216	E1151	A1068	Q965	L883	E801	T709	I630	E541	T467	P400
PRO	PRO	VAL	S1415	V1319	D1223	I1152	A1068	Q965	L883	E801	T709	I630	E541	T467	P400
THR	GLY	ASN	A1416	V1319	D1223	I1152	A1068	Q965	L883	E801	T709	I630	E541	T467	P400
SER	PHE	ALA	A1416	V1319	D1223	I1152	A1068	Q965	L883	E801	T709	I630	E541	T467	P400
PRO	SER	ASP	D1419	I1322	I1227	D1155	G1073	T970	A892	F814	R711	V633	L543	R468	K403
SER	PRO	ASP	D1420	I1323	I1228	P1156	G1073	T970	A892	F814	R711	V633	L543	R468	K403
TYR	THR	ASP	G1421	P1324	W1228	D1157	E1074	H972	E894	A817	R711	V633	L543	R468	K403
SER	SER	VAL	D1421	P1324	W1228	D1157	E1074	H972	E894	A817	R711	V633	L543	R468	K403
PRO	PRO	LYS	V1424	T1325	ASN	P1158	P1075	H972	E894	A817	R711	V633	L543	R468	K403
THR	THR	GLU	S1425	T1326	ASP	S1160	T1077	D974	R896	G819	L722	Q640	W551	Y478	Y478
SER	TYR	GLU	E1426	T1327	GLU	T1161	T1079	T976	R898	R821	K728	V641	W552	N479	N479
PRO	SER	LEU	M1427	T1328	LYS	V1162	M1080	K977	R898	R821	K728	V641	W552	N479	N479
SER	PRO	MET	V1428	T1328	LYS	V1162	M1080	K977	R898	R821	K728	V641	W552	N479	N479
TYR	THR	PHE	I1429	I1333	L1236	I1163	L1081	P978	D900	E833	R731	G642	W556	D481	D481
SER	SER	THR	L1430	D1334	I1237	P1164	M1082	S979	L901	L824	N736	F646	P561	F462	D483
PRO	PRO	PRO	L1430	D1334	I1237	P1164	M1082	S979	L901	L824	N736	F646	P561	F462	D483
THR	ALA	VAL	A1434	M1336	R1241	E1166	F1084	V987	N903	D826	L737	N648	P563	G484	D423
SER	VAL	VAL	P1435	M1336	R1241	E1166	F1084	V987	N903	D826	L737	N648	P563	G484	D423
PRO	ASP	ASP	T1436	G1340	ARG	I1168	A1087	L988	T907	E828	I739	I649	I565	M487	Q425
SER	PRO	ASP	T1436	G1340	ARG	I1168	A1087	L988	T907	E828	I739	I649	I565	M487	Q425
TYR	THR	GLY	G1437	L1341	PRO	I1170	A1087	G989	L908	E829	L740	Q650	I566	N488	L426
SER	SER	GLY	T1438	E1342	LYS	Q1171	V1089	L993	D909	K830	M741	K651	I567	L489	Q427
PRO	PRO	ASN	F1441	A1343	SER	L1172	A1090	Q994	S911	T831	M741	K651	I567	L489	Q427
THR	SER	ASN	D1442	L1348	LEU	H1173	S1091	E995	S911	T831	M741	K651	I567	L489	Q427
SER	ALA	ASP	V1443	L1348	ALA	F1174	K1092	N996	L912	E833	K744	P568	K569	H490	G429
PRO	THR	ALA	M1444	S1358	GLU	S1175	K1093	L997	E914	T834	Q745	V491	K569	P492	W430
SER	SER	MET	M1444	S1358	GLU	S1175	K1093	L997	E914	T834	Q745	V491	K569	P492	W430
PRO	PRO	ALA	T1445	N1364	THR	LEU	V1094	L998	S915	Y836	S751	N660	W572	S494	K431
TYR	THR	GLY	ASP	N1364	THR	LEU	V1094	L998	S915	Y836	S751	N660	W572	S494	K431
SER	SER	GLY	GLU	Y1365	GLU	ASP	S1096	K1003	E918	Q838	S754	S663	G574	L501	E433
PRO	PRO	PHE	GLU	Y1365	GLU	ASP	S1096	K1003	E918	Q838	S754	S663	G574	L501	E433
THR	SER	THR	SER	R1366	GLU	GLU	G1097	D1013	E919	Q839	F755	I666	Q576	S502	R434
SER	THR	THR	SER	K1261	ALA	ALA	V1099	A1014	E921	R840	I756	G667	I577	Q503	H435
PRO	ALA	ALA	K1262	Y1263	GLU	GLU	P1099	A1014	E921	R840	I756	G667	I577	Q503	H435
PRO	VAL	TYR	L1370	L1263	GLU	GLU	A1100	V1015	D922	L841	I758	T689	S579	C505	I436
PRO	VAL	TYR	L1371	L1263	GLU	GLU	A1100	V1015	D922	L841	I758	T689	S579	C505	I436
PRO	GLY	GLY	V1372	V1372	SER	GLN	R1104	T1016	Q926	E846	C764	I670	I582	A506	D438
TYR	TYR	GLY	D1373	D1373	PHE	PHE	I1104	T1016	Q926	E846	C764	I670	I582	A506	D438

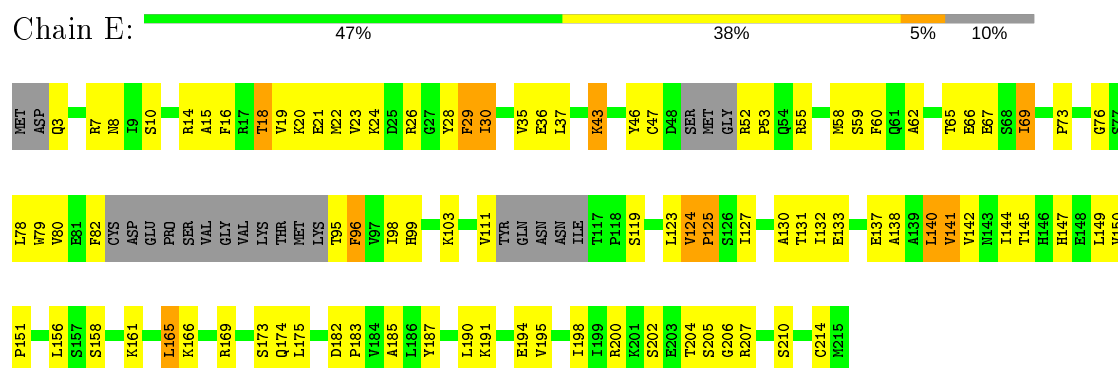




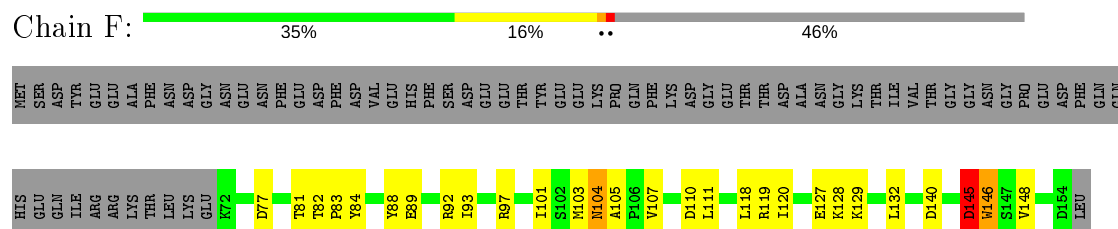
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



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

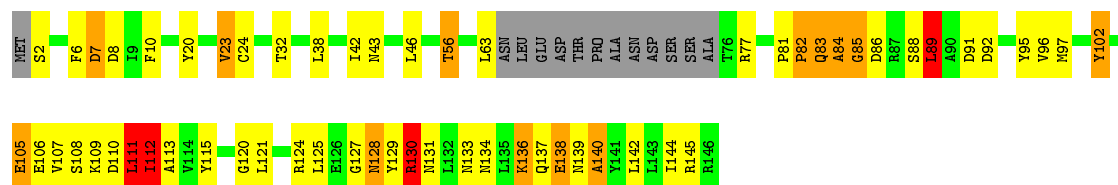


• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



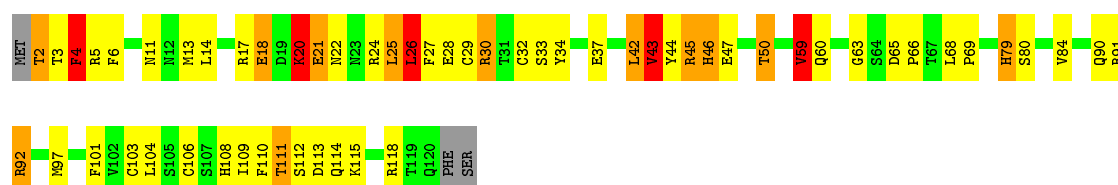
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 



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

Chain I: 



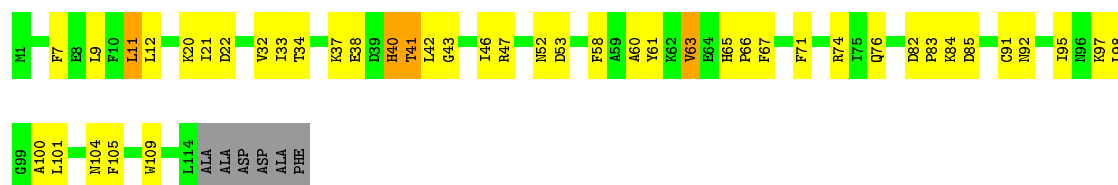
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J: 



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

Chain K: 



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

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.30 39.94 – 4.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.30) 86.4 (39.94-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.332 0.277 , 0.330	Depositor DCC
R_{free} test set	4179 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29002	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.81	0/243	1.33	0/378
2	T	0.87	0/634	1.63	17/975 (1.7%)
3	N	0.77	0/317	1.35	1/488 (0.2%)
4	A	0.45	1/11180 (0.0%)	0.67	3/15117 (0.0%)
5	B	0.45	0/8866	0.65	1/11956 (0.0%)
6	C	0.43	0/2133	0.60	0/2891
7	E	0.44	0/1625	0.61	0/2182
8	F	0.43	0/682	0.61	1/922 (0.1%)
9	H	0.47	0/1086	0.77	2/1470 (0.1%)
10	I	0.48	0/989	0.74	0/1331
11	J	0.47	0/541	0.62	0/727
12	K	0.46	0/937	0.60	0/1265
13	L	0.53	0/365	0.79	0/485
All	All	0.47	1/29598 (0.0%)	0.72	25/40187 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1158	PRO	CG-CD	5.94	1.70	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	23	DC	O4'-C4'-C3'	-9.30	100.42	106.00
2	T	16	DC	O4'-C1'-N1	9.29	114.50	108.00
2	T	11	DG	O4'-C1'-N9	8.90	114.23	108.00
2	T	23	DC	O4'-C1'-N1	8.24	113.77	108.00
2	T	20	DC	O4'-C4'-C3'	-8.15	101.11	106.00
2	T	19	DT	C4-C5-C7	8.11	123.86	119.00
2	T	15	DA	P-O3'-C3'	7.71	128.96	119.70
2	T	19	DT	C6-C5-C7	-7.40	118.46	122.90
2	T	27	DA	O4'-C4'-C3'	-7.23	101.61	104.50
2	T	20	DC	C4'-C3'-C2'	-6.19	97.53	103.10
5	B	883	LEU	CA-CB-CG	6.16	129.46	115.30
2	T	23	DC	C4'-C3'-C2'	-6.04	97.66	103.10
2	T	16	DC	O4'-C4'-C3'	-6.00	102.10	104.50
3	N	1	DC	O4'-C1'-N1	5.97	112.18	108.00
4	A	1070	GLN	N-CA-C	-5.95	94.95	111.00
2	T	4	DC	O4'-C1'-N1	5.54	111.88	108.00
2	T	5	DC	C1'-O4'-C4'	-5.42	104.69	110.10
4	A	1069	ALA	N-CA-C	-5.38	96.46	111.00
2	T	24	DT	N3-C4-O4	5.37	123.12	119.90
9	H	89	LEU	CA-CB-CG	5.32	127.54	115.30
2	T	5	DC	O4'-C1'-N1	5.20	111.64	108.00
4	A	701	LEU	CA-CB-CG	5.09	127.02	115.30
8	F	118	LEU	CA-CB-CG	5.07	126.97	115.30
9	H	111	LEU	CA-CB-CG	5.04	126.89	115.30
2	T	4	DC	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
9	H	130	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	6	0
2	T	566	0	316	18	0
3	N	284	0	161	2	0
4	A	10984	0	11069	568	0
5	B	8701	0	8728	479	0
6	C	2095	0	2051	92	0
7	E	1594	0	1622	52	0
8	F	670	0	690	15	0
9	H	1068	0	1040	52	0
10	I	971	0	928	63	0
11	J	532	0	542	38	0
12	K	919	0	929	32	0
13	L	363	0	387	13	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	B	29	0	11	2	0
All	All	29002	0	28583	1299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1299) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:701:LEU:HA	4:A:702:LEU:CB	1.68	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:975:HIS:HB3	4:A:976:THR:OG1	1.41	1.19
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.27	1.16
4:A:1167:GLU:CB	4:A:1168:GLU:HA	1.75	1.15
5:B:1019:SER:HB2	5:B:1020:ARG:HB2	1.24	1.15
4:A:707:GLY:HA2	4:A:709:THR:H	0.99	1.14
4:A:712:GLU:H	4:A:713:SER:HB2	0.98	1.14
4:A:709:THR:HA	4:A:710:LEU:HB3	1.19	1.13
5:B:227:LYS:HA	5:B:228:LYS:HB2	1.29	1.12
10:I:3:THR:HA	10:I:4:PHE:CG	1.85	1.11
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.33	1.11
4:A:1167:GLU:HB2	4:A:1168:GLU:CA	1.81	1.09
5:B:705:MET:HB3	5:B:706:GLN:HB2	1.08	1.08
4:A:1080:THR:O	4:A:1082:ASN:N	1.86	1.08
5:B:877:PRO:HA	5:B:878:GLN:CB	1.84	1.07
9:H:85:GLY:HA2	9:H:86:ASP:HB2	1.14	1.06
5:B:868:MET:H	5:B:869:SER:HB3	0.92	1.06
10:I:20:LYS:HA	10:I:21:GLU:O	1.57	1.05
4:A:707:GLY:HA2	4:A:709:THR:N	1.72	1.04
5:B:327:ARG:HB3	5:B:328:GLU:HB2	1.09	1.04
5:B:293:PRO:HA	5:B:294:ASP:HB2	1.40	1.03
4:A:701:LEU:CA	4:A:702:LEU:HB2	1.88	1.03
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.04	1.03
13:L:42:ARG:HB2	13:L:43:THR:HB	1.35	1.03
10:I:25:LEU:HA	10:I:26:LEU:CB	1.89	1.02
5:B:256:VAL:HG11	5:B:382:ILE:HD11	1.40	1.02
4:A:712:GLU:N	4:A:713:SER:HB2	1.73	1.02
10:I:45:ARG:HA	10:I:46:HIS:HB2	1.05	1.02
5:B:868:MET:N	5:B:869:SER:HB3	1.74	1.02
5:B:636:PRO:HB2	5:B:637:LEU:HB3	1.43	1.00
5:B:1019:SER:CB	5:B:1020:ARG:HB2	1.91	1.00
5:B:868:MET:H	5:B:869:SER:CB	1.75	1.00
9:H:111:LEU:HB3	9:H:128:ASN:HB2	1.41	0.99
9:H:85:GLY:CA	9:H:86:ASP:HB2	1.91	0.99
4:A:709:THR:HA	4:A:710:LEU:CB	1.92	0.99
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.26	0.99
5:B:877:PRO:HA	5:B:878:GLN:HB2	1.44	0.98
10:I:45:ARG:HA	10:I:46:HIS:CB	1.93	0.98
4:A:1091:SER:HB2	4:A:1092:LYS:C	1.84	0.98
5:B:635:ARG:CB	5:B:636:PRO:HD2	1.92	0.98
4:A:712:GLU:H	4:A:713:SER:CB	1.76	0.98
10:I:25:LEU:HA	10:I:26:LEU:HB2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:635:ARG:HB2	5:B:636:PRO:CD	1.94	0.97
4:A:802:ASN:HD21	5:B:729:ILE:H	0.98	0.97
4:A:67:CYS:CB	4:A:70:CYS:HB2	1.93	0.97
9:H:85:GLY:HA2	9:H:86:ASP:CB	1.94	0.97
4:A:1071:SER:H	4:A:1072:ILE:HB	1.26	0.96
10:I:63:GLY:HA3	10:I:104:LEU:HD21	1.45	0.96
10:I:45:ARG:CA	10:I:46:HIS:HB2	1.95	0.96
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.30	0.95
4:A:1236:LEU:HA	4:A:1237:ILE:HB	1.46	0.95
4:A:782:ARG:HB3	4:A:789:LYS:HA	1.46	0.95
5:B:766:ARG:HH21	5:B:1020:ARG:HA	1.26	0.95
4:A:284:ALA:H	4:A:285:PRO:HD3	1.29	0.94
5:B:350:GLN:HB3	5:B:351:TYR:HB2	1.48	0.94
4:A:284:ALA:H	4:A:285:PRO:CD	1.80	0.94
4:A:701:LEU:HA	4:A:702:LEU:HB2	0.95	0.94
6:C:58:LEU:HD11	11:J:2:ILE:HD12	1.50	0.93
5:B:882:THR:HB	5:B:883:LEU:HA	1.49	0.92
4:A:709:THR:CA	4:A:710:LEU:HB3	2.00	0.91
6:C:67:LEU:O	6:C:70:ILE:HG22	1.69	0.91
5:B:327:ARG:CB	5:B:328:GLU:HB2	2.01	0.90
1:R:10:A:H61	2:T:19:DT:H3	1.16	0.90
4:A:282:ASN:HB3	4:A:283:GLY:CA	2.02	0.90
9:H:84:ALA:HA	9:H:85:GLY:C	1.92	0.90
4:A:108:MET:HE3	4:A:167:CYS:HB2	1.52	0.90
5:B:122:LEU:HD22	5:B:958:GLN:HG3	1.51	0.89
1:R:4:G:H2'	1:R:5:A:H8	1.38	0.89
5:B:124:TYR:HH	5:B:179:CYS:HG	1.17	0.89
6:C:74:SER:O	6:C:77:ILE:HB	1.74	0.87
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.55	0.87
5:B:636:PRO:HB2	5:B:637:LEU:CB	2.05	0.86
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.76	0.86
1:R:4:G:H2'	1:R:5:A:C8	2.10	0.85
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.56	0.85
4:A:1085:HIS:CD2	4:A:1085:HIS:H	1.88	0.85
4:A:1152:ILE:HA	4:A:1153:TYR:HB2	1.57	0.84
5:B:705:MET:HB3	5:B:706:GLN:CB	2.01	0.84
4:A:630:ILE:HD12	4:A:630:ILE:H	1.43	0.84
5:B:705:MET:CB	5:B:706:GLN:HB2	2.03	0.84
4:A:67:CYS:HB2	4:A:70:CYS:HB2	1.59	0.83
1:R:9:G:N2	2:T:21:DC:H1'	1.92	0.83
4:A:1082:ASN:N	4:A:1083:THR:HA	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1191:TRP:HA	4:A:1192:LEU:HB2	1.58	0.83
5:B:782:LEU:HD13	5:B:784:ASN:HD21	1.43	0.83
5:B:557:PHE:O	5:B:561:TRP:HB3	1.79	0.83
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.61	0.83
4:A:1083:THR:OG1	4:A:1084:PHE:HB3	1.79	0.83
4:A:1097:GLY:H	4:A:1100:ARG:HB2	1.41	0.83
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.60	0.83
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.12	0.82
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.59	0.82
7:E:165:LEU:HD21	7:E:175:LEU:HD21	1.61	0.82
10:I:25:LEU:CA	10:I:26:LEU:HB2	2.08	0.82
4:A:335:ARG:HD2	5:B:1202:LEU:CD1	2.06	0.82
6:C:184:ASN:ND2	6:C:189:THR:O	2.13	0.82
5:B:877:PRO:HA	5:B:878:GLN:HB3	1.62	0.81
5:B:973:ILE:HG22	5:B:974:PRO:HD2	1.63	0.81
4:A:1191:TRP:HA	4:A:1192:LEU:CB	2.10	0.81
5:B:571:PRO:HB2	5:B:572:HIS:HA	1.60	0.81
5:B:498:THR:HB	5:B:537:LYS:O	1.81	0.81
10:I:20:LYS:HA	10:I:21:GLU:C	2.01	0.81
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.60	0.81
6:C:248:ILE:HG23	12:K:98:LEU:HD22	1.61	0.81
5:B:327:ARG:HB3	5:B:328:GLU:CB	2.04	0.81
10:I:43:VAL:HB	10:I:44:TYR:HA	1.61	0.81
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.16	0.80
5:B:349:ILE:HA	5:B:352:ALA:HB2	1.63	0.80
1:R:9:G:H22	2:T:21:DC:H1'	1.46	0.80
4:A:902:LEU:O	4:A:903:ASN:HB2	1.81	0.80
16:B:3000:UTP:H4'	16:B:3000:UTP:O2A	1.79	0.80
4:A:423:ASP:CG	4:A:424:ILE:H	1.85	0.79
4:A:1159:ARG:HB2	4:A:1161:THR:N	1.97	0.79
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.45	0.79
5:B:955:THR:HG22	5:B:956:THR:H	1.46	0.79
4:A:1083:THR:N	4:A:1084:PHE:O	2.16	0.79
4:A:1089:VAL:N	4:A:1090:ALA:HA	1.98	0.78
5:B:1008:PRO:HB3	5:B:1087:PHE:HE1	1.45	0.78
4:A:707:GLY:CA	4:A:709:THR:H	1.91	0.78
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.64	0.78
5:B:493:SER:OG	5:B:751:VAL:HB	1.83	0.78
5:B:600:LEU:HB3	5:B:615:MET:SD	2.24	0.78
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.66	0.77
4:A:351:THR:HG22	4:A:352:VAL:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.50	0.77
5:B:256:VAL:HG11	5:B:382:ILE:CD1	2.14	0.77
6:C:58:LEU:HD11	11:J:2:ILE:CD1	2.13	0.77
10:I:17:ARG:O	10:I:26:LEU:HB3	1.85	0.77
5:B:572:HIS:H	5:B:573:GLN:C	1.88	0.77
4:A:834:THR:HG21	4:A:1080:THR:HG21	1.66	0.77
5:B:801:LYS:O	11:J:52:THR:HG22	1.83	0.77
4:A:681:GLU:HA	4:A:684:ALA:HB3	1.66	0.77
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.67	0.77
4:A:278:THR:O	4:A:279:LEU:HB2	1.86	0.76
5:B:705:MET:H	5:B:710:LEU:HD13	1.51	0.76
5:B:277:LYS:HD2	5:B:335:GLY:H	1.50	0.76
13:L:32:ALA:H	13:L:55:ILE:HD13	1.50	0.76
13:L:42:ARG:CB	13:L:43:THR:HB	2.16	0.76
4:A:1228:TRP:HD1	4:A:1228:TRP:O	1.68	0.76
5:B:877:PRO:CA	5:B:878:GLN:CB	2.63	0.75
6:C:93:ASP:OD1	6:C:122:SER:HB2	1.87	0.75
4:A:675:THR:HG21	4:A:736:ASN:HD21	1.49	0.75
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.68	0.75
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.66	0.75
4:A:1072:ILE:HG22	4:A:1073:GLY:N	2.02	0.75
5:B:572:HIS:H	5:B:573:GLN:CA	1.99	0.75
4:A:1167:GLU:HB2	4:A:1168:GLU:HA	0.86	0.75
4:A:701:LEU:CA	4:A:702:LEU:CB	2.58	0.75
4:A:1159:ARG:HB2	4:A:1160:SER:C	2.07	0.75
4:A:1155:ASP:CG	4:A:1190:PRO:HA	2.07	0.75
4:A:1427:ASN:HB2	4:A:1434:ALA:HB2	1.69	0.74
4:A:579:SER:HA	4:A:582:ILE:CG1	2.17	0.74
4:A:1069:ALA:HB1	4:A:1070:GLN:HA	1.69	0.74
4:A:630:ILE:HD12	4:A:630:ILE:N	2.02	0.74
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.23	0.74
4:A:446:ARG:HH12	4:A:448:PRO:HD2	1.52	0.74
6:C:34:ARG:O	6:C:38:ILE:HG12	1.87	0.74
5:B:227:LYS:HA	5:B:228:LYS:CB	2.15	0.74
10:I:3:THR:HA	10:I:4:PHE:CB	2.17	0.74
9:H:111:LEU:HA	9:H:112:ILE:HB	1.70	0.73
4:A:1071:SER:N	4:A:1072:ILE:HB	2.02	0.73
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.51	0.73
6:C:58:LEU:HD12	6:C:145:CYS:SG	2.28	0.73
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.70	0.73
4:A:1092:LYS:HB3	4:A:1093:LYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1093:LYS:HB3	4:A:1094:VAL:HB	1.71	0.73
2:T:6:DG:H2"	2:T:7:DA:C8	2.23	0.73
4:A:751:SER:HB2	5:B:1015:HIS:HE1	1.53	0.73
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.53	0.73
5:B:864:LYS:H	5:B:872:GLU:HB2	1.54	0.73
4:A:282:ASN:HB3	4:A:283:GLY:HA3	1.70	0.73
10:I:20:LYS:HG2	10:I:24:ARG:H	1.54	0.73
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.70	0.72
10:I:43:VAL:CB	10:I:44:TYR:HA	2.17	0.72
13:L:42:ARG:HB2	13:L:43:THR:CB	2.16	0.72
4:A:638:GLY:H	4:A:641:VAL:HB	1.54	0.72
4:A:915:SER:HB2	4:A:919:ILE:HG12	1.72	0.72
5:B:636:PRO:CB	5:B:637:LEU:HA	2.18	0.72
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.70	0.72
5:B:1001:PHE:HE1	6:C:178:PHE:HB3	1.53	0.72
4:A:1091:SER:HB2	4:A:1092:LYS:O	1.88	0.72
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.52	0.72
11:J:43:ARG:HG3	11:J:46:CYS:SG	2.29	0.72
4:A:975:HIS:HB3	4:A:976:THR:HG1	1.51	0.72
5:B:882:THR:HG21	5:B:935:ARG:HA	1.70	0.72
4:A:579:SER:HA	4:A:582:ILE:HG13	1.71	0.72
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.72	0.72
5:B:705:MET:O	5:B:742:GLU:HB3	1.90	0.72
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.25	0.71
5:B:636:PRO:CB	5:B:637:LEU:CA	2.69	0.71
5:B:126:SER:OG	5:B:172:ILE:HD11	1.90	0.71
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.54	0.71
5:B:642:ASP:HA	5:B:649:LYS:HA	1.72	0.71
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.05	0.71
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.72	0.71
4:A:288:ALA:HA	4:A:290:GLU:N	2.06	0.70
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.56	0.70
4:A:1072:ILE:HG22	4:A:1073:GLY:H	1.56	0.70
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.74	0.70
10:I:4:PHE:HD1	10:I:4:PHE:C	1.94	0.70
5:B:842:ASN:HB3	5:B:845:SER:OG	1.91	0.70
4:A:1075:PRO:O	4:A:1079:MET:N	2.24	0.70
5:B:1156:ASP:HB2	5:B:1198:TYR:H	1.55	0.70
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.73	0.70
5:B:1019:SER:CA	5:B:1020:ARG:HB2	2.22	0.70
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:ASN:HD21	5:B:729:ILE:N	1.83	0.69
5:B:636:PRO:HB2	5:B:637:LEU:CA	2.23	0.69
4:A:288:ALA:HA	4:A:290:GLU:H	1.57	0.69
5:B:1177:HIS:HA	5:B:1178:ASN:HB2	1.74	0.69
6:C:142:VAL:HG13	11:J:15:GLY:HA3	1.73	0.69
5:B:986:GLN:HE21	5:B:1025:HIS:CD2	2.10	0.69
9:H:105:GLU:HG3	9:H:106:GLU:H	1.58	0.69
5:B:168:GLY:H	5:B:450:ALA:HB1	1.57	0.69
5:B:997:GLU:OE1	6:C:39:ALA:HB2	1.92	0.69
4:A:657:LEU:HD21	5:B:829:CYS:HB3	1.75	0.69
10:I:25:LEU:HA	10:I:26:LEU:HB3	1.72	0.69
4:A:1064:VAL:O	4:A:1068:ALA:N	2.26	0.69
10:I:25:LEU:CA	10:I:26:LEU:CB	2.70	0.68
10:I:33:SER:HA	10:I:34:TYR:HB3	1.75	0.68
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.76	0.68
5:B:363:HIS:O	5:B:364:ILE:HB	1.93	0.68
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.59	0.68
4:A:1083:THR:N	4:A:1084:PHE:C	2.47	0.68
4:A:446:ARG:NH1	4:A:448:PRO:HD2	2.09	0.68
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.74	0.67
4:A:1200:ALA:HB2	4:A:1203:ASN:HB2	1.77	0.67
5:B:827:ILE:HG12	5:B:1012:ILE:CD1	2.25	0.67
5:B:65:GLU:O	5:B:66:ASP:HB3	1.95	0.67
4:A:711:ARG:HA	4:A:713:SER:HB2	1.77	0.67
4:A:834:THR:HG21	4:A:1080:THR:CG2	2.25	0.67
4:A:1084:PHE:CD1	4:A:1085:HIS:HA	2.30	0.67
6:C:21:ILE:HG22	6:C:22:LEU:H	1.59	0.67
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.77	0.67
5:B:852:ARG:HG2	5:B:973:ILE:HG23	1.76	0.67
10:I:17:ARG:HB2	10:I:26:LEU:HD12	1.77	0.66
4:A:1085:HIS:CD2	4:A:1085:HIS:N	2.63	0.66
4:A:1085:HIS:H	4:A:1085:HIS:HD2	1.41	0.66
5:B:287:ARG:NH1	5:B:324:ILE:O	2.28	0.66
6:C:101:LEU:HD23	6:C:155:LEU:HD12	1.78	0.66
4:A:1069:ALA:HA	4:A:1072:ILE:HG21	1.77	0.66
4:A:1143:LEU:HB3	4:A:1268:LEU:HA	1.76	0.66
4:A:1228:TRP:CD1	4:A:1228:TRP:O	2.48	0.66
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.78	0.66
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.76	0.65
4:A:630:ILE:H	4:A:630:ILE:CD1	2.09	0.65
5:B:1137:CYS:O	5:B:1140:ALA:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:230:ALA:N	5:B:231:PRO:HD3	2.12	0.65
4:A:1104:ILE:HG22	4:A:1105:LEU:HD12	1.79	0.65
4:A:1159:ARG:HD2	4:A:1161:THR:HG23	1.77	0.65
4:A:994:GLN:HG3	4:A:1019:CYS:SG	2.36	0.65
9:H:88:SER:O	9:H:89:LEU:HB3	1.95	0.65
4:A:782:ARG:NH2	5:B:699:GLU:O	2.29	0.65
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.78	0.65
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.79	0.65
5:B:313:MET:HE2	5:B:386:LEU:HD22	1.78	0.65
5:B:709:ASP:HB3	5:B:710:LEU:HD12	1.79	0.65
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.78	0.65
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.62	0.65
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.78	0.64
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.78	0.64
4:A:381:THR:HG22	4:A:382:PRO:HD2	1.79	0.64
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.79	0.64
4:A:407:ARG:HD2	4:A:413:ILE:HD13	1.79	0.64
6:C:112:ASN:HD21	6:C:146:LYS:HE2	1.62	0.64
8:F:145:ASP:O	8:F:146:TRP:HB2	1.97	0.64
4:A:545:GLN:O	4:A:549:MET:HG3	1.97	0.64
5:B:421:PHE:O	5:B:424:LEU:HD23	1.96	0.64
5:B:572:HIS:N	5:B:573:GLN:HB3	2.12	0.64
5:B:711:GLU:H	5:B:712:PRO:CD	2.09	0.64
5:B:728:ARG:NH1	5:B:760:ASP:OD2	2.28	0.64
4:A:1092:LYS:HB3	4:A:1093:LYS:CA	2.26	0.64
4:A:1197:LEU:HA	4:A:1198:ASP:HB3	1.78	0.64
5:B:848:ARG:NH1	11:J:8:PHE:O	2.30	0.64
5:B:778:MET:HE1	5:B:853:SER:HB3	1.78	0.64
4:A:802:ASN:ND2	5:B:729:ILE:H	1.82	0.64
5:B:474:SER:HB2	5:B:476:ARG:HG3	1.79	0.64
5:B:886:LYS:HG2	5:B:940:PRO:HG3	1.78	0.64
6:C:84:ARG:HD2	12:K:11:LEU:HD11	1.79	0.64
5:B:572:HIS:H	5:B:573:GLN:HB3	1.61	0.64
5:B:579:ARG:HA	5:B:589:VAL:HA	1.80	0.64
4:A:849:MET:HB3	4:A:1063:MET:SD	2.38	0.64
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.79	0.64
4:A:845:LEU:HB2	4:A:1065:GLY:O	1.98	0.63
4:A:282:ASN:CB	4:A:283:GLY:HA3	2.28	0.63
5:B:286:PHE:HB3	5:B:297:ILE:HD11	1.81	0.63
4:A:10:PRO:HG2	5:B:1192:TYR:HA	1.81	0.63
5:B:882:THR:CG2	5:B:935:ARG:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:472:LEU:HD13	5:B:835:GLN:NE2	2.13	0.63
4:A:868:TYR:HE2	4:A:1366:ARG:HE	1.45	0.63
4:A:975:HIS:CB	4:A:976:THR:OG1	2.34	0.63
4:A:1421:CYS:HA	4:A:1426:GLU:HG2	1.81	0.62
5:B:572:HIS:H	5:B:573:GLN:CB	2.12	0.62
5:B:67:SER:HB2	5:B:92:PHE:H	1.63	0.62
4:A:265:LYS:HZ1	4:A:323:LYS:HE2	1.64	0.62
4:A:282:ASN:HB3	4:A:283:GLY:HA2	1.79	0.62
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.80	0.62
5:B:913:GLY:HA2	5:B:938:SER:HB3	1.81	0.62
10:I:4:PHE:C	10:I:4:PHE:CD1	2.69	0.62
4:A:269:ILE:HD11	4:A:300:VAL:HG23	1.81	0.62
5:B:785:TYR:HE2	11:J:60:PHE:CE1	2.17	0.62
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.34	0.62
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.35	0.62
5:B:524:PRO:HG3	5:B:748:ILE:HD12	1.79	0.62
5:B:785:TYR:CE2	11:J:60:PHE:CE1	2.87	0.62
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.64	0.62
5:B:782:LEU:HD13	5:B:784:ASN:ND2	2.13	0.62
4:A:1084:PHE:HA	4:A:1085:HIS:C	2.19	0.62
4:A:845:LEU:O	4:A:848:ILE:HG12	2.00	0.62
5:B:1082:MET:HG2	6:C:188:HIS:O	1.99	0.62
5:B:1008:PRO:HB3	5:B:1087:PHE:CE1	2.32	0.62
4:A:466:SER:O	5:B:1103:ILE:HD11	1.99	0.62
6:C:20:PHE:HD1	6:C:21:ILE:O	1.82	0.62
7:E:16:PHE:CE2	7:E:20:LYS:HE2	2.34	0.62
5:B:877:PRO:CA	5:B:878:GLN:HB3	2.29	0.62
4:A:1083:THR:HG23	4:A:1084:PHE:HD2	1.64	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.88	0.62
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.63	0.62
4:A:1093:LYS:H	4:A:1095:THR:H	1.49	0.61
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.34	0.61
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	1.80	0.61
5:B:778:MET:CE	5:B:853:SER:HB3	2.29	0.61
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.82	0.61
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.30	0.61
5:B:955:THR:HG22	5:B:956:THR:N	2.13	0.61
9:H:82:PRO:O	9:H:83:GLN:HB3	2.00	0.61
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.64	0.61
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.35	0.61
6:C:166:GLU:O	6:C:167:HIS:HB2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.83	0.61
12:K:20:LYS:HB3	12:K:34:THR:HB	1.81	0.61
4:A:68:GLN:HG2	4:A:68:GLN:O	2.01	0.61
5:B:227:LYS:CA	5:B:228:LYS:HB2	2.18	0.61
9:H:111:LEU:HD12	9:H:127:GLY:HA2	1.82	0.61
4:A:1162:VAL:HA	4:A:1163:ILE:O	2.00	0.61
4:A:320:ARG:HB2	4:A:321:PRO:HA	1.83	0.61
4:A:840:ARG:HG2	4:A:1402:PHE:HZ	1.65	0.61
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.82	0.61
6:C:171:GLY:C	6:C:173:ALA:H	2.03	0.61
5:B:351:TYR:H	5:B:354:ASP:HB2	1.66	0.61
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.82	0.61
4:A:523:ILE:HD13	4:A:622:VAL:HG22	1.83	0.60
5:B:803:LEU:N	5:B:822:ASN:HD21	1.99	0.60
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.81	0.60
9:H:109:LYS:CG	9:H:110:ASP:HB2	2.31	0.60
5:B:785:TYR:CE2	11:J:60:PHE:HE1	2.18	0.60
4:A:961:ARG:NH1	4:A:965:GLN:HE22	2.00	0.60
5:B:123:THR:HG23	5:B:205:ILE:HA	1.81	0.60
6:C:56:THR:HG21	6:C:145:CYS:SG	2.40	0.60
4:A:1070:GLN:O	4:A:1074:GLU:HB2	2.01	0.60
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.66	0.60
5:B:549:THR:HB	5:B:628:THR:CG2	2.31	0.60
5:B:779:GLY:O	5:B:795:ILE:HA	2.01	0.60
4:A:834:THR:OG1	4:A:1077:THR:HA	2.02	0.60
4:A:901:LEU:H	4:A:926:GLN:NE2	1.99	0.60
6:C:45:ALA:HA	6:C:72:LEU:HD13	1.83	0.60
11:J:43:ARG:HH11	11:J:43:ARG:HB3	1.66	0.60
4:A:68:GLN:HE22	4:A:80:HIS:CE1	2.20	0.60
2:T:6:DG:H2"	2:T:7:DA:H8	1.65	0.60
4:A:440:ASP:O	4:A:460:VAL:HG23	2.02	0.60
1:R:10:A:N6	2:T:19:DT:H3	1.92	0.60
4:A:675:THR:CG2	4:A:736:ASN:HD21	2.14	0.60
9:H:83:GLN:O	9:H:83:GLN:HG3	2.01	0.60
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.67	0.59
5:B:1176:ASN:O	5:B:1177:HIS:CG	2.55	0.59
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.68	0.59
4:A:855:THR:HG23	4:A:857:ARG:HE	1.65	0.59
5:B:977:GLY:HA3	5:B:1099:VAL:CG1	2.32	0.59
5:B:1156:ASP:OD2	5:B:1156:ASP:N	2.34	0.59
5:B:391:ASP:CA	5:B:392:ARG:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.84	0.59
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.31	0.59
5:B:806:THR:HG22	5:B:1046:PRO:HD3	1.83	0.59
5:B:706:GLN:HB3	5:B:709:ASP:HB2	1.85	0.59
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.84	0.59
4:A:451:HIS:HB3	4:A:453:MET:N	2.16	0.59
9:H:84:ALA:HA	9:H:86:ASP:N	2.16	0.59
5:B:801:LYS:O	11:J:52:THR:CG2	2.50	0.59
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.85	0.59
4:A:567:LYS:O	4:A:569:LYS:N	2.34	0.59
5:B:424:LEU:O	5:B:428:ILE:HG12	2.02	0.59
5:B:882:THR:CB	5:B:883:LEU:HA	2.23	0.59
8:F:81:THR:HG22	8:F:82:THR:H	1.67	0.59
4:A:1223:ASP:O	4:A:1224:LEU:HB2	2.02	0.59
5:B:25:ILE:HD12	5:B:651:LEU:HD13	1.84	0.59
5:B:213:ILE:HD13	5:B:497:ARG:HB3	1.85	0.59
4:A:90:VAL:HG13	4:A:297:GLN:OE1	2.03	0.59
4:A:579:SER:OG	4:A:612:ILE:HG22	2.02	0.59
4:A:699:ALA:N	4:A:700:ASN:HA	2.17	0.59
5:B:1031:LEU:HD13	5:B:1055:ILE:HD12	1.85	0.59
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.84	0.59
4:A:1093:LYS:HB3	4:A:1094:VAL:CB	2.33	0.59
5:B:287:ARG:HH21	5:B:294:ASP:CG	2.06	0.59
7:E:111:VAL:HG12	7:E:137:GLU:HG2	1.84	0.59
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.03	0.58
5:B:558:LEU:HB3	5:B:563:MET:SD	2.42	0.58
4:A:449:SER:HB2	5:B:1137:CYS:SG	2.43	0.58
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.38	0.58
4:A:579:SER:HA	4:A:582:ILE:HG12	1.85	0.58
5:B:292:ILE:HD12	5:B:326:ASP:HA	1.84	0.58
5:B:709:ASP:HB3	5:B:710:LEU:HB2	1.85	0.58
5:B:831:SER:HB2	5:B:833:TYR:HD1	1.66	0.58
7:E:65:THR:C	7:E:67:GLU:H	2.06	0.58
4:A:364:VAL:HG12	4:A:459:ARG:O	2.02	0.58
5:B:239:GLU:HG3	5:B:255:GLN:HG2	1.84	0.58
5:B:351:TYR:CD2	5:B:355:ILE:HD11	2.38	0.58
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.38	0.58
5:B:1162:ILE:HG12	5:B:1194:ILE:HD12	1.85	0.58
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.18	0.58
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.69	0.58
4:A:1084:PHE:HD1	4:A:1086:PHE:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:35:SER:HA	5:B:811:TYR:HE2	1.69	0.58
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.85	0.58
8:F:127:GLU:O	8:F:129:LYS:N	2.36	0.58
4:A:800:VAL:HG11	4:A:808:LEU:HG	1.86	0.58
4:A:928:LEU:HA	4:A:931:GLU:HB2	1.86	0.58
7:E:198:ILE:HB	7:E:210:SER:HB3	1.86	0.58
2:T:27:DA:N3	2:T:27:DA:H2'	2.19	0.58
4:A:1154:TYR:O	4:A:1192:LEU:HG	2.04	0.57
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.86	0.57
5:B:975:GLN:O	5:B:990:ILE:HD12	2.03	0.57
5:B:1168:LEU:HD21	5:B:1214:PRO:HD2	1.86	0.57
6:C:251:LEU:O	6:C:255:VAL:HG23	2.05	0.57
9:H:56:THR:O	9:H:144:ILE:HA	2.05	0.57
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.85	0.57
7:E:144:ILE:HG13	7:E:145:THR:H	1.69	0.57
4:A:115:LEU:HD11	4:A:145:LYS:HD2	1.87	0.57
5:B:1177:HIS:CA	5:B:1178:ASN:HB2	2.34	0.57
11:J:57:ILE:O	11:J:61:LEU:HG	2.05	0.57
5:B:977:GLY:HA3	5:B:1099:VAL:HG13	1.87	0.57
5:B:391:ASP:N	5:B:392:ARG:HB2	2.20	0.57
5:B:941:LEU:HD23	5:B:942:ARG:H	1.70	0.57
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.86	0.57
5:B:270:LYS:HA	5:B:281:PRO:HA	1.86	0.57
4:A:534:LEU:O	4:A:574:GLY:HA3	2.05	0.57
4:A:901:LEU:HA	4:A:907:THR:HG23	1.87	0.57
5:B:525:ALA:O	5:B:768:THR:HG23	2.03	0.57
4:A:1077:THR:O	4:A:1081:LEU:HB3	2.05	0.56
4:A:1092:LYS:CB	4:A:1093:LYS:HB2	2.35	0.56
4:A:313:GLN:HE21	4:A:322:VAL:HG11	1.70	0.56
5:B:1019:SER:CA	5:B:1020:ARG:CB	2.82	0.56
10:I:20:LYS:HG2	10:I:24:ARG:N	2.20	0.56
4:A:648:ASN:O	4:A:652:VAL:HG23	2.05	0.56
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.88	0.56
4:A:698:GLN:HA	10:I:97:MET:O	2.06	0.56
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.40	0.56
4:A:596:THR:C	4:A:598:LEU:H	2.09	0.56
4:A:95:PHE:O	4:A:99:ILE:HG13	2.05	0.56
10:I:14:LEU:HD23	10:I:27:PHE:HB3	1.87	0.56
10:I:92:ARG:NE	10:I:92:ARG:HA	2.20	0.56
4:A:663:SER:CB	5:B:827:ILE:O	2.54	0.56
5:B:354:ASP:O	5:B:358:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:969:GLN:HA	4:A:972:HIS:HB3	1.88	0.56
4:A:351:THR:HG22	4:A:352:VAL:H	1.70	0.56
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.88	0.56
10:I:3:THR:HA	10:I:4:PHE:CD2	2.37	0.56
4:A:731:ARG:CG	4:A:755:PHE:HE1	2.19	0.56
5:B:764:SER:N	5:B:765:PRO:HD2	2.21	0.56
5:B:974:PRO:HA	5:B:1094:ARG:HH21	1.70	0.56
4:A:1096:SER:N	4:A:1097:GLY:HA3	2.21	0.56
4:A:855:THR:CG2	4:A:857:ARG:HE	2.18	0.56
5:B:180:TYR:HD1	5:B:180:TYR:H	1.54	0.56
7:E:15:ALA:HA	7:E:141:VAL:H	1.70	0.56
11:J:53:HIS:HE1	11:J:55:ASP:OD1	1.89	0.56
4:A:1092:LYS:HB3	4:A:1093:LYS:CB	2.36	0.55
4:A:596:THR:HB	4:A:598:LEU:HB2	1.88	0.55
4:A:731:ARG:HG3	4:A:755:PHE:CZ	2.40	0.55
5:B:1019:SER:N	5:B:1020:ARG:HB3	2.20	0.55
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.71	0.55
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.41	0.55
4:A:1319:VAL:HB	4:A:1322:ILE:HD12	1.88	0.55
5:B:1120:GLU:HB3	5:B:1124:ARG:HH12	1.71	0.55
5:B:469:GLN:HE21	5:B:470:LYS:HE3	1.71	0.55
9:H:109:LYS:H	9:H:110:ASP:C	2.10	0.55
4:A:1105:LEU:HB3	4:A:1384:VAL:HB	1.89	0.55
5:B:485:ARG:NH2	5:B:782:LEU:HD11	2.21	0.55
4:A:868:TYR:CE1	4:A:1064:VAL:HG21	2.41	0.55
4:A:284:ALA:N	4:A:285:PRO:CD	2.56	0.55
4:A:442:VAL:HG12	4:A:491:VAL:HG22	1.88	0.55
5:B:708:GLU:HA	5:B:711:GLU:HG2	1.88	0.55
5:B:879:ARG:O	5:B:880:THR:HG22	2.06	0.55
6:C:18:VAL:HG12	6:C:20:PHE:CD2	2.41	0.55
6:C:82:TYR:HB2	6:C:85:ASP:HB2	1.88	0.55
11:J:3:VAL:HG22	11:J:53:HIS:CE1	2.42	0.55
4:A:1151:GLU:HA	10:I:45:ARG:HB3	1.89	0.55
4:A:456:MET:HB2	4:A:478:TYR:OH	2.06	0.55
4:A:389:THR:OG1	4:A:426:LEU:HD12	2.07	0.55
4:A:667:GLY:HA2	4:A:670:ILE:HG13	1.89	0.55
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.71	0.55
4:A:351:THR:CG2	4:A:352:VAL:N	2.68	0.55
4:A:617:VAL:HG12	4:A:622:VAL:HB	1.89	0.55
4:A:683:ILE:HG22	4:A:687:LYS:HG3	1.88	0.55
5:B:518:HIS:CE1	5:B:537:LYS:HE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:614:SER:HB3	5:B:694:ASP:OD1	2.07	0.55
5:B:878:GLN:HG3	5:B:881:ASN:HB2	1.87	0.55
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.72	0.55
4:A:219:PHE:O	4:A:222:LEU:O	2.24	0.55
5:B:303:TYR:HH	5:B:586:TRP:HH2	1.55	0.55
5:B:512:ARG:NH2	5:B:532:ALA:HA	2.21	0.55
10:I:42:LEU:CD2	10:I:43:VAL:H	2.20	0.55
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.88	0.55
7:E:29:PHE:O	7:E:30:ILE:HB	2.07	0.55
10:I:101:PHE:HB2	10:I:110:PHE:CZ	2.41	0.55
4:A:1075:PRO:O	4:A:1079:MET:HG3	2.07	0.54
5:B:350:GLN:HB3	5:B:351:TYR:CB	2.31	0.54
4:A:1092:LYS:HB2	4:A:1093:LYS:HB2	1.90	0.54
4:A:1093:LYS:CB	4:A:1094:VAL:HB	2.36	0.54
4:A:438:ASP:HA	4:A:460:VAL:O	2.07	0.54
5:B:391:ASP:HA	5:B:392:ARG:HB2	1.88	0.54
5:B:707:PRO:HA	5:B:741:CYS:SG	2.47	0.54
5:B:851:PHE:CD2	5:B:1094:ARG:HB2	2.42	0.54
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.31	0.54
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.42	0.54
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.88	0.54
4:A:1287:TYR:HD2	4:A:1305:VAL:HB	1.72	0.54
4:A:629:LEU:O	4:A:633:VAL:HG23	2.08	0.54
7:E:35:VAL:C	7:E:37:LEU:H	2.11	0.54
11:J:6:ARG:HA	11:J:12:LYS:O	2.07	0.54
4:A:1227:ILE:HA	4:A:1228:TRP:CG	2.42	0.54
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.37	0.54
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.07	0.54
4:A:827:THR:OG1	4:A:1083:THR:HG21	2.07	0.54
4:A:909:ASP:C	4:A:911:SER:H	2.11	0.54
6:C:173:ALA:O	6:C:233:GLU:O	2.24	0.54
4:A:1073:GLY:O	4:A:1077:THR:OG1	2.15	0.54
4:A:232:GLU:HG3	4:A:233:TRP:CD1	2.43	0.54
4:A:350:ARG:HD3	4:A:488:ASN:OD1	2.07	0.54
4:A:375:THR:HA	4:A:434:ARG:O	2.08	0.54
6:C:66:ARG:NH2	11:J:4:PRO:HA	2.23	0.54
4:A:8:SER:O	4:A:10:PRO:HD3	2.08	0.53
5:B:515:HIS:H	5:B:518:HIS:CD2	2.25	0.53
10:I:17:ARG:HA	10:I:18:GLU:HB3	1.90	0.53
5:B:237:VAL:HG22	5:B:257:LYS:HG2	1.90	0.53
5:B:573:GLN:O	5:B:575:PRO:HD3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1194:ARG:O	4:A:1195:LEU:HB2	2.08	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HD13	1.90	0.53
5:B:973:ILE:CG2	5:B:974:PRO:HD2	2.37	0.53
9:H:96:VAL:HA	9:H:142:LEU:O	2.09	0.53
4:A:1264:GLU:HA	4:A:1267:MET:HB2	1.91	0.53
4:A:278:THR:O	4:A:279:LEU:CB	2.57	0.53
4:A:930:ASP:HA	4:A:933:TYR:HB3	1.91	0.53
4:A:973:ILE:HG23	4:A:974:ASP:HA	1.90	0.53
5:B:115:GLN:CD	5:B:118:ARG:HH21	2.12	0.53
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.42	0.53
9:H:81:PRO:HB2	9:H:82:PRO:CD	2.39	0.53
5:B:515:HIS:H	5:B:518:HIS:HD2	1.57	0.53
6:C:182:PRO:HG3	6:C:206:ASN:O	2.09	0.53
10:I:43:VAL:CG1	10:I:44:TYR:HA	2.38	0.53
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.72	0.53
4:A:573:SER:O	4:A:576:GLN:HB2	2.08	0.53
6:C:64:ALA:HA	6:C:67:LEU:HD12	1.90	0.53
7:E:7:ARG:HA	7:E:10:SER:HB3	1.91	0.53
4:A:1115:SER:HA	4:A:1308:THR:O	2.08	0.53
4:A:847:ASP:HB3	4:A:1424:VAL:HG23	1.90	0.53
6:C:13:ALA:HA	6:C:17:ASN:O	2.09	0.53
13:L:60:ARG:HG3	13:L:61:THR:H	1.73	0.53
4:A:1236:LEU:CA	4:A:1237:ILE:HB	2.30	0.53
5:B:223:VAL:HG22	5:B:240:ILE:HD12	1.91	0.53
7:E:35:VAL:O	7:E:37:LEU:N	2.38	0.53
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.91	0.53
4:A:482:PHE:C	4:A:484:GLY:H	2.12	0.53
5:B:1159:ARG:HE	5:B:1193:GLN:NE2	2.08	0.53
5:B:637:LEU:HA	5:B:743:ILE:HD11	1.91	0.53
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.44	0.53
4:A:1067:LEU:O	4:A:1069:ALA:O	2.28	0.52
4:A:380:VAL:HG22	4:A:430:TRP:H	1.74	0.52
4:A:794:PRO:C	4:A:796:SER:H	2.12	0.52
4:A:818:MET:HG2	5:B:514:LEU:HD23	1.91	0.52
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.92	0.52
5:B:293:PRO:HA	5:B:294:ASP:CB	2.25	0.52
5:B:785:TYR:HE2	11:J:60:PHE:CZ	2.25	0.52
5:B:122:LEU:CD2	5:B:958:GLN:HG3	2.32	0.52
7:E:194:GLU:O	7:E:214:CYS:HB2	2.08	0.52
5:B:408:LEU:HD23	5:B:545:ILE:HG21	1.92	0.52
5:B:589:VAL:HG12	5:B:590:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:17:ARG:HB3	10:I:18:GLU:O	2.09	0.52
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.90	0.52
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.37	0.52
5:B:649:LYS:HE2	5:B:737:THR:HA	1.92	0.52
9:H:109:LYS:HG2	9:H:110:ASP:HB2	1.90	0.52
4:A:266:LEU:O	4:A:269:ILE:HG22	2.09	0.52
4:A:579:SER:HB3	4:A:611:GLN:HA	1.91	0.52
4:A:623:GLY:C	4:A:625:SER:H	2.13	0.52
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.91	0.52
5:B:557:PHE:O	5:B:561:TRP:CB	2.53	0.52
12:K:82:ASP:OD1	12:K:83:PRO:HD2	2.10	0.52
4:A:98:LYS:O	4:A:102:VAL:HG23	2.09	0.52
4:A:446:ARG:HD2	4:A:480:ALA:HB2	1.92	0.52
5:B:571:PRO:N	5:B:572:HIS:HB2	2.25	0.52
6:C:62:PHE:O	6:C:66:ARG:HG3	2.08	0.52
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.90	0.52
5:B:708:GLU:O	5:B:712:PRO:HD3	2.09	0.52
10:I:21:GLU:O	10:I:22:ASN:HB3	2.10	0.52
4:A:1156:PRO:O	4:A:1157:ASP:HB2	2.09	0.52
4:A:681:GLU:HA	4:A:684:ALA:CB	2.39	0.52
6:C:3:GLU:HG3	6:C:4:GLU:H	1.75	0.52
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.91	0.52
4:A:1200:ALA:HA	4:A:1201:ALA:C	2.29	0.52
4:A:1100:ARG:O	4:A:1103:GLU:HB2	2.10	0.52
5:B:498:THR:O	5:B:536:VAL:HA	2.10	0.52
2:T:26:DG:C2	2:T:27:DA:H1'	2.44	0.52
4:A:768:GLN:NE2	4:A:1087:ALA:HB1	2.25	0.52
4:A:1093:LYS:HB3	4:A:1094:VAL:CG2	2.39	0.52
4:A:642:CYS:O	4:A:645:LEU:HB3	2.10	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.10	0.52
4:A:751:SER:CB	5:B:1015:HIS:CE1	2.93	0.52
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.91	0.52
5:B:471:LYS:O	5:B:474:SER:HB3	2.10	0.52
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.92	0.52
5:B:40:GLU:OE1	5:B:682:SER:HB2	2.10	0.51
6:C:37:MET:HA	6:C:41:ILE:HD11	1.92	0.51
9:H:129:TYR:O	9:H:130:ARG:HG2	2.09	0.51
4:A:387:ARG:O	4:A:391:LEU:HD23	2.11	0.51
4:A:423:ASP:CG	4:A:424:ILE:N	2.59	0.51
4:A:663:SER:HA	5:B:1014:PRO:HG3	1.91	0.51
11:J:6:ARG:HB3	11:J:11:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:407:ARG:HD3	4:A:411:ASP:HB2	1.93	0.51
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.92	0.51
5:B:1177:HIS:HA	5:B:1178:ASN:CB	2.38	0.51
5:B:603:LEU:HB3	5:B:609:ILE:HG12	1.93	0.51
6:C:48:SER:HB3	6:C:158:VAL:HB	1.92	0.51
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.93	0.51
5:B:638:PHE:O	5:B:740:HIS:HB2	2.10	0.51
5:B:1075:GLY:O	6:C:35:ARG:HD2	2.11	0.51
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.43	0.51
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.39	0.51
13:L:55:ILE:HD12	13:L:56:LEU:H	1.76	0.51
4:A:1156:PRO:HG2	4:A:1163:ILE:HG12	1.93	0.51
4:A:1394:THR:HG22	4:A:1398:MET:HE1	1.92	0.51
4:A:550:LEU:HD12	4:A:556:TRP:NE1	2.25	0.51
4:A:546:VAL:HG21	4:A:572:TRP:CE3	2.46	0.51
5:B:613:VAL:HG22	5:B:628:THR:HG23	1.93	0.51
6:C:66:ARG:NH2	11:J:3:VAL:O	2.43	0.51
2:T:16:DC:C6	2:T:17:DG:C8	2.98	0.51
4:A:710:LEU:HA	4:A:713:SER:HB2	1.92	0.51
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.11	0.51
5:B:1019:SER:N	5:B:1020:ARG:CB	2.74	0.51
5:B:288:ALA:HB1	5:B:331:LEU:HG	1.93	0.51
5:B:518:HIS:HE1	5:B:537:LYS:HE2	1.75	0.51
5:B:815:ARG:HD3	5:B:1041:GLU:OE2	2.11	0.51
4:A:1391:ARG:O	4:A:1393:ASN:N	2.43	0.51
4:A:1411:GLU:HA	4:A:1414:ALA:HB3	1.92	0.51
4:A:1434:ALA:O	4:A:1436:ILE:N	2.44	0.51
5:B:1156:ASP:CB	5:B:1198:TYR:H	2.21	0.51
4:A:403:LYS:O	4:A:433:GLU:O	2.29	0.51
4:A:731:ARG:HG2	4:A:755:PHE:HE1	1.76	0.51
4:A:834:THR:O	4:A:837:ILE:HB	2.11	0.51
5:B:983:ARG:HH11	5:B:1091:TYR:HB3	1.76	0.51
5:B:637:LEU:O	5:B:690:VAL:HG13	2.10	0.51
5:B:745:PRO:O	5:B:747:MET:N	2.44	0.51
10:I:29:CYS:H	10:I:33:SER:HB2	1.76	0.51
10:I:43:VAL:HB	10:I:44:TYR:CA	2.38	0.51
11:J:43:ARG:NH1	11:J:43:ARG:HB3	2.26	0.51
4:A:1071:SER:H	4:A:1072:ILE:CB	2.11	0.50
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.46	0.50
4:A:814:PHE:HB2	5:B:519:TRP:HZ3	1.76	0.50
5:B:552:MET:HB2	5:B:553:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:115:TYR:HE2	9:H:124:ARG:HG3	1.76	0.50
6:C:66:ARG:HH21	11:J:4:PRO:HA	1.75	0.50
12:K:65:HIS:O	12:K:67:PHE:N	2.44	0.50
4:A:1091:SER:HB2	4:A:1093:LYS:N	2.26	0.50
4:A:330:LYS:O	4:A:334:GLY:HA3	2.10	0.50
4:A:663:SER:HB2	5:B:827:ILE:O	2.11	0.50
6:C:133:ILE:HD11	6:C:237:SER:HA	1.92	0.50
6:C:57:VAL:HG11	11:J:60:PHE:CD1	2.46	0.50
4:A:1171:GLN:C	4:A:1173:HIS:N	2.64	0.50
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.52	0.50
5:B:364:ILE:O	5:B:365:THR:HB	2.11	0.50
6:C:36:VAL:HG21	6:C:251:LEU:HD13	1.93	0.50
9:H:105:GLU:CG	9:H:106:GLU:H	2.23	0.50
9:H:6:PHE:O	9:H:7:ASP:HB3	2.11	0.50
13:L:29:TYR:HB3	13:L:56:LEU:HD22	1.93	0.50
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.93	0.50
4:A:1069:ALA:C	4:A:1071:SER:N	2.65	0.50
4:A:374:LEU:O	4:A:436:ILE:HG13	2.11	0.50
4:A:407:ARG:HD2	4:A:413:ILE:CD1	2.42	0.50
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.11	0.50
6:C:77:ILE:HD12	6:C:161:LYS:HE3	1.93	0.50
8:F:103:MET:O	8:F:105:ALA:N	2.45	0.50
4:A:1390:ASN:ND2	4:A:1402:PHE:HB3	2.26	0.50
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.24	0.50
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.42	0.50
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.93	0.50
4:A:1157:ASP:C	4:A:1159:ARG:N	2.65	0.50
4:A:1167:GLU:CB	4:A:1168:GLU:CA	2.62	0.50
4:A:667:GLY:HA2	4:A:670:ILE:CG1	2.42	0.50
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.10	0.50
5:B:635:ARG:O	5:B:636:PRO:O	2.30	0.50
10:I:33:SER:HA	10:I:34:TYR:CB	2.39	0.50
4:A:407:ARG:CD	4:A:413:ILE:HD13	2.41	0.50
4:A:712:GLU:H	4:A:713:SER:CA	2.24	0.50
4:A:822:GLU:O	4:A:825:ILE:HB	2.11	0.50
4:A:452:LYS:HB3	5:B:1140:ALA:HB1	1.93	0.50
5:B:124:TYR:OH	5:B:179:CYS:SG	2.49	0.50
5:B:190:TYR:CZ	5:B:196:PRO:HG3	2.47	0.50
5:B:54:PHE:HB2	5:B:410:GLY:HA2	1.93	0.50
10:I:111:THR:HG22	10:I:112:SER:H	1.76	0.50
4:A:350:ARG:O	4:A:351:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.46	0.49
4:A:528:LEU:HD23	4:A:751:SER:HA	1.94	0.49
13:L:28:LYS:HB2	13:L:39:SER:HA	1.94	0.49
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	2.15	0.49
5:B:108:VAL:HG12	5:B:109:THR:H	1.77	0.49
5:B:179:CYS:SG	5:B:181:LEU:HG	2.52	0.49
5:B:549:THR:HG22	5:B:550:ASP:H	1.76	0.49
9:H:102:TYR:N	9:H:102:TYR:CD2	2.80	0.49
10:I:3:THR:HG22	10:I:4:PHE:CE2	2.47	0.49
10:I:42:LEU:HD22	10:I:43:VAL:H	1.76	0.49
4:A:1082:ASN:C	4:A:1084:PHE:O	2.51	0.49
4:A:1086:PHE:N	4:A:1086:PHE:CD1	2.79	0.49
4:A:455:MET:CE	5:B:1134:GLU:HG3	2.42	0.49
5:B:1177:HIS:CB	5:B:1178:ASN:HB2	2.42	0.49
5:B:357:GLN:HA	5:B:374:LYS:HZ1	1.76	0.49
5:B:579:ARG:HB3	5:B:589:VAL:HG22	1.94	0.49
5:B:708:GLU:O	5:B:708:GLU:HG2	2.12	0.49
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.93	0.49
10:I:5:ARG:HG2	10:I:6:PHE:H	1.77	0.49
4:A:754:SER:N	4:A:757:ASN:HD22	2.11	0.49
4:A:826:ASP:HA	4:A:830:LYS:H	1.76	0.49
4:A:961:ARG:O	4:A:965:GLN:NE2	2.45	0.49
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.94	0.49
4:A:575:LYS:HD2	9:H:120:GLY:HA3	1.94	0.49
4:A:1436:ILE:HG22	4:A:1437:GLY:N	2.27	0.49
4:A:903:ASN:O	4:A:907:THR:OG1	2.30	0.49
4:A:976:THR:H	4:A:1036:ARG:NH1	2.11	0.49
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.48	0.49
5:B:549:THR:HB	5:B:628:THR:HG21	1.95	0.49
5:B:59:LEU:HA	5:B:62:ILE:HD12	1.93	0.49
5:B:955:THR:CG2	5:B:956:THR:H	2.23	0.49
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.95	0.49
4:A:853:ASP:OD2	4:A:855:THR:HG22	2.12	0.49
5:B:976:ILE:HD11	5:B:992:ILE:HA	1.94	0.49
4:A:731:ARG:CG	4:A:755:PHE:CE1	2.95	0.49
5:B:291:ILE:HD12	5:B:291:ILE:H	1.78	0.49
4:A:1152:ILE:CA	4:A:1153:TYR:HB2	2.36	0.49
5:B:880:THR:H	5:B:883:LEU:HD12	1.77	0.49
4:A:1070:GLN:O	4:A:1074:GLU:N	2.46	0.49
4:A:1161:THR:O	4:A:1163:ILE:HG12	2.12	0.49
5:B:811:TYR:N	5:B:811:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:81:THR:HG22	8:F:82:THR:N	2.27	0.49
4:A:788:SER:HB3	10:I:69:PRO:HD3	1.93	0.49
13:L:62:LYS:H	13:L:62:LYS:HD2	1.78	0.49
4:A:1311:VAL:HG22	4:A:1329:THR:HG21	1.95	0.49
5:B:302:CYS:HB2	5:B:310:MET:HG2	1.95	0.49
4:A:1341:ILE:HB	7:E:182:ASP:OD1	2.13	0.49
11:J:23:ASN:O	11:J:27:GLU:HB3	2.11	0.49
4:A:1411:GLU:O	4:A:1415:SER:N	2.38	0.48
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.43	0.48
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.78	0.48
6:C:239:PRO:O	6:C:243:VAL:HG23	2.13	0.48
4:A:987:VAL:C	4:A:989:GLY:H	2.16	0.48
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.43	0.48
4:A:320:ARG:CB	4:A:321:PRO:HA	2.43	0.48
4:A:707:GLY:CA	4:A:709:THR:N	2.62	0.48
5:B:825:VAL:HG21	5:B:1090:THR:HB	1.95	0.48
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.95	0.48
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.31	0.48
5:B:230:ALA:C	5:B:232:SER:HB3	2.33	0.48
5:B:487:THR:HG22	5:B:488:TYR:N	2.27	0.48
5:B:872:GLU:HG2	5:B:916:THR:HB	1.94	0.48
4:A:517:ASN:ND2	4:A:1364:ASN:OD1	2.44	0.48
5:B:640:VAL:HG13	5:B:650:GLU:O	2.14	0.48
4:A:663:SER:HB3	5:B:827:ILE:O	2.14	0.48
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.95	0.48
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.13	0.48
4:A:442:VAL:CG1	4:A:491:VAL:HG22	2.43	0.48
4:A:775:ILE:HB	4:A:797:LYS:O	2.13	0.48
4:A:821:ARG:O	4:A:825:ILE:HG12	2.13	0.48
4:A:491:VAL:H	5:B:1150:ARG:NH2	2.11	0.48
7:E:43:LYS:O	7:E:47:CYS:HB3	2.12	0.48
4:A:332:LYS:C	4:A:334:GLY:H	2.17	0.48
4:A:492:PRO:O	4:A:493:GLN:NE2	2.46	0.48
4:A:754:SER:H	4:A:757:ASN:HD22	1.60	0.48
4:A:768:GLN:HE22	4:A:1087:ALA:HB1	1.79	0.48
6:C:173:ALA:O	6:C:174:ALA:HB3	2.13	0.48
12:K:38:GLU:HG3	12:K:42:LEU:HD22	1.96	0.48
4:A:1082:ASN:HB3	4:A:1084:PHE:O	2.12	0.48
4:A:350:ARG:HH11	4:A:488:ASN:HD21	1.60	0.48
4:A:515:GLN:HG3	4:A:1071:SER:HB3	1.96	0.48
5:B:636:PRO:CB	5:B:637:LEU:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.95	0.48
5:B:1175:LEU:HB2	5:B:1176:ASN:HA	1.94	0.48
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.46	0.48
6:C:3:GLU:HG2	12:K:104:ASN:OD1	2.13	0.48
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.94	0.48
4:A:1030:ARG:HD3	4:A:1034:GLU:HG3	1.94	0.48
4:A:702:LEU:HG	4:A:704:ALA:HB2	1.96	0.48
5:B:520:GLY:HA2	5:B:748:ILE:HA	1.94	0.48
4:A:332:LYS:H	4:A:337:ARG:HB2	1.79	0.48
4:A:897:TYR:CD2	4:A:936:LEU:HD21	2.48	0.48
5:B:571:PRO:HB2	5:B:572:HIS:CA	2.36	0.48
10:I:103:CYS:SG	10:I:106:CYS:CB	3.00	0.48
2:T:17:DG:H5"	2:T:18:DA:OP1	2.13	0.48
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.18	0.47
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.14	0.47
4:A:56:PRO:HA	4:A:57:ARG:HA	1.62	0.47
5:B:95:ILE:HD12	5:B:130:VAL:HG22	1.96	0.47
5:B:839:MET:O	5:B:990:ILE:HA	2.14	0.47
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.79	0.47
4:A:623:GLY:O	4:A:625:SER:N	2.44	0.47
4:A:818:MET:CG	5:B:514:LEU:HD23	2.43	0.47
5:B:996:ARG:HH12	6:C:173:ALA:CB	2.27	0.47
7:E:55:ARG:HB3	7:E:82:PHE:HB3	1.96	0.47
6:C:35:ARG:HH12	12:K:41:THR:N	2.13	0.47
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.14	0.47
7:E:18:THR:HG21	7:E:140:LEU:HB2	1.96	0.47
4:A:1081:LEU:O	4:A:1083:THR:HG22	2.13	0.47
4:A:707:GLY:O	4:A:1283:VAL:HG21	2.14	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.49	0.47
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.47	0.47
5:B:294:ASP:H	5:B:297:ILE:HB	1.78	0.47
4:A:1343:ALA:HB2	7:E:150:VAL:HG22	1.97	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.95	0.47
5:B:841:MET:HA	5:B:1009:ASP:O	2.13	0.47
4:A:490:HIS:ND1	5:B:1150:ARG:NH1	2.63	0.47
5:B:638:PHE:O	5:B:740:HIS:CB	2.63	0.47
6:C:173:ALA:O	6:C:174:ALA:CB	2.63	0.47
7:E:144:ILE:HG13	7:E:145:THR:N	2.30	0.47
10:I:30:ARG:HB2	10:I:30:ARG:NH1	2.29	0.47
2:T:26:DG:C6	2:T:27:DA:C8	3.02	0.47
4:A:1069:ALA:CB	4:A:1070:GLN:HA	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:420:ARG:O	4:A:424:ILE:HG13	2.14	0.47
4:A:380:VAL:HG21	4:A:427:GLN:O	2.15	0.47
4:A:833:GLU:O	4:A:837:ILE:HG12	2.14	0.47
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.95	0.47
5:B:95:ILE:HD12	5:B:130:VAL:CG2	2.45	0.47
7:E:131:THR:HG21	7:E:191:LYS:HD3	1.96	0.47
7:E:140:LEU:HA	7:E:141:VAL:HB	1.96	0.47
4:A:1076:ALA:O	4:A:1080:THR:HG22	2.15	0.47
4:A:1084:PHE:CD1	4:A:1086:PHE:HA	2.49	0.47
4:A:1261:LYS:C	4:A:1263:ILE:H	2.17	0.47
4:A:350:ARG:NH1	4:A:488:ASN:HD21	2.11	0.47
4:A:867:ILE:HG22	4:A:872:GLY:CA	2.45	0.47
5:B:256:VAL:CG1	5:B:382:ILE:HD11	2.29	0.47
5:B:38:PHE:O	5:B:42:GLY:N	2.47	0.47
6:C:124:LEU:C	6:C:126:GLY:H	2.17	0.47
5:B:487:THR:O	5:B:490:SER:OG	2.14	0.47
9:H:63:LEU:C	9:H:89:LEU:HB2	2.35	0.47
4:A:399:HIS:O	4:A:435:HIS:HD2	1.97	0.47
4:A:503:GLN:O	4:A:504:LEU:HD12	2.14	0.47
5:B:51:PHE:CD2	5:B:173:MET:HB3	2.50	0.47
5:B:570:VAL:C	5:B:572:HIS:HB2	2.35	0.47
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.80	0.47
7:E:10:SER:O	7:E:14:ARG:HG3	2.15	0.47
4:A:975:HIS:HB3	4:A:976:THR:CB	2.39	0.47
5:B:243:ALA:HB2	5:B:251:ILE:HD13	1.96	0.47
10:I:43:VAL:HG12	10:I:44:TYR:HA	1.97	0.47
11:J:9:SER:CB	11:J:45:CYS:HB2	2.45	0.47
4:A:61:ILE:HG13	4:A:62:ASP:N	2.30	0.47
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.80	0.47
5:B:32:ALA:O	5:B:35:SER:HB2	2.15	0.47
5:B:979:LYS:HA	5:B:989:THR:HG22	1.96	0.47
5:B:777:ALA:HB1	5:B:819:ALA:HB1	1.97	0.46
7:E:205:SER:O	7:E:207:ARG:N	2.47	0.46
10:I:101:PHE:HB2	10:I:110:PHE:CE1	2.50	0.46
4:A:792:TYR:OH	10:I:91:ARG:NH2	2.48	0.46
4:A:457:ALA:O	4:A:507:VAL:HG23	2.16	0.46
5:B:1120:GLU:HB3	5:B:1124:ARG:NH1	2.30	0.46
5:B:1209:ALA:C	5:B:1211:ASN:H	2.19	0.46
4:A:1342:GLU:HG3	7:E:198:ILE:HG21	1.98	0.46
4:A:1191:TRP:CA	4:A:1192:LEU:CB	2.90	0.46
4:A:58:LEU:HD22	4:A:244:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:O	4:A:302:THR:OG1	2.33	0.46
4:A:416:ARG:HG3	4:A:417:TYR:CD1	2.49	0.46
4:A:793:SER:CB	4:A:794:PRO:HD2	2.45	0.46
5:B:265:SER:O	5:B:266:ALA:HB3	2.14	0.46
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.97	0.46
5:B:785:TYR:HA	5:B:788:ARG:HB2	1.96	0.46
4:A:254:GLU:HA	4:A:255:SER:HA	1.70	0.46
4:A:617:VAL:CG1	4:A:622:VAL:HB	2.45	0.46
9:H:139:ASN:O	9:H:140:ALA:HB2	2.15	0.46
9:H:23:VAL:HA	9:H:43:ASN:HA	1.95	0.46
4:A:370:ILE:HG22	4:A:374:LEU:CD1	2.45	0.46
4:A:396:PRO:HB3	4:A:403:LYS:HG2	1.96	0.46
4:A:445:ASN:CB	4:A:455:MET:HG2	2.46	0.46
4:A:666:ILE:H	4:A:666:ILE:HD12	1.79	0.46
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.45	0.46
4:A:1170:ILE:HA	4:A:1171:GLN:O	2.16	0.46
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.96	0.46
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.98	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:CZ	2.45	0.46
5:B:328:GLU:HA	5:B:329:THR:HA	1.63	0.46
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.97	0.46
5:B:950:ASP:O	5:B:951:GLN:HG3	2.16	0.46
10:I:114:GLN:HA	10:I:115:LYS:HA	1.69	0.46
4:A:312:PRO:O	4:A:313:GLN:HB2	2.15	0.46
4:A:767:GLN:NE2	4:A:774:ARG:HB2	2.31	0.46
5:B:471:LYS:HG2	5:B:471:LYS:O	2.16	0.46
5:B:704:ALA:HB1	5:B:710:LEU:HB3	1.98	0.46
5:B:892:LYS:O	5:B:899:ILE:HG23	2.16	0.46
6:C:50:GLU:HB2	6:C:156:THR:OG1	2.15	0.46
9:H:106:GLU:HA	9:H:112:ILE:H	1.81	0.46
9:H:6:PHE:HZ	9:H:134:ASN:HB2	1.81	0.46
4:A:838:GLN:O	4:A:840:ARG:N	2.49	0.46
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.79	0.46
5:B:213:ILE:CD1	5:B:497:ARG:HB3	2.45	0.46
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.98	0.46
4:A:1050:GLU:O	4:A:1054:LEU:HD13	2.16	0.46
4:A:1116:LEU:HB3	4:A:1308:THR:HB	1.98	0.46
4:A:345:VAL:HA	5:B:1154:ALA:O	2.16	0.46
4:A:892:ALA:O	4:A:896:ARG:HB2	2.16	0.46
5:B:230:ALA:O	5:B:232:SER:O	2.34	0.46
4:A:637:LYS:HA	4:A:638:GLY:HA2	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:125:SER:HB2	5:B:169:ARG:HB3	1.97	0.46
5:B:707:PRO:HB3	5:B:741:CYS:SG	2.55	0.46
5:B:955:THR:HG23	13:L:54:ARG:O	2.16	0.46
6:C:41:ILE:CG2	6:C:246:ARG:HB3	2.46	0.46
2:T:9:DA:H61	3:N:6:DT:H3	1.63	0.46
4:A:1015:VAL:O	4:A:1017:LEU:N	2.49	0.45
4:A:282:ASN:CB	4:A:283:GLY:CA	2.78	0.45
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.97	0.45
4:A:513:SER:HB3	4:A:518:LYS:O	2.16	0.45
4:A:722:LEU:HD11	4:A:794:PRO:HB3	1.98	0.45
4:A:901:LEU:H	4:A:926:GLN:HE21	1.62	0.45
5:B:709:ASP:CB	5:B:710:LEU:HB2	2.46	0.45
4:A:824:LEU:HD21	5:B:769:TYR:HE1	1.81	0.45
5:B:845:SER:HB2	11:J:8:PHE:HB3	1.96	0.45
4:A:452:LYS:HD2	4:A:510:GLN:HE22	1.81	0.45
5:B:996:ARG:CG	5:B:1007:VAL:HG21	2.41	0.45
4:A:10:PRO:HD2	5:B:1193:GLN:HB2	1.96	0.45
5:B:372:SER:O	5:B:376:PHE:HD1	1.99	0.45
5:B:492:LEU:HD13	5:B:812:LEU:HD12	1.98	0.45
10:I:79:HIS:HA	10:I:80:SER:O	2.16	0.45
2:T:11:DG:N2	3:N:5:DT:O2	2.49	0.45
4:A:563:PRO:HD3	4:A:572:TRP:CZ2	2.52	0.45
4:A:712:GLU:N	4:A:713:SER:CB	2.53	0.45
4:A:741:ASN:HD22	4:A:744:LYS:H	1.62	0.45
4:A:907:THR:HG22	4:A:908:LEU:N	2.31	0.45
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.51	0.45
5:B:212:LEU:HA	5:B:479:VAL:O	2.15	0.45
5:B:331:LEU:HB3	5:B:352:ALA:HB1	1.97	0.45
5:B:61:ASP:HA	5:B:64:CYS:HB2	1.98	0.45
5:B:680:THR:HB	5:B:681:TRP:H	1.56	0.45
6:C:88:CYS:SG	6:C:89:GLU:N	2.89	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.45
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.99	0.45
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.99	0.45
12:K:37:LYS:O	12:K:38:GLU:HG2	2.16	0.45
5:B:1076:HIS:ND1	12:K:40:HIS:NE2	2.64	0.45
4:A:1068:ALA:C	4:A:1069:ALA:O	2.53	0.45
4:A:663:SER:OG	5:B:1085:ILE:HA	2.16	0.45
5:B:831:SER:HB2	5:B:833:TYR:CD1	2.49	0.45
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.81	0.45
6:C:215:GLU:HG3	6:C:216:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1191:TRP:HA	4:A:1192:LEU:HB3	1.96	0.45
4:A:199:LEU:HB3	4:A:200:ARG:H	1.56	0.45
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.98	0.45
4:A:959:ASN:OD1	4:A:961:ARG:HB3	2.17	0.45
8:F:93:ILE:HG12	8:F:148:VAL:HG21	1.98	0.45
10:I:59:VAL:HG12	10:I:60:GLN:H	1.81	0.45
4:A:1080:THR:HG23	4:A:1081:LEU:H	1.81	0.45
4:A:868:TYR:C	4:A:868:TYR:CD2	2.90	0.45
5:B:1177:HIS:HB2	5:B:1178:ASN:HB2	1.98	0.45
5:B:572:HIS:N	5:B:573:GLN:C	2.64	0.45
7:E:69:ILE:HD13	7:E:73:PRO:HA	1.99	0.45
9:H:108:SER:HB3	9:H:111:LEU:H	1.81	0.45
4:A:975:HIS:NE2	9:H:136:LYS:CB	2.80	0.45
5:B:1166:CYS:O	5:B:1168:LEU:N	2.48	0.45
5:B:1175:LEU:HA	5:B:1177:HIS:O	2.16	0.45
12:K:97:LYS:O	12:K:100:ALA:HB3	2.16	0.45
12:K:7:PHE:C	12:K:9:LEU:H	2.19	0.45
13:L:32:ALA:H	13:L:55:ILE:CD1	2.26	0.45
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	1.98	0.45
4:A:630:ILE:N	4:A:630:ILE:CD1	2.72	0.45
5:B:579:ARG:HA	5:B:589:VAL:HG13	1.97	0.45
5:B:814:PHE:C	5:B:816:GLU:H	2.20	0.45
6:C:127:ARG:HG3	6:C:129:ILE:HG22	1.99	0.45
4:A:783:THR:O	5:B:516:ASN:OD1	2.35	0.45
5:B:600:LEU:HD22	5:B:615:MET:SD	2.57	0.45
4:A:1069:ALA:CB	4:A:1070:GLN:CA	2.95	0.44
4:A:1072:ILE:CG2	4:A:1073:GLY:N	2.72	0.44
4:A:68:GLN:O	4:A:68:GLN:CG	2.65	0.44
5:B:476:ARG:O	5:B:477:ALA:C	2.55	0.44
6:C:265:MET:C	6:C:267:GLN:H	2.20	0.44
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.64	0.44
10:I:50:THR:HB	10:I:90:GLN:HE22	1.81	0.44
4:A:1069:ALA:HA	4:A:1072:ILE:CG2	2.45	0.44
4:A:1083:THR:H	4:A:1084:PHE:C	2.17	0.44
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.17	0.44
4:A:324:SER:O	4:A:326:ARG:N	2.45	0.44
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	2.00	0.44
5:B:1148:LYS:O	5:B:1152:MET:HB2	2.17	0.44
5:B:459:TYR:O	5:B:463:THR:OG1	2.35	0.44
9:H:88:SER:O	9:H:89:LEU:CB	2.63	0.44
4:A:1197:LEU:HA	4:A:1198:ASP:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1074:ASN:OD1	5:B:1074:ASN:C	2.54	0.44
6:C:124:LEU:O	6:C:127:ARG:HG2	2.17	0.44
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.48	0.44
4:A:222:LEU:O	4:A:224:PHE:N	2.50	0.44
4:A:265:LYS:NZ	4:A:323:LYS:HE2	2.32	0.44
4:A:915:SER:HB2	4:A:919:ILE:CG1	2.45	0.44
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.46	0.44
5:B:1176:ASN:O	5:B:1177:HIS:ND1	2.51	0.44
7:E:173:SER:O	7:E:175:LEU:N	2.51	0.44
7:E:46:TYR:CD2	7:E:58:MET:HG3	2.53	0.44
4:A:351:THR:HB	4:A:468:PHE:CD1	2.52	0.44
4:A:692:ASP:O	4:A:695:LYS:HG2	2.17	0.44
5:B:638:PHE:HB3	5:B:651:LEU:HD21	1.99	0.44
6:C:46:ILE:O	6:C:169:LYS:HE3	2.18	0.44
4:A:1327:ILE:O	7:E:147:HIS:HE1	2.01	0.44
10:I:21:GLU:O	10:I:22:ASN:CB	2.65	0.44
4:A:1171:GLN:C	4:A:1173:HIS:H	2.21	0.44
5:B:1124:ARG:O	5:B:1125:ASP:C	2.55	0.44
5:B:487:THR:CG2	5:B:488:TYR:N	2.80	0.44
5:B:999:MET:CE	5:B:1000:PRO:HD2	2.47	0.44
6:C:101:LEU:HB3	6:C:155:LEU:HB2	2.00	0.44
4:A:451:HIS:HB3	4:A:453:MET:H	1.81	0.44
4:A:541:ILE:CD1	4:A:577:ILE:HD11	2.48	0.44
4:A:855:THR:O	4:A:855:THR:HG23	2.18	0.44
5:B:756:ILE:O	5:B:759:PRO:HD3	2.17	0.44
8:F:145:ASP:O	8:F:146:TRP:CB	2.65	0.44
9:H:129:TYR:O	9:H:130:ARG:CG	2.65	0.44
10:I:63:GLY:CA	10:I:104:LEU:HD21	2.32	0.44
4:A:1325:THR:HG23	4:A:1326:ARG:HG3	2.00	0.44
4:A:344:ARG:HB3	5:B:1118:PRO:HD2	1.99	0.44
4:A:304:MET:SD	5:B:1210:MET:HG3	2.58	0.44
16:B:3000:UTP:H6	16:B:3000:UTP:H5'1	1.83	0.44
4:A:1150:SER:HB3	10:I:46:HIS:CD2	2.53	0.44
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.00	0.44
4:A:1327:ILE:O	7:E:147:HIS:CE1	2.71	0.44
4:A:366:VAL:O	4:A:463:ILE:HG13	2.18	0.44
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.99	0.44
5:B:387:LEU:HD13	5:B:392:ARG:HD2	1.99	0.44
5:B:459:TYR:C	5:B:459:TYR:CD2	2.91	0.44
5:B:547:VAL:CG1	5:B:548:GLY:N	2.81	0.44
5:B:865:LYS:HB2	5:B:865:LYS:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1070:GLN:O	4:A:1074:GLU:CB	2.64	0.43
4:A:479:ASN:ND2	4:A:1078:GLN:OE1	2.50	0.43
4:A:1083:THR:C	4:A:1084:PHE:O	2.57	0.43
4:A:365:GLY:HA3	4:A:469:ARG:HB2	2.00	0.43
4:A:873:MET:C	4:A:1058:VAL:HG13	2.38	0.43
5:B:242:SER:HB2	5:B:362:PRO:HD2	2.00	0.43
6:C:43:THR:HG22	6:C:44:LEU:H	1.83	0.43
6:C:71:PRO:HB2	6:C:133:ILE:HB	1.98	0.43
7:E:19:VAL:O	7:E:23:VAL:HG23	2.17	0.43
11:J:43:ARG:HD2	11:J:46:CYS:SG	2.58	0.43
4:A:451:HIS:O	4:A:1070:GLN:NE2	2.52	0.43
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.50	0.43
4:A:413:ILE:HG22	4:A:413:ILE:O	2.18	0.43
4:A:956:LEU:HA	4:A:957:PRO:HD3	1.68	0.43
5:B:273:LEU:HD21	5:B:360:PHE:HB2	1.99	0.43
5:B:572:HIS:N	5:B:573:GLN:CB	2.77	0.43
5:B:986:GLN:HE21	5:B:1025:HIS:HD2	1.64	0.43
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.46	0.43
7:E:52:ARG:HA	7:E:53:PRO:HD3	1.74	0.43
4:A:668:ASP:HB3	4:A:743:VAL:CG2	2.46	0.43
4:A:870:GLU:OE2	7:E:200:ARG:NH1	2.51	0.43
5:B:1194:ILE:H	5:B:1194:ILE:HD13	1.84	0.43
5:B:46:GLN:OE1	5:B:47:GLN:HG2	2.18	0.43
5:B:563:MET:HA	5:B:590:HIS:ND1	2.33	0.43
9:H:105:GLU:HB3	9:H:113:ALA:HB3	1.99	0.43
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.83	0.43
5:B:898:LEU:HD22	5:B:964:VAL:HG11	2.00	0.43
4:A:1089:VAL:H	4:A:1090:ALA:HA	1.77	0.43
4:A:383:TYR:OH	8:F:107:VAL:HG21	2.19	0.43
4:A:751:SER:CB	5:B:1015:HIS:HE1	2.26	0.43
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.99	0.43
5:B:1209:ALA:C	5:B:1211:ASN:N	2.71	0.43
5:B:31:TRP:O	5:B:34:ILE:HB	2.17	0.43
5:B:53:GLN:HG3	5:B:53:GLN:O	2.16	0.43
4:A:816:HIS:CD2	5:B:764:SER:H	2.36	0.43
12:K:58:PHE:HE2	12:K:74:ARG:HB3	1.84	0.43
4:A:1091:SER:CB	4:A:1092:LYS:C	2.72	0.43
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.48	0.43
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.54	0.43
5:B:463:THR:HB	5:B:465:ASN:H	1.84	0.43
5:B:790:ASP:N	5:B:790:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:2:THR:OG1	10:I:43:VAL:HG13	2.18	0.43
11:J:2:ILE:HG13	11:J:57:ILE:HG21	1.99	0.43
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.84	0.43
4:A:1159:ARG:CB	4:A:1160:SER:C	2.83	0.43
4:A:1277:GLU:HG2	4:A:1277:GLU:H	1.70	0.43
4:A:135:PHE:HA	4:A:138:ILE:HD12	2.00	0.43
4:A:304:MET:SD	5:B:1210:MET:HA	2.59	0.43
4:A:313:GLN:HB3	4:A:314:ALA:H	1.66	0.43
4:A:374:LEU:CB	4:A:436:ILE:HD11	2.49	0.43
4:A:567:LYS:HD2	9:H:46:LEU:HD13	2.01	0.43
5:B:172:ILE:HG22	5:B:173:MET:O	2.19	0.43
5:B:124:TYR:HB2	5:B:204:ILE:HB	2.01	0.43
5:B:230:ALA:N	5:B:231:PRO:CD	2.81	0.43
12:K:40:HIS:CE1	12:K:63:VAL:HG11	2.53	0.43
4:A:1092:LYS:CB	4:A:1093:LYS:CB	2.97	0.43
4:A:353:ILE:HA	4:A:468:PHE:O	2.19	0.43
4:A:88:LYS:HA	4:A:89:PRO:HD3	1.91	0.43
5:B:1010:LEU:HA	5:B:1010:LEU:HD12	1.75	0.43
5:B:1213:THR:HB	5:B:1215:ARG:NH1	2.34	0.43
5:B:555:ILE:HA	5:B:558:LEU:HD12	2.00	0.43
6:C:91:HIS:HB2	6:C:96:SER:OG	2.19	0.43
7:E:138:ALA:HA	7:E:140:LEU:N	2.33	0.43
8:F:93:ILE:HD11	8:F:132:LEU:HB2	2.00	0.43
9:H:43:ASN:ND2	9:H:46:LEU:HD12	2.34	0.43
12:K:65:HIS:C	12:K:67:PHE:H	2.22	0.43
2:T:19:DT:H2'	2:T:20:DC:C6	2.54	0.43
4:A:1171:GLN:O	4:A:1173:HIS:N	2.52	0.43
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.54	0.43
4:A:77:CYS:SG	4:A:80:HIS:NE2	2.91	0.43
4:A:826:ASP:HB2	4:A:830:LYS:HB3	2.01	0.43
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.19	0.43
5:B:1098:MET:O	5:B:1099:VAL:C	2.57	0.43
5:B:890:TYR:CE2	5:B:910:VAL:HG11	2.54	0.43
4:A:38:PRO:CB	4:A:39:GLU:HA	2.47	0.43
4:A:819:GLY:O	4:A:820:GLY:C	2.57	0.43
4:A:961:ARG:HH11	4:A:965:GLN:HE22	1.65	0.43
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	2.01	0.43
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	2.01	0.42
4:A:867:ILE:HG22	4:A:872:GLY:HA3	2.01	0.42
4:A:979:SER:OG	4:A:980:ASP:N	2.53	0.42
5:B:802:PRO:HA	5:B:1091:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.24	0.42
5:B:846:ILE:HG23	5:B:974:PRO:HG2	2.01	0.42
6:C:34:ARG:HG3	6:C:35:ARG:N	2.34	0.42
7:E:59:SER:HB3	7:E:80:VAL:O	2.18	0.42
10:I:3:THR:CA	10:I:4:PHE:CB	2.93	0.42
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.42
4:A:502:SER:HA	4:A:506:ALA:HB2	2.01	0.42
5:B:999:MET:HE2	5:B:1000:PRO:HD2	2.01	0.42
5:B:820:GLY:N	5:B:1091:TYR:OH	2.49	0.42
5:B:37:PHE:O	5:B:38:PHE:HB2	2.19	0.42
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.49	0.42
10:I:4:PHE:HD1	10:I:5:ARG:N	2.17	0.42
12:K:40:HIS:HB3	12:K:61:TYR:HE1	1.84	0.42
12:K:82:ASP:OD2	12:K:84:LYS:HB2	2.20	0.42
4:A:562:THR:HA	4:A:563:PRO:HD2	1.81	0.42
4:A:647:GLY:O	4:A:651:LYS:HG3	2.19	0.42
4:A:711:ARG:CA	4:A:713:SER:HB2	2.48	0.42
5:B:31:TRP:HA	5:B:34:ILE:HG13	2.01	0.42
8:F:82:THR:HA	8:F:83:PRO:HD3	1.87	0.42
12:K:32:VAL:HG22	12:K:74:ARG:HG3	2.00	0.42
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.84	0.42
4:A:465:TYR:HB3	5:B:976:ILE:HG21	2.01	0.42
7:E:141:VAL:HG12	7:E:142:VAL:HG23	2.00	0.42
13:L:60:ARG:HG3	13:L:61:THR:N	2.34	0.42
2:T:18:DA:H2'	2:T:19:DT:C6	2.55	0.42
4:A:1155:ASP:OD1	4:A:1190:PRO:HA	2.18	0.42
5:B:254:LEU:HD12	5:B:272:THR:O	2.20	0.42
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.02	0.42
5:B:886:LYS:O	5:B:888:GLY:N	2.42	0.42
6:C:43:THR:HG22	6:C:44:LEU:N	2.34	0.42
4:A:1078:GLN:O	4:A:1082:ASN:HB2	2.20	0.42
4:A:351:THR:CG2	4:A:352:VAL:H	2.32	0.42
4:A:589:GLN:HB3	4:A:961:ARG:HH22	1.84	0.42
5:B:483:LEU:HD22	5:B:484:ASN:H	1.85	0.42
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.85	0.42
5:B:745:PRO:HB2	5:B:1047:PHE:HD1	1.84	0.42
5:B:973:ILE:HG13	5:B:973:ILE:H	1.47	0.42
6:C:21:ILE:O	6:C:22:LEU:HB2	2.18	0.42
5:B:1011:ILE:N	5:B:1011:ILE:HD12	2.34	0.42
5:B:1139:ILE:H	5:B:1139:ILE:HG13	1.66	0.42
5:B:867:GLY:HA2	5:B:868:MET:HA	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:620:ARG:HH21	10:I:68:LEU:HD21	1.84	0.42
4:A:14:VAL:HG21	4:A:1430:LEU:HD22	2.01	0.42
4:A:606:LEU:HD23	4:A:613:ILE:HG21	2.01	0.42
4:A:841:LEU:HD22	4:A:1072:ILE:HG21	2.01	0.42
5:B:232:SER:HA	5:B:233:PRO:HD3	2.00	0.42
5:B:911:ILE:HG22	5:B:912:ILE:CG1	2.43	0.42
7:E:22:MET:HG3	7:E:187:TYR:CD1	2.54	0.42
9:H:111:LEU:HB2	9:H:112:ILE:HG22	2.01	0.42
4:A:538:ASP:HB2	9:H:20:TYR:CD2	2.54	0.42
10:I:42:LEU:HD22	10:I:43:VAL:N	2.34	0.42
4:A:1197:LEU:HB3	4:A:1198:ASP:O	2.19	0.42
4:A:964:ILE:O	4:A:968:GLN:HG2	2.20	0.42
5:B:265:SER:O	5:B:266:ALA:CB	2.68	0.42
6:C:61:GLU:HA	6:C:64:ALA:HB3	2.01	0.42
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.49	0.42
4:A:1057:VAL:HG12	4:A:1058:VAL:O	2.19	0.42
4:A:582:ILE:HG22	4:A:610:GLY:HA2	2.02	0.42
4:A:745:GLN:HG2	4:A:745:GLN:H	1.62	0.42
5:B:826:ALA:O	5:B:1011:ILE:HA	2.20	0.42
5:B:211:VAL:O	5:B:480:SER:HA	2.20	0.42
5:B:796:LEU:HD22	5:B:799:PRO:HA	2.02	0.42
5:B:802:PRO:HA	5:B:822:ASN:ND2	2.35	0.42
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.66	0.42
4:A:1414:ALA:C	4:A:1416:ALA:H	2.23	0.41
4:A:482:PHE:C	4:A:484:GLY:N	2.73	0.41
4:A:704:ALA:HB1	4:A:710:LEU:HD22	2.01	0.41
4:A:858:ASN:ND2	4:A:860:LEU:H	2.18	0.41
5:B:123:THR:O	5:B:125:SER:N	2.43	0.41
5:B:67:SER:HB2	5:B:92:PHE:CD1	2.55	0.41
6:C:18:VAL:HG23	6:C:240:VAL:HB	2.02	0.41
7:E:161:LYS:HG3	7:E:195:VAL:HG21	2.02	0.41
7:E:202:SER:OG	7:E:204:THR:HG22	2.20	0.41
4:A:1096:SER:O	4:A:1100:ARG:HG3	2.21	0.41
4:A:1364:ASN:O	4:A:1365:TYR:C	2.57	0.41
4:A:831:THR:O	4:A:834:THR:HG23	2.20	0.41
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.52	0.41
5:B:831:SER:CB	5:B:833:TYR:HD1	2.32	0.41
5:B:977:GLY:HA3	5:B:1099:VAL:HG11	2.02	0.41
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.55	0.41
5:B:125:SER:HA	5:B:171:PRO:HA	2.01	0.41
5:B:789:MET:HE2	5:B:965:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:537:ARG:HG2	4:A:575:LYS:HE3	2.00	0.41
4:A:575:LYS:O	4:A:576:GLN:C	2.59	0.41
4:A:754:SER:H	4:A:757:ASN:ND2	2.18	0.41
4:A:777:PHE:CE2	4:A:782:ARG:HA	2.55	0.41
5:B:1150:ARG:HA	5:B:1150:ARG:HD3	1.90	0.41
5:B:363:HIS:O	5:B:364:ILE:CB	2.66	0.41
6:C:234:SER:HB3	6:C:240:VAL:HG13	2.02	0.41
6:C:245:VAL:HA	6:C:248:ILE:HD12	2.03	0.41
6:C:250:THR:HA	6:C:253:LYS:HB2	2.02	0.41
7:E:149:LEU:O	7:E:151:PRO:HD3	2.20	0.41
4:A:1441:PHE:HZ	8:F:88:TYR:C	2.24	0.41
4:A:323:LYS:HD3	4:A:323:LYS:N	2.35	0.41
4:A:365:GLY:N	4:A:469:ARG:O	2.50	0.41
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.83	0.41
4:A:847:ASP:HA	4:A:1063:MET:HE1	2.03	0.41
5:B:195:CYS:HB3	5:B:198:ASP:HB2	2.02	0.41
5:B:391:ASP:HA	5:B:393:LYS:N	2.36	0.41
5:B:757:PRO:HD3	5:B:983:ARG:HE	1.85	0.41
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.55	0.41
4:A:23:SER:O	4:A:27:VAL:HG23	2.21	0.41
2:T:20:DC:OP1	5:B:1131:GLY:HA3	2.19	0.41
5:B:128:LEU:HB2	5:B:167:ILE:O	2.21	0.41
5:B:183:GLU:CA	5:B:184:ALA:HB3	2.51	0.41
5:B:636:PRO:HB3	5:B:743:ILE:CG1	2.51	0.41
9:H:23:VAL:HG11	9:H:121:LEU:HD22	2.02	0.41
9:H:84:ALA:CA	9:H:85:GLY:C	2.76	0.41
12:K:42:LEU:O	12:K:46:ILE:HB	2.21	0.41
4:A:1083:THR:CA	4:A:1084:PHE:O	2.68	0.41
4:A:552:TRP:CE3	4:A:651:LYS:HB3	2.55	0.41
4:A:909:ASP:C	4:A:911:SER:N	2.74	0.41
5:B:1103:ILE:O	5:B:1103:ILE:HG22	2.21	0.41
5:B:1177:HIS:CA	5:B:1178:ASN:CB	2.98	0.41
5:B:273:LEU:HD23	5:B:274:PRO:HD2	2.01	0.41
5:B:549:THR:HB	5:B:628:THR:HG22	2.02	0.41
6:C:102:GLN:OE1	6:C:154:LYS:HD2	2.20	0.41
6:C:73:GLN:HB3	6:C:131:HIS:H	1.86	0.41
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.51	0.41
9:H:92:ASP:O	9:H:145:ARG:HD3	2.20	0.41
10:I:103:CYS:SG	10:I:106:CYS:HB2	2.60	0.41
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	2.03	0.41
4:A:1193:LEU:HD21	4:A:1264:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:645:LEU:HD11	4:A:649:ILE:HD11	2.02	0.41
4:A:710:LEU:HA	4:A:712:GLU:N	2.36	0.41
5:B:1023:VAL:O	5:B:1026:LEU:HB2	2.21	0.41
4:A:16:GLU:HB2	5:B:1217:TYR:HB2	2.03	0.41
5:B:51:PHE:CE1	5:B:203:PHE:HE2	2.39	0.41
5:B:523:CYS:SG	5:B:750:GLY:N	2.94	0.41
9:H:105:GLU:HG3	9:H:106:GLU:N	2.30	0.41
11:J:3:VAL:HA	11:J:4:PRO:HD3	1.88	0.41
4:A:858:ASN:HD22	4:A:858:ASN:C	2.24	0.41
4:A:857:ARG:HA	4:A:864:ILE:HG12	2.03	0.41
5:B:997:GLU:C	5:B:999:MET:H	2.24	0.41
4:A:1438:THR:CG2	8:F:92:ARG:HB2	2.51	0.41
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.56	0.41
4:A:619:LYS:O	4:A:623:GLY:HA3	2.21	0.41
5:B:29:ASP:HB3	5:B:658:ILE:HD13	2.03	0.41
7:E:140:LEU:HA	7:E:142:VAL:H	1.84	0.41
12:K:40:HIS:HB3	12:K:61:TYR:CE1	2.56	0.41
4:A:1072:ILE:HD13	4:A:1072:ILE:HA	1.86	0.41
4:A:1200:ALA:CB	4:A:1203:ASN:HB2	2.50	0.41
4:A:61:ILE:HG13	4:A:62:ASP:H	1.86	0.41
4:A:675:THR:HG21	4:A:736:ASN:ND2	2.26	0.41
4:A:452:LYS:HB3	5:B:1140:ALA:CB	2.50	0.41
5:B:634:TYR:HE1	5:B:692:TYR:CD1	2.36	0.41
6:C:258:ILE:H	6:C:258:ILE:HG13	1.60	0.41
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.02	0.41
4:A:256:GLN:HB3	4:A:256:GLN:HE21	1.62	0.40
4:A:347:PHE:H	5:B:1107:ALA:HA	1.86	0.40
4:A:481:ASP:HA	5:B:836:GLU:HG2	2.03	0.40
4:A:527:THR:HG23	4:A:650:GLN:HA	2.04	0.40
4:A:814:PHE:O	4:A:817:ALA:HB3	2.22	0.40
4:A:86:LEU:HD23	4:A:273:ASN:HD22	1.86	0.40
5:B:183:GLU:N	5:B:184:ALA:HB3	2.36	0.40
5:B:212:LEU:HD21	5:B:461:LEU:CD1	2.50	0.40
5:B:238:ALA:HB3	5:B:256:VAL:HB	2.03	0.40
5:B:293:PRO:CA	5:B:294:ASP:HB2	2.29	0.40
5:B:550:ASP:HA	5:B:551:PRO:HD3	1.97	0.40
4:A:1192:LEU:HD13	4:A:1193:LEU:N	2.35	0.40
4:A:1366:ARG:H	4:A:1366:ARG:HG2	1.77	0.40
4:A:794:PRO:C	4:A:796:SER:N	2.73	0.40
4:A:764:CYS:HA	4:A:802:ASN:O	2.21	0.40
6:C:124:LEU:C	6:C:126:GLY:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:59:SER:O	7:E:60:PHE:HB3	2.21	0.40
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.56	0.40
4:A:977:LYS:HA	4:A:977:LYS:HD3	1.69	0.40
4:A:993:LEU:HA	4:A:996:ASN:HD21	1.86	0.40
5:B:421:PHE:HA	5:B:453:ILE:HD11	2.03	0.40
7:E:21:GLU:O	7:E:24:LYS:HG2	2.21	0.40
7:E:79:TRP:CZ2	7:E:99:HIS:NE2	2.90	0.40
9:H:137:GLN:HG2	9:H:138:GLU:H	1.85	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.90	0.40
2:T:18:DA:H8	4:A:832:ALA:HA	1.87	0.40
4:A:1189:SER:HB2	4:A:1242:VAL:O	2.22	0.40
4:A:1271:ILE:HA	4:A:1271:ILE:HD13	1.99	0.40
4:A:560:ILE:HG12	4:A:560:ILE:H	1.58	0.40
5:B:327:ARG:O	5:B:331:LEU:HD12	2.21	0.40
6:C:166:GLU:O	6:C:167:HIS:CB	2.69	0.40
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	2.03	0.40
4:A:380:VAL:HG12	4:A:388:LEU:HD13	2.03	0.40
4:A:38:PRO:HG3	4:A:270:LEU:HB3	2.04	0.40
4:A:71:GLN:O	4:A:73:GLY:N	2.53	0.40
4:A:818:MET:HA	5:B:514:LEU:HB3	2.03	0.40
4:A:841:LEU:O	4:A:845:LEU:HG	2.22	0.40
4:A:894:GLU:C	4:A:896:ARG:H	2.25	0.40
4:A:975:HIS:NE2	9:H:136:LYS:HB2	2.36	0.40
5:B:108:VAL:HG12	5:B:109:THR:N	2.37	0.40
8:F:82:THR:HG22	8:F:84:TYR:HB2	2.04	0.40
9:H:111:LEU:HD12	9:H:127:GLY:CA	2.50	0.40
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1384/1733 (80%)	1055 (76%)	224 (16%)	105 (8%)	1	15
5	B	1074/1224 (88%)	855 (80%)	161 (15%)	58 (5%)	2	22
6	C	264/318 (83%)	217 (82%)	35 (13%)	12 (4%)	2	24
7	E	185/215 (86%)	146 (79%)	26 (14%)	13 (7%)	1	17
8	F	81/155 (52%)	62 (76%)	15 (18%)	4 (5%)	2	23
9	H	129/146 (88%)	87 (67%)	30 (23%)	12 (9%)	0	12
10	I	117/122 (96%)	73 (62%)	32 (27%)	12 (10%)	0	9
11	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2	23
12	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	17	56
13	L	44/70 (63%)	29 (66%)	11 (25%)	4 (9%)	1	12
All	All	3453/4173 (83%)	2678 (78%)	551 (16%)	224 (6%)	1	18

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	63	ARG
4	A	223	GLY
4	A	284	ALA
4	A	313	GLN
4	A	404	TYR
4	A	517	ASN
4	A	525	GLN
4	A	568	PRO
4	A	702	LEU
4	A	710	LEU
4	A	903	ASN
4	A	998	LEU
4	A	1016	THR
4	A	1081	LEU
4	A	1084	PHE
4	A	1085	HIS
4	A	1156	PRO
4	A	1158	PRO
4	A	1163	ILE
4	A	1165	GLU
4	A	1172	LEU
4	A	1191	TRP
4	A	1365	TYR
4	A	1392	SER

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Mol	Chain	Res	Type
4	A	1393	ASN
5	B	66	ASP
5	B	184	ALA
5	B	231	PRO
5	B	274	PRO
5	B	636	PRO
5	B	711	GLU
5	B	878	GLN
5	B	882	THR
5	B	1178	ASN
6	C	110	THR
6	C	167	HIS
6	C	173	ALA
6	C	174	ALA
7	E	130	ALA
8	F	104	ASN
8	F	128	LYS
9	H	77	ARG
9	H	84	ALA
10	I	21	GLU
10	I	26	LEU
10	I	46	HIS
10	I	47	GLU
13	L	26	THR
4	A	55	ASP
4	A	71	GLN
4	A	250	ILE
4	A	279	LEU
4	A	288	ALA
4	A	312	PRO
4	A	423	ASP
4	A	424	ILE
4	A	479	ASN
4	A	543	LEU
4	A	576	GLN
4	A	624	SER
4	A	637	LYS
4	A	713	SER
4	A	1069	ALA
4	A	1072	ILE
4	A	1094	VAL
4	A	1127	ASP

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Mol	Chain	Res	Type
4	A	1153	TYR
4	A	1154	TYR
4	A	1160	SER
4	A	1167	GLU
4	A	1192	LEU
4	A	1224	LEU
4	A	1391	ARG
5	B	228	LYS
5	B	266	ALA
5	B	276	ILE
5	B	301	ILE
5	B	391	ASP
5	B	410	GLY
5	B	474	SER
5	B	478	GLY
5	B	705	MET
5	B	708	GLU
5	B	864	LYS
5	B	996	ARG
5	B	1020	ARG
5	B	1021	MET
5	B	1167	GLY
5	B	1177	HIS
6	C	22	LEU
6	C	142	VAL
6	C	266	ASP
7	E	30	ILE
7	E	36	GLU
7	E	141	VAL
7	E	174	GLN
7	E	206	GLY
8	F	145	ASP
9	H	82	PRO
9	H	85	GLY
9	H	89	LEU
9	H	107	VAL
9	H	112	ILE
9	H	140	ALA
4	A	48	ALA
4	A	72	GLU
4	A	214	ILE
4	A	257	ARG

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Mol	Chain	Res	Type
4	A	289	ILE
4	A	465	TYR
4	A	741	ASN
4	A	972	HIS
4	A	1206	ASP
5	B	477	ALA
5	B	482	VAL
5	B	531	GLN
5	B	792	MET
6	C	88	CYS
6	C	90	ASP
9	H	91	ASP
9	H	131	ASN
10	I	4	PHE
13	L	56	LEU
4	A	54	ASN
4	A	287	HIS
4	A	321	PRO
4	A	591	PHE
4	A	651	LYS
4	A	708	MET
4	A	775	ILE
4	A	975	HIS
4	A	1003	LYS
4	A	1262	LYS
4	A	1270	ASN
4	A	1435	PRO
5	B	100	PRO
5	B	124	TYR
5	B	458	LYS
5	B	572	HIS
5	B	635	ARG
5	B	710	LEU
5	B	865	LYS
5	B	887	HIS
5	B	1017	ILE
5	B	1046	PRO
5	B	1103	ILE
5	B	1112	GLN
7	E	125	PRO
8	F	146	TRP
10	I	20	LYS

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Mol	Chain	Res	Type
10	I	113	ASP
11	J	10	CYS
11	J	29	GLU
12	K	66	PRO
4	A	10	PRO
4	A	58	LEU
4	A	178	GLY
4	A	213	HIS
4	A	254	GLU
4	A	306	ASN
4	A	332	LYS
4	A	333	GLU
4	A	639	PRO
4	A	650	GLN
4	A	673	GLY
4	A	870	GLU
4	A	902	LEU
4	A	910	PRO
4	A	920	LEU
4	A	922	ASP
4	A	958	VAL
4	A	969	GLN
4	A	1013	ASP
4	A	1155	ASP
4	A	1164	PRO
4	A	1366	ARG
5	B	64	CYS
5	B	232	SER
5	B	476	ARG
5	B	652	LYS
5	B	786	ASN
5	B	870	ILE
5	B	974	PRO
6	C	21	ILE
6	C	38	ILE
7	E	29	PHE
7	E	66	GLU
7	E	96	PHE
7	E	166	LYS
9	H	7	ASP
9	H	23	VAL
10	I	11	ASN

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1218/1520 (80%)	1055 (87%)	163 (13%)	4	20
5	B	951/1061 (90%)	827 (87%)	124 (13%)	4	21
6	C	234/274 (85%)	207 (88%)	27 (12%)	5	24
7	E	177/197 (90%)	160 (90%)	17 (10%)	8	30
8	F	73/137 (53%)	65 (89%)	8 (11%)	6	25
9	H	117/128 (91%)	103 (88%)	14 (12%)	5	23
10	I	113/116 (97%)	92 (81%)	21 (19%)	1	10
11	J	60/65 (92%)	51 (85%)	9 (15%)	3	17
12	K	99/102 (97%)	88 (89%)	11 (11%)	6	25
13	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
All	All	3082/3657 (84%)	2679 (87%)	403 (13%)	4	21

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	TYR
4	A	13	THR
4	A	41	MET
4	A	49	LYS
4	A	50	ILE
4	A	53	LEU
4	A	62	ASP
4	A	65	LEU
4	A	66	LYS
4	A	68	GLN
4	A	69	THR
4	A	80	HIS
4	A	84	ILE
4	A	100	LYS
4	A	108	MET
4	A	122	MET
4	A	133	LYS
4	A	140	THR
4	A	161	LEU
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	256	GLN
4	A	260	ASP

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Mol	Chain	Res	Type
4	A	264	PHE
4	A	270	LEU
4	A	279	LEU
4	A	286	HIS
4	A	289	ILE
4	A	302	THR
4	A	303	TYR
4	A	306	ASN
4	A	308	ILE
4	A	313	GLN
4	A	320	ARG
4	A	322	VAL
4	A	323	LYS
4	A	348	SER
4	A	373	THR
4	A	381	THR
4	A	391	LEU
4	A	443	LEU
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	481	ASP
4	A	487	MET
4	A	494	SER
4	A	501	LEU
4	A	509	LEU
4	A	535	THR
4	A	541	ILE
4	A	544	ASP
4	A	560	ILE
4	A	566	ILE
4	A	573	SER
4	A	576	GLN
4	A	582	ILE
4	A	596	THR
4	A	618	GLU
4	A	635	ARG
4	A	645	LEU
4	A	660	ASN
4	A	666	ILE

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Mol	Chain	Res	Type
4	A	675	THR
4	A	680	THR
4	A	687	LYS
4	A	708	MET
4	A	714	PHE
4	A	721	PHE
4	A	728	LYS
4	A	738	LYS
4	A	740	LEU
4	A	758	ILE
4	A	765	VAL
4	A	774	ARG
4	A	795	GLU
4	A	821	ARG
4	A	826	ASP
4	A	834	THR
4	A	839	ARG
4	A	856	THR
4	A	858	ASN
4	A	859	SER
4	A	867	ILE
4	A	880	LYS
4	A	881	GLN
4	A	896	ARG
4	A	902	LEU
4	A	913	LEU
4	A	915	SER
4	A	918	GLU
4	A	920	LEU
4	A	927	VAL
4	A	929	LEU
4	A	941	LYS
4	A	945	GLU
4	A	949	ASP
4	A	964	ILE
4	A	971	PHE
4	A	973	ILE
4	A	974	ASP
4	A	988	LEU
4	A	996	ASN
4	A	1016	THR
4	A	1017	LEU

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Mol	Chain	Res	Type
4	A	1025	ARG
4	A	1028	THR
4	A	1035	TYR
4	A	1054	LEU
4	A	1058	VAL
4	A	1078	GLN
4	A	1083	THR
4	A	1085	HIS
4	A	1086	PHE
4	A	1104	ILE
4	A	1113	THR
4	A	1116	LEU
4	A	1127	ASP
4	A	1128	GLN
4	A	1141	THR
4	A	1142	THR
4	A	1156	PRO
4	A	1158	PRO
4	A	1159	ARG
4	A	1161	THR
4	A	1166	ASP
4	A	1167	GLU
4	A	1168	GLU
4	A	1172	LEU
4	A	1187	GLN
4	A	1188	GLN
4	A	1192	LEU
4	A	1215	ARG
4	A	1224	LEU
4	A	1227	ILE
4	A	1228	TRP
4	A	1241	ARG
4	A	1242	VAL
4	A	1262	LYS
4	A	1276	VAL
4	A	1281	ARG
4	A	1284	MET
4	A	1295	THR
4	A	1312	ASN
4	A	1322	ILE
4	A	1329	THR
4	A	1333	ILE

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Mol	Chain	Res	Type
4	A	1334	ASP
4	A	1335	ILE
4	A	1336	MET
4	A	1358	SER
4	A	1364	ASN
4	A	1366	ARG
4	A	1376	THR
4	A	1385	THR
4	A	1391	ARG
4	A	1394	THR
4	A	1426	GLU
4	A	1442	ASP
4	A	1443	VAL
5	B	28	GLU
5	B	44	VAL
5	B	46	GLN
5	B	49	ASP
5	B	66	ASP
5	B	94	LYS
5	B	102	VAL
5	B	131	ASP
5	B	167	ILE
5	B	175	ARG
5	B	178	ASN
5	B	180	TYR
5	B	185	THR
5	B	188	ASP
5	B	191	LYS
5	B	199	MET
5	B	217	ARG
5	B	225	VAL
5	B	234	ILE
5	B	242	SER
5	B	264	SER
5	B	268	THR
5	B	273	LEU
5	B	291	ILE
5	B	297	ILE
5	B	302	CYS
5	B	304	ASP
5	B	322	PHE
5	B	346	GLU

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Mol	Chain	Res	Type
5	B	347	LYS
5	B	351	TYR
5	B	361	LEU
5	B	367	LEU
5	B	373	ARG
5	B	387	LEU
5	B	391	ASP
5	B	393	LYS
5	B	394	ASP
5	B	398	ARG
5	B	415	GLN
5	B	424	LEU
5	B	425	THR
5	B	432	MET
5	B	448	ILE
5	B	463	THR
5	B	466	TRP
5	B	473	MET
5	B	475	SER
5	B	483	LEU
5	B	502	ILE
5	B	537	LYS
5	B	547	VAL
5	B	549	THR
5	B	561	TRP
5	B	572	HIS
5	B	616	ILE
5	B	618	ASP
5	B	624	LEU
5	B	628	THR
5	B	635	ARG
5	B	637	LEU
5	B	650	GLU
5	B	651	LEU
5	B	655	LYS
5	B	680	THR
5	B	701	ILE
5	B	728	ARG
5	B	736	THR
5	B	740	HIS
5	B	741	CYS
5	B	787	VAL

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Mol	Chain	Res	Type
5	B	796	LEU
5	B	797	TYR
5	B	812	LEU
5	B	837	ASP
5	B	844	SER
5	B	864	LYS
5	B	866	TYR
5	B	880	THR
5	B	883	LEU
5	B	898	LEU
5	B	899	ILE
5	B	905	VAL
5	B	916	THR
5	B	918	ILE
5	B	941	LEU
5	B	943	SER
5	B	953	LEU
5	B	959	ASP
5	B	970	THR
5	B	973	ILE
5	B	975	GLN
5	B	982	SER
5	B	1004	GLU
5	B	1012	ILE
5	B	1021	MET
5	B	1051	THR
5	B	1060	ARG
5	B	1065	GLN
5	B	1072	MET
5	B	1082	MET
5	B	1092	TYR
5	B	1096	ARG
5	B	1099	VAL
5	B	1103	ILE
5	B	1113	VAL
5	B	1115	THR
5	B	1122	ARG
5	B	1123	SER
5	B	1124	ARG
5	B	1133	MET
5	B	1135	ARG
5	B	1153	GLU

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Mol	Chain	Res	Type
5	B	1156	ASP
5	B	1159	ARG
5	B	1160	VAL
5	B	1166	CYS
5	B	1183	LYS
5	B	1189	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1219	ASP
5	B	1220	ARG
5	B	1222	ARG
6	C	10	ILE
6	C	27	LEU
6	C	41	ILE
6	C	55	THR
6	C	56	THR
6	C	57	VAL
6	C	77	ILE
6	C	81	GLU
6	C	106	GLU
6	C	119	VAL
6	C	120	ILE
6	C	123	ASN
6	C	154	LYS
6	C	185	LYS
6	C	195	GLN
6	C	208	GLU
6	C	210	GLU
6	C	221	TYR
6	C	235	VAL
6	C	240	VAL
6	C	249	ASP
6	C	250	THR
6	C	258	ILE
6	C	259	LEU
6	C	265	MET
6	C	266	ASP
6	C	268	ASP
7	E	3	GLN
7	E	8	ASN
7	E	18	THR
7	E	43	LYS

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Mol	Chain	Res	Type
7	E	69	ILE
7	E	95	THR
7	E	98	ILE
7	E	103	LYS
7	E	119	SER
7	E	123	LEU
7	E	127	ILE
7	E	132	ILE
7	E	140	LEU
7	E	156	LEU
7	E	158	SER
7	E	165	LEU
7	E	169	ARG
8	F	77	ASP
8	F	97	ARG
8	F	104	ASN
8	F	110	ASP
8	F	111	LEU
8	F	119	ARG
8	F	140	ASP
8	F	145	ASP
9	H	2	SER
9	H	24	CYS
9	H	32	THR
9	H	56	THR
9	H	83	GLN
9	H	89	LEU
9	H	102	TYR
9	H	105	GLU
9	H	111	LEU
9	H	112	ILE
9	H	130	ARG
9	H	133	ASN
9	H	136	LYS
9	H	138	GLU
10	I	2	THR
10	I	4	PHE
10	I	13	MET
10	I	20	LYS
10	I	25	LEU
10	I	26	LEU
10	I	28	GLU

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Mol	Chain	Res	Type
10	I	30	ARG
10	I	32	CYS
10	I	37	GLU
10	I	42	LEU
10	I	43	VAL
10	I	45	ARG
10	I	50	THR
10	I	59	VAL
10	I	79	HIS
10	I	84	VAL
10	I	92	ARG
10	I	108	HIS
10	I	109	ILE
10	I	111	THR
11	J	2	ILE
11	J	7	CYS
11	J	9	SER
11	J	36	LEU
11	J	43	ARG
11	J	48	ARG
11	J	51	LEU
11	J	52	THR
11	J	55	ASP
12	K	11	LEU
12	K	12	LEU
12	K	22	ASP
12	K	40	HIS
12	K	41	THR
12	K	52	ASN
12	K	53	ASP
12	K	63	VAL
12	K	85	ASP
12	K	91	CYS
12	K	101	LEU
13	L	31	CYS
13	L	33	GLU
13	L	48	CYS
13	L	53	HIS
13	L	61	THR
13	L	62	LYS
13	L	63	ARG
13	L	65	VAL

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Mol	Chain	Res	Type
13	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	68	GLN
4	A	83	HIS
4	A	109	HIS
4	A	225	ASN
4	A	256	GLN
4	A	273	ASN
4	A	313	GLN
4	A	390	GLN
4	A	397	ASN
4	A	399	HIS
4	A	435	HIS
4	A	510	GLN
4	A	517	ASN
4	A	576	GLN
4	A	654	ASN
4	A	660	ASN
4	A	700	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	802	ASN
4	A	838	GLN
4	A	858	ASN
4	A	926	GLN
4	A	965	GLN
4	A	966	ASN
4	A	968	GLN
4	A	972	HIS
4	A	996	ASN
4	A	1085	HIS
4	A	1110	ASN
4	A	1128	GLN
4	A	1222	ASN
4	A	1312	ASN
4	A	1364	ASN
4	A	1390	ASN
5	B	121	ASN

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Mol	Chain	Res	Type
5	B	325	GLN
5	B	363	HIS
5	B	366	GLN
5	B	469	GLN
5	B	481	GLN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	531	GLN
5	B	744	HIS
5	B	763	GLN
5	B	776	GLN
5	B	794	ASN
5	B	822	ASN
5	B	835	GLN
5	B	975	GLN
5	B	984	HIS
5	B	1013	ASN
5	B	1015	HIS
5	B	1025	HIS
5	B	1084	GLN
5	B	1177	HIS
6	C	7	GLN
6	C	73	GLN
6	C	112	ASN
6	C	188	HIS
6	C	203	GLN
6	C	224	GLN
6	C	242	GLN
6	C	252	GLN
7	E	8	ASN
7	E	101	GLN
7	E	147	HIS
8	F	78	GLN
9	H	33	GLN
9	H	128	ASN
10	I	90	GLN
10	I	116	ASN
11	J	53	HIS
12	K	65	HIS

5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	UTP	B	3000	15	26,30,30	2.09	7 (26%)	34,47,47	1.85	8 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	UTP	B	3000	15	-	6/22/38/38	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	3000	UTP	C6-C5	-4.92	1.39	1.52
16	B	3000	UTP	C5-C4	-4.56	1.39	1.50
16	B	3000	UTP	C2-N1	4.45	1.42	1.35
16	B	3000	UTP	PG-O2G	3.32	1.61	1.50
16	B	3000	UTP	C6-N1	-2.63	1.42	1.47
16	B	3000	UTP	C4-N3	2.50	1.41	1.37
16	B	3000	UTP	C1'-N1	2.22	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	3000	UTP	C4-N3-C2	-6.29	120.57	125.79
16	B	3000	UTP	PB-O3B-PG	-3.37	121.26	132.83
16	B	3000	UTP	C5-C4-N3	3.27	120.32	116.65
16	B	3000	UTP	C5-C6-N1	3.08	121.76	111.61
16	B	3000	UTP	O1G-PG-O3B	2.57	113.25	104.64
16	B	3000	UTP	PB-O3A-PA	-2.46	124.38	132.83
16	B	3000	UTP	N3-C2-N1	2.38	119.17	116.65
16	B	3000	UTP	C5'-C4'-C3'	-2.01	107.63	115.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

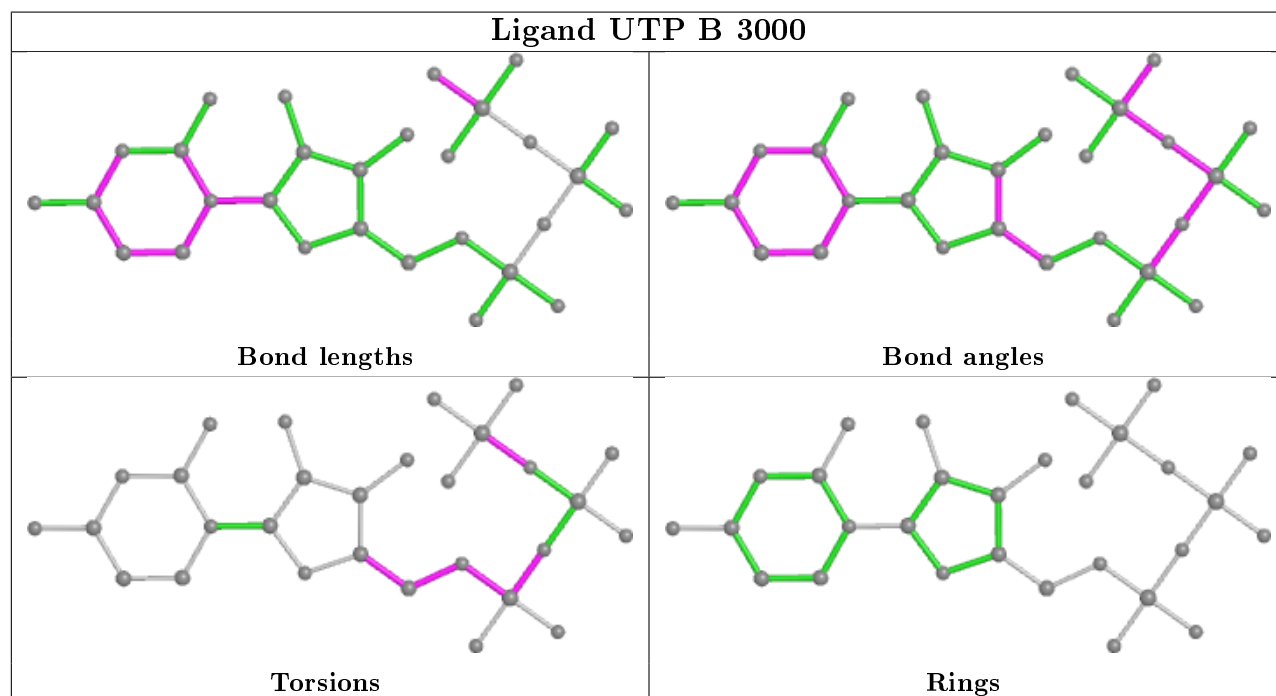
Mol	Chain	Res	Type	Atoms
16	B	3000	UTP	C5'-O5'-PA-O1A
16	B	3000	UTP	C4'-C5'-O5'-PA
16	B	3000	UTP	O4'-C4'-C5'-O5'
16	B	3000	UTP	C3'-C4'-C5'-O5'
16	B	3000	UTP	PB-O3A-PA-O5'
16	B	3000	UTP	PB-O3B-PG-O2G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

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



5.7 Other polymers ⓘ

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%)	-0.36	0 100 100	89, 111, 136, 141	0
2	T	28/28 (100%)	0.73	8 (28%) 0 0	81, 200, 285, 291	0
3	N	14/14 (100%)	1.65	7 (50%) 0 0	265, 273, 291, 292	0
4	A	1398/1733 (80%)	-0.38	4 (0%) 94 90	84, 118, 171, 184	0
5	B	1096/1224 (89%)	-0.38	1 (0%) 95 95	86, 114, 151, 165	0
6	C	266/318 (83%)	-0.42	1 (0%) 92 87	99, 118, 146, 150	0
7	E	193/215 (89%)	-0.32	0 100 100	98, 130, 163, 167	0
8	F	83/155 (53%)	-0.36	0 100 100	111, 127, 138, 144	0
9	H	133/146 (91%)	-0.26	0 100 100	120, 141, 176, 181	0
10	I	119/122 (97%)	-0.22	0 100 100	118, 149, 168, 173	0
11	J	65/70 (92%)	-0.56	0 100 100	103, 119, 134, 136	0
12	K	114/120 (95%)	-0.34	0 100 100	99, 118, 134, 136	0
13	L	46/70 (65%)	-0.06	0 100 100	137, 178, 191, 193	0
All	All	3565/4225 (84%)	-0.35	21 (0%) 89 84	81, 120, 168, 292	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	2	DT	4.9
2	T	3	DA	3.7
2	T	10	DA	3.2
3	N	11	DG	3.2
2	T	1	DC	3.1
4	A	168	GLY	2.8
3	N	1	DC	2.8
3	N	12	DT	2.7
3	N	10	DG	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	1175	SER	2.4
2	T	12	DC	2.4
3	N	2	DT	2.2
3	N	9	DC	2.1
5	B	1221	SER	2.1
2	T	11	DG	2.1
4	A	44	THR	2.1
2	T	4	DC	2.1
6	C	203	GLN	2.1
4	A	1174	PHE	2.0
3	N	14	DG	2.0
2	T	8	DT	2.0

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

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

6.3 Carbohydrates ⓘ

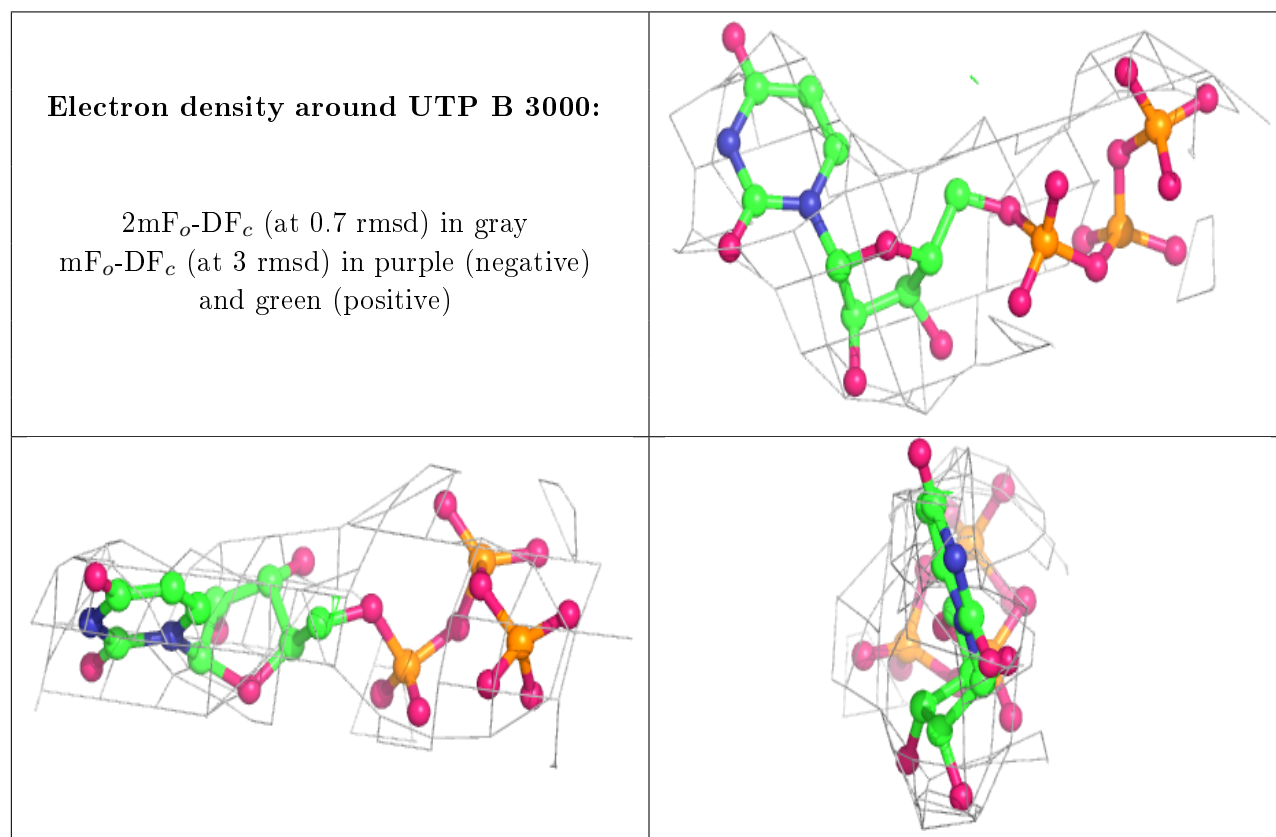
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	A	2001	1/1	0.84	0.14	97,97,97,97	0
15	MG	A	2002	1/1	0.88	0.19	102,102,102,102	0
14	ZN	A	1734	1/1	0.92	0.07	177,177,177,177	0
14	ZN	I	204	1/1	0.95	0.04	157,157,157,157	0
14	ZN	L	105	1/1	0.95	0.11	181,181,181,181	0
14	ZN	I	203	1/1	0.95	0.09	121,121,121,121	0
14	ZN	A	1735	1/1	0.95	0.05	165,165,165,165	0
16	UTP	B	3000	29/29	0.96	0.16	110,112,113,113	0
14	ZN	J	101	1/1	0.97	0.12	112,112,112,112	0
14	ZN	B	1307	1/1	0.97	0.05	147,147,147,147	0
14	ZN	C	319	1/1	0.98	0.03	117,117,117,117	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.