



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 05:25 AM UTC

PDB ID : 2E2H / pdb_00002e2h
Title : RNA polymerase II elongation complex at 5 mM Mg²⁺ with GTP
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-14
Resolution : 3.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

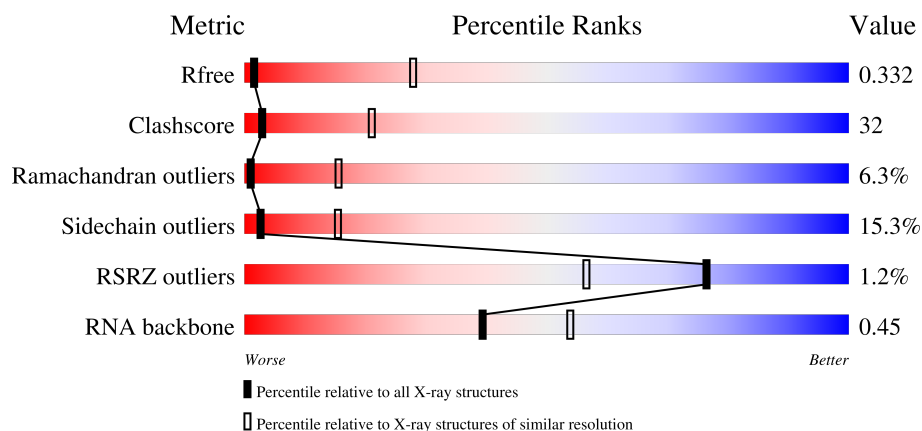
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)
RNA backbone	3983	1016 (4.80-3.10)

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

Mol	Chain	Length	Quality of chain
1	R	10	20% 80%
2	T	28	50% 46% .
3	N	14	7% 86% 14%
4	A	1733	% 39% 30% 10% . 19%

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29003 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
			564	270	102	165	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.

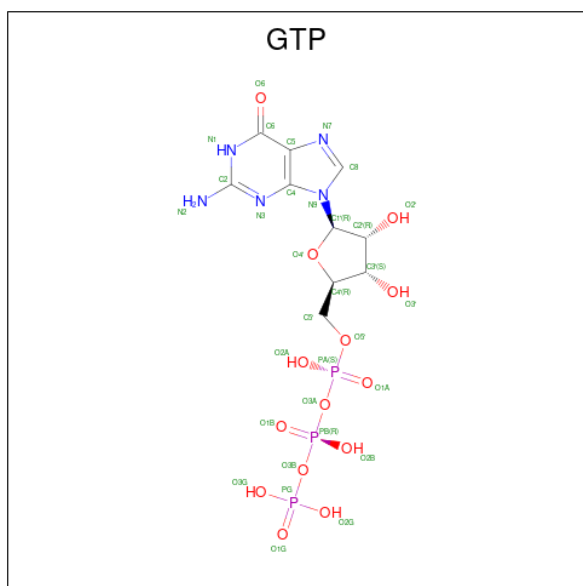
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- 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 GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

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

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

3 Residue-property plots

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

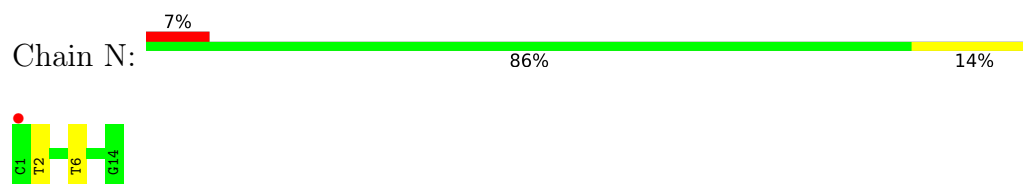
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'



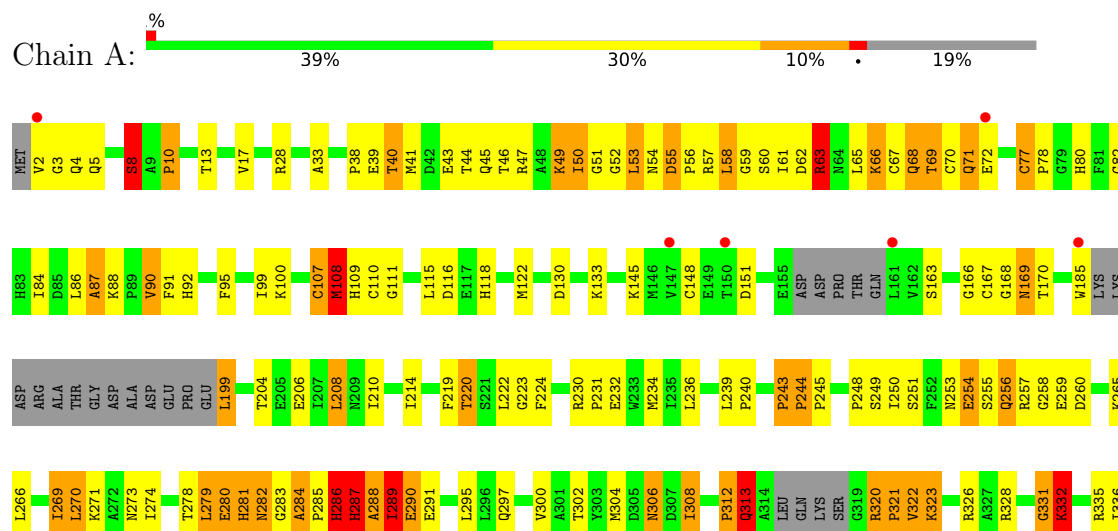
- Molecule 2: 28-MER DNA template strand



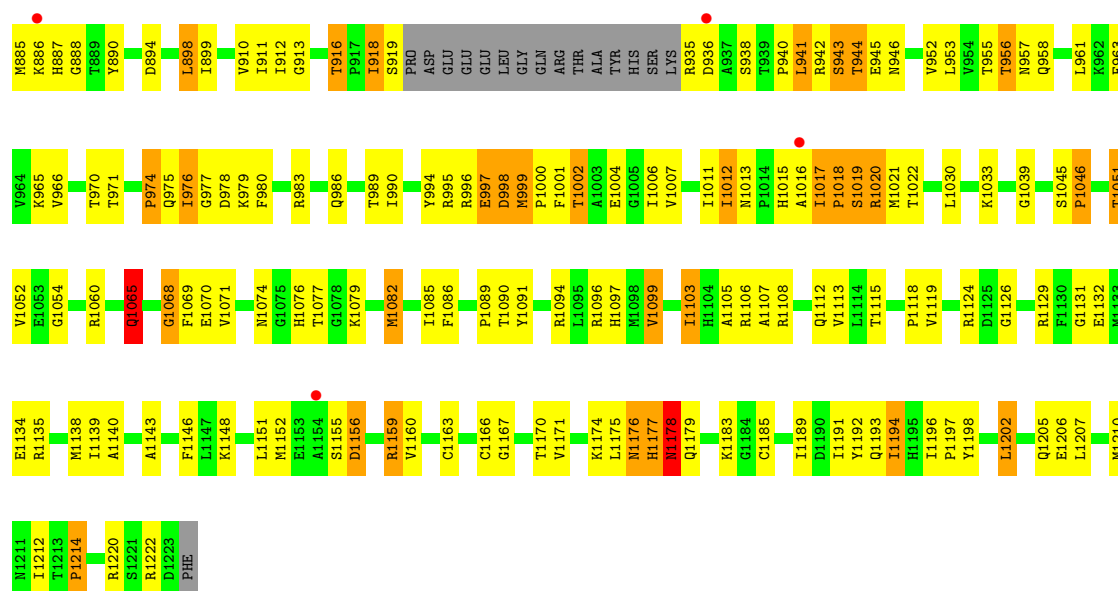
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'



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

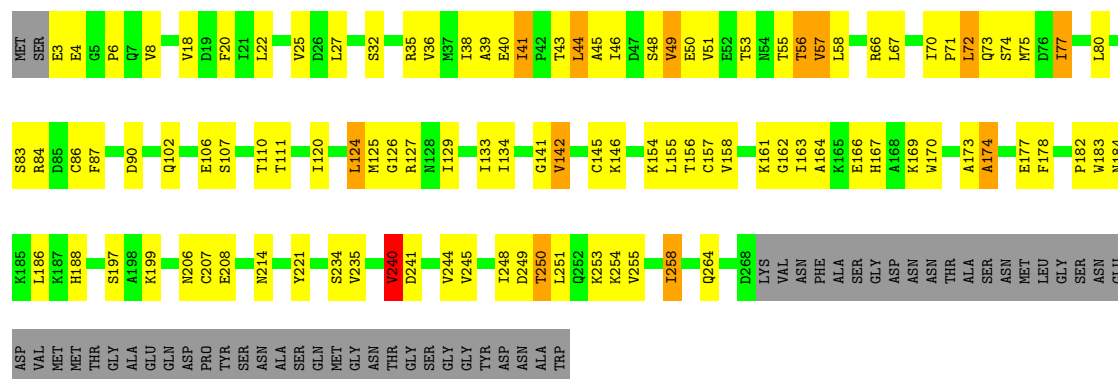


VAL	V1372	L1273	R1199	E1129	P1060	K984	L901	A817	K738	S663	R590	A506	R337
LYS	T1376	R1274	A1200	Q1130	G1061	D985	L902	M618	D739	S666	F591	L509	G338
TYR	M1201	N1278	A1201	L1133	M1062	V986	N903	G819	N741	T667	T595	L509	N339
MET	Q1378	N1278	M1202	L1133	M1063	V987	N903	G820	N741	T667	T595	L509	L340
PRO	T1385	R1281	D1206	T1141	V1064	G988	T907	R821	N742	D668	T596	S513	M341
GLU	T1385	V1282	L1207	T1142	V1066	V990	D909	R822	N744	D669	L597	P514	Y428
GLN	G1388	M1284	L1208	L1143	L1067	A991	P910	D826	Q745	L670	L598	Q515	R344
ILE	G1389	V1283	T1208	L1143	L1068	D992	S911	T827	P674	T675	P600	N517	F347
THR	F1390	D1288	M1209	T1146	A1068	D992	S911	T827	P674	T675	K601	P600	R434
GLY	F1391	D1288	M1209	T1146	A1068	D992	S911	T827	P674	T675	K601	P600	H435
ASP	S1392	S1293	Q1211	E1151	L1072	V996	S915	E833	S751	E678	G604	I523	R350
GLY	T1394	P1294	G1213	L1152	G1073	L997	S915	T834	S754	E678	G604	I523	T351
GLN	M1398	T1295	R1215	Y1154	P1075	V999	I919	G835	L756	T680	M605	D526	V352
ASP	M1398	L1306	P1156	D1155	A1076	L1000	L920	V836	N757	L683	T607	L528	I353
GLY	S1401	L1307	P1156	D1155	A1076	L1000	L920	V836	N757	L683	T607	L528	S354
VAL	V1406	T1308	D1223	E1165	M1078	E1005	D922	R840	V765	A686	G610	I531	D356
THR	E1407	D1309	L1224	P1158	M1078	E1005	D922	R840	V765	A686	G610	I531	Q363
PRO	N1408	V1311	L1225	S1160	T1080	M1009	L925	L841	Q766	K687	G611	L534	V364
TYR	L1409	N1312	V1226	T1161	M1082	Q1011	Q926	V690	Q768	V690	I612	T535	G365
SER	F1410	L1313	I1227	V1162	T1083	L929	D930	E846	S769	V693	G615	R537	V366
ASN	F1410	S1314	M1228	V1163	F1084	L929	D930	E846	S769	V693	G615	R537	P367
GLY	A1414	E1315	D1231	P1164	H1085	T1016	D930	E846	S769	V693	G615	R537	L370
SER	S1415	M1317	ASN	E1166	F1086	L1017	Y933	D847	I775	A697	V622	I541	A371
GLY	A1416	G1318	GLU	E1167	G1088	F1018	Y933	D847	I775	A697	V622	I541	A457
LEU	A1417	V1319	ASP	E1168	V1089	C1020	Y937	Y852	G777	A699	G623	L543	K372
VAL	L1418	L1319	LYS	T1169	A1090	L1021	Y937	Y852	G777	A699	G623	L543	K373
ASN	D1419	I1322	L1236	T1170	S1091	L1022	D939	R854	V780	L702	S625	Q545	L374
ASP	D1420	D1323	L1237	Q1171	K1092	A1027	L943	T855	D781	L703	T630	V546	T375
LEU	C1421	P1324	R1238	L1172	K1093	T1028	L944	T856	R782	A704	H631	M549	V380
VAL	V1424	T1325	C1240	F1173	V1094	R1029	E945	R857	L784	K705	H631	M549	T381
LYS	S1425	T1329	R1241	S1175	T1095	R1030	V946	S858	L785	K706	H631	M549	P382
ASP	E1426	T1329	V1242	L1176	S1096	V1031	F947	L860	P785	G707	T634	W556	Y383
LEU	N1427	F1332	ARG	ASP	G1097	L1032	E951	G861	K789	L710	K637	I560	N384
GLY	L1430	T1333	PRO	GLU	P1099	Q1033	E951	G861	D790	L710	K637	I560	R387
PHE	T1431	M1336	LYS	GLU	R1100	E1034	W954	V863	S793	E712	G638	I566	L388
SER	G1432	G1340	SER	ALA	L1101	Y1035	W954	V863	P794	S713	G641	K567	L391
LEU	H1433	ASP	LEU	GLN	T1104	T1038	L956	I867	F799	D716	C642	P568	E398
VAL	A1434	R1345	ASP	GLN	L1105	A1041	P957	Y868	W800	N717	C642	P568	H399
ASP	P1435	ALA	ALA	SER	N1106	A1041	V958	G869	E801	N718	L645	S573	P400
SER	T1436	T1356	THR	PHE	V1107	V1045	N959	M873	N802	V719	F646	K575	Y404
GLY	G1437	A1357	ASP	ASP	A1108	V1045	I960	M873	N802	V719	F646	K575	V405
SER	T1438	S1358	GLU	Q1187	K1109	N1048	R961	D874	L805	R721	G647	T577	T406
ASN	G1439	D1359	ASP	Q1188	K1112	N1048	R961	D874	L805	R721	G647	T577	R407
ASP	A1440	K1261	ASP	S1189	K1112	N1048	R961	D874	L805	R721	G647	T577	M487
ALA	F1441	K1262	ALA	P1190	T1113	E1050	T970	I878	L808	N723	V652	S578	D411
MET	T1445	I1263	MET	W1191	P1114	F1053	F971	I886	T809	E724	V653	I582	I412
ALA	ASP	T1266	ALA	L1193	S1115	L1054	H972	I886	P810	K728	V656	I582	I413
GLY	GLU	M1267	GLY	R1194	T1117	R1055	D974	R896	Q811	K728	V656	I582	I413
PHE	THR	R1366	THR	L1195	V1118	S1056	H975	Y897	F813	R731	L658	N584	A499
THR	GLU	E1196	GLU	E1196	V1118	S1056	H975	Y897	F813	R731	L658	N584	A499
ALA	LEU	L1370	LEU	L1197	D1127	V1058	K976	R898	F814	R731	L658	N584	A499
		L1371		D1198	Q1128	H1059	T977	V899	F815	N736	N660	H587	Q503
													L588
													S418
													C505



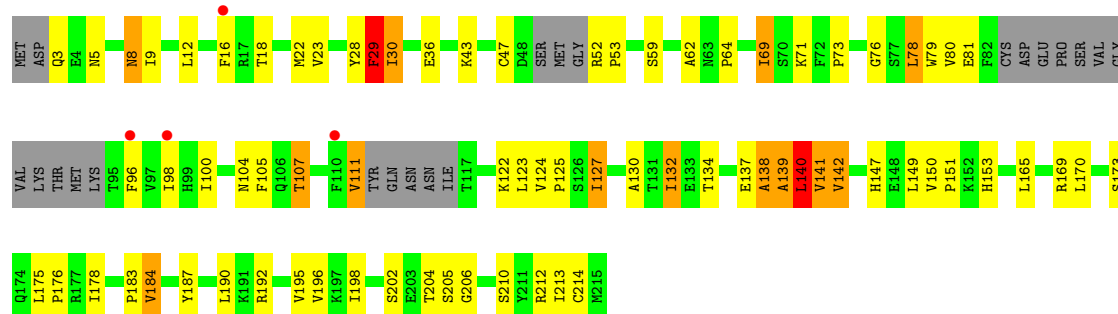
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 51% 29% 16%

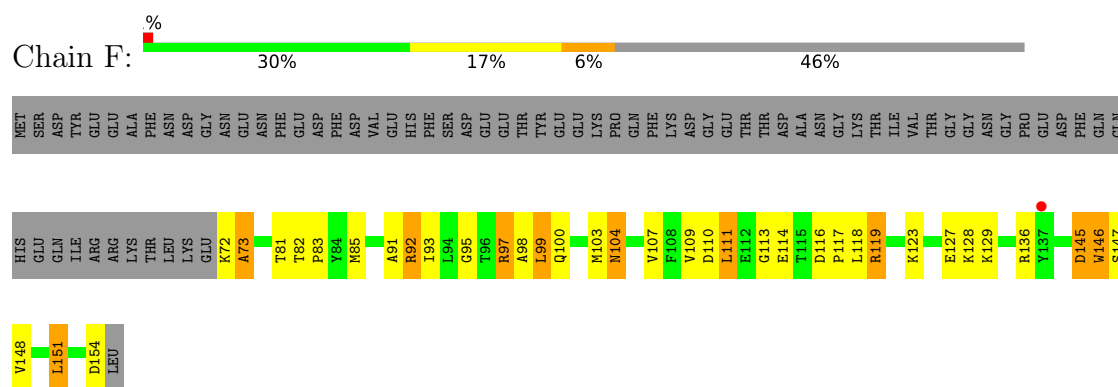


• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

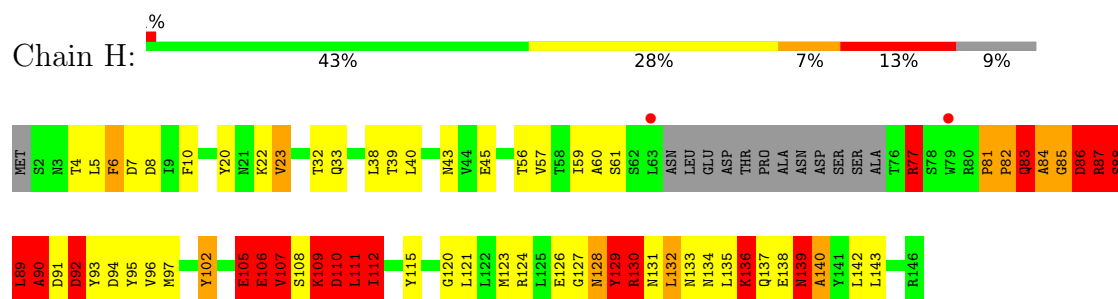
Chain E: 2% 54% 29% 6% 10%



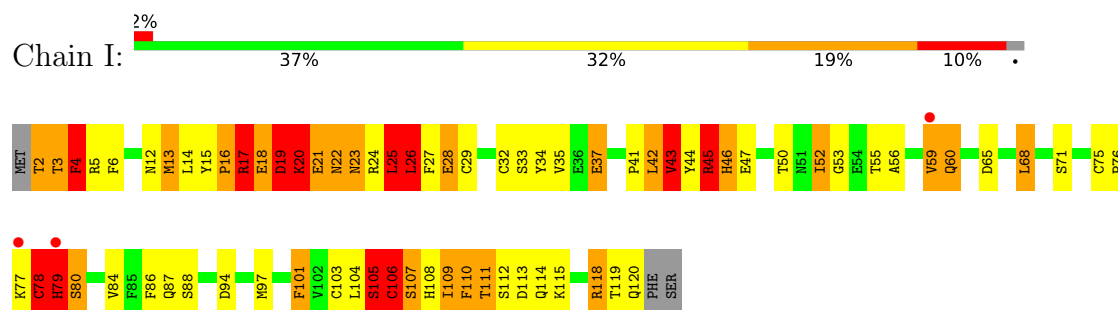
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



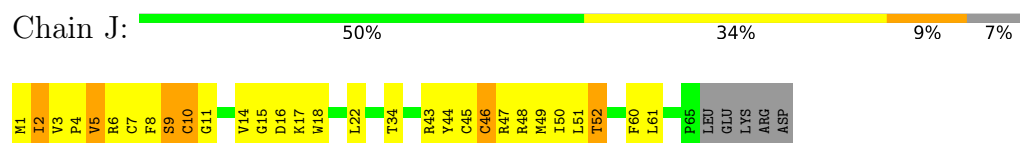
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



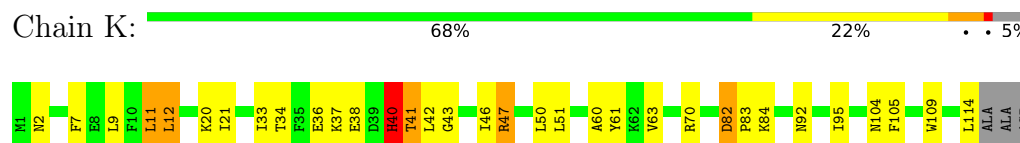
- Molecule 10: DNA-directed RNA polymerase II subunit 9



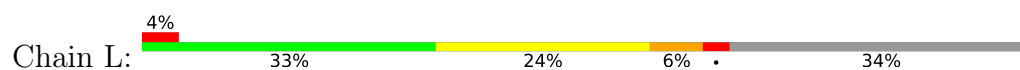
- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

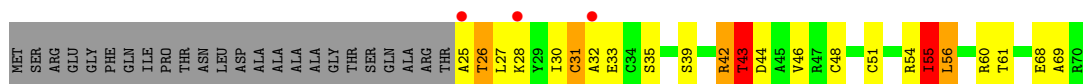


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.11Å 222.00Å 195.16Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	45.08 – 3.95 45.08 – 3.95	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.08-3.95) 97.7 (45.08-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.290 , 0.368 0.270 , 0.332	Depositor DCC
R_{free} test set	3078 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	115.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29003	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GTP, 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	0.49	0/243	0.86	0/378
2	T	0.34	0/631	0.87	1/970 (0.1%)
3	N	0.30	0/317	0.81	0/488
4	A	0.56	0/11180	0.90	18/15117 (0.1%)
5	B	0.57	0/8866	0.88	8/11956 (0.1%)
6	C	0.54	0/2133	0.88	2/2891 (0.1%)
7	E	0.57	0/1625	0.87	2/2182 (0.1%)
8	F	0.54	0/682	0.82	0/922
9	H	0.61	0/1086	0.83	1/1470 (0.1%)
10	I	0.58	0/989	0.86	4/1331 (0.3%)
11	J	0.45	0/541	0.85	0/727
12	K	0.54	0/937	0.92	2/1265 (0.2%)
13	L	0.51	0/365	0.81	0/485
All	All	0.55	0/29595	0.88	38/40182 (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	42
5	B	0	26
7	E	0	2
9	H	0	14
10	I	0	15
12	K	0	1
13	L	0	2
All	All	0	102

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	452	LYS	N-CA-C	-6.75	105.33	113.97
4	A	243	PRO	CA-C-N	6.72	127.30	120.38
4	A	243	PRO	C-N-CA	6.72	127.30	120.38
4	A	244	PRO	N-CA-C	6.68	118.85	110.70
12	K	82	ASP	CA-C-N	6.61	126.38	119.05
12	K	82	ASP	C-N-CA	6.61	126.38	119.05
4	A	331	GLY	N-CA-C	6.56	119.47	111.93
5	B	635	ARG	CA-C-N	6.11	127.47	119.84
5	B	635	ARG	C-N-CA	6.11	127.47	119.84
10	I	68	LEU	CA-C-N	5.94	126.77	120.11
10	I	68	LEU	C-N-CA	5.94	126.77	120.11
6	C	240	VAL	N-CA-C	5.92	117.37	110.62
5	B	99	LYS	CA-C-N	5.86	127.17	119.84
5	B	99	LYS	C-N-CA	5.86	127.17	119.84
4	A	584	ASN	N-CA-C	5.81	118.22	108.23
9	H	6	PHE	N-CA-C	5.66	117.81	108.48
10	I	28	GLU	N-CA-C	5.63	118.25	109.52
5	B	56	ASP	N-CA-C	5.62	118.34	111.82
10	I	110	PHE	N-CA-C	5.54	115.86	108.38
7	E	52	ARG	CA-C-N	5.54	126.76	119.84
7	E	52	ARG	C-N-CA	5.54	126.76	119.84
4	A	525	GLN	N-CA-C	5.53	116.18	108.00
4	A	1130	GLN	N-CA-C	-5.53	106.04	112.89
5	B	580	VAL	N-CA-C	5.49	115.76	107.80
4	A	809	THR	CA-C-N	5.37	124.83	119.24
4	A	809	THR	C-N-CA	5.37	124.83	119.24
4	A	1311	VAL	N-CA-C	5.35	115.79	107.28
5	B	699	GLU	N-CA-C	5.21	117.63	111.33
4	A	1189	SER	CA-C-N	5.19	125.11	119.76
4	A	1189	SER	C-N-CA	5.19	125.11	119.76
4	A	88	LYS	CA-C-N	5.16	126.29	119.84
4	A	88	LYS	C-N-CA	5.16	126.29	119.84
6	C	41	ILE	N-CA-C	5.16	113.06	108.63
4	A	460	VAL	N-CA-C	5.13	116.08	108.23
2	T	15	DA	P-O3'-C3'	5.11	127.86	120.20
4	A	829	VAL	N-CA-C	5.11	116.28	111.48
4	A	587	HIS	N-CA-C	5.05	116.65	108.26
5	B	21	GLU	N-CA-C	5.04	117.16	111.11

There are no chirality outliers.

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1068	ALA	Peptide
4	A	1069	ALA	Peptide
4	A	107	CYS	Peptide
4	A	1070	GLN	Peptide
4	A	1071	SER	Peptide
4	A	1079	MET	Peptide
4	A	108	MET	Peptide
4	A	1081	LEU	Peptide
4	A	1082	ASN	Peptide
4	A	1083	THR	Peptide
4	A	1084	PHE	Peptide
4	A	1089	VAL	Peptide
4	A	1091	SER	Peptide
4	A	1093	LYS	Peptide
4	A	1152	ILE	Peptide
4	A	1155	ASP	Peptide
4	A	1156	PRO	Peptide
4	A	1158	PRO	Peptide
4	A	1159	ARG	Peptide
4	A	1162	VAL	Peptide
4	A	1163	ILE	Peptide
4	A	1171	GLN	Peptide
4	A	1197	LEU	Peptide
4	A	166	GLY	Peptide
4	A	256	GLN	Peptide
4	A	257	ARG	Peptide
4	A	258	GLY	Peptide
4	A	286	HIS	Peptide
4	A	287	HIS	Peptide
4	A	288	ALA	Peptide
4	A	289	ILE	Peptide
4	A	383	TYR	Peptide
4	A	398	GLU	Peptide
4	A	451	HIS	Peptide
4	A	701	LEU	Peptide
4	A	705	LYS	Peptide
4	A	707	GLY	Peptide
4	A	709	THR	Peptide
4	A	8	SER	Peptide
4	A	975	HIS	Peptide
4	A	976	THR	Peptide
4	A	977	LYS	Peptide
5	B	1018	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	B	1019	SER	Peptide
5	B	1065	GLN	Peptide
5	B	1068	GLY	Peptide
5	B	1176	ASN	Peptide
5	B	1177	HIS	Peptide
5	B	1178	ASN	Peptide
5	B	182	SER	Peptide
5	B	183	GLU	Peptide
5	B	184	ALA	Peptide
5	B	229	ALA	Peptide
5	B	231	PRO	Peptide
5	B	327	ARG	Peptide
5	B	388	CYS	Peptide
5	B	510	LYS	Peptide
5	B	571	PRO	Peptide
5	B	572	HIS	Peptide
5	B	573	GLN	Peptide
5	B	705	MET	Peptide
5	B	709	ASP	Peptide
5	B	710	LEU	Peptide
5	B	863	GLU	Peptide
5	B	865	LYS	Peptide
5	B	866	TYR	Peptide
5	B	867	GLY	Peptide
5	B	868	MET	Peptide
7	E	138	ALA	Peptide
7	E	140	LEU	Peptide
9	H	105	GLU	Peptide
9	H	109	LYS	Peptide
9	H	110	ASP	Peptide
9	H	111	LEU	Peptide
9	H	128	ASN	Peptide
9	H	129	TYR	Peptide
9	H	130	ARG	Peptide
9	H	132	LEU	Peptide
9	H	136	LYS	Peptide
9	H	86	ASP	Peptide
9	H	87	ARG	Peptide
9	H	88	SER	Peptide
9	H	90	ALA	Peptide
9	H	92	ASP	Peptide
10	I	105	SER	Peptide

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Mol	Chain	Res	Type	Group
10	I	106	CYS	Peptide
10	I	107	SER	Peptide
10	I	16	PRO	Peptide
10	I	17	ARG	Peptide
10	I	19	ASP	Peptide
10	I	20	LYS	Peptide
10	I	3	THR	Peptide
10	I	4	PHE	Peptide
10	I	41	PRO	Peptide
10	I	43	VAL	Peptide
10	I	45	ARG	Peptide
10	I	56	ALA	Peptide
10	I	77	LYS	Peptide
10	I	79	HIS	Peptide
12	K	40	HIS	Peptide
13	L	42	ARG	Peptide
13	L	43	THR	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	10	0
2	T	564	0	316	13	0
3	N	284	0	161	2	0
4	A	10984	0	11070	896	0
5	B	8701	0	8729	537	0
6	C	2095	0	2051	72	0
7	E	1594	0	1622	60	0
8	F	670	0	690	33	0
9	H	1068	0	1040	132	0
10	I	971	0	930	128	0
11	J	532	0	543	32	0
12	K	919	0	929	25	0
13	L	363	0	387	26	0
14	T	32	0	12	4	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29003	0	28589	1861	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 32.

All (1861) 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:289:ILE:CG2	4:A:290:GLU:HB3	1.38	1.50
11:J:43:ARG:HG3	11:J:46:CYS:SG	1.49	1.49
4:A:1191:TRP:CA	4:A:1192:LEU:HB2	1.35	1.48
4:A:973:ILE:CG2	4:A:974:ASP:HA	1.43	1.46
4:A:287:HIS:HA	4:A:289:ILE:CB	1.46	1.45
5:B:1019:SER:CB	5:B:1020:ARG:HB2	1.45	1.44
4:A:286:HIS:CD2	4:A:287:HIS:HB3	1.52	1.44
4:A:1191:TRP:HA	4:A:1192:LEU:CB	1.31	1.42
4:A:709:THR:HA	4:A:710:LEU:CB	1.42	1.42
4:A:709:THR:CA	4:A:710:LEU:HB3	1.43	1.40
9:H:109:LYS:CB	9:H:110:ASP:HB2	1.54	1.38
13:L:42:ARG:HB2	13:L:43:THR:CB	1.54	1.38
4:A:1167:GLU:HB2	4:A:1168:GLU:CA	1.47	1.37
5:B:327:ARG:HB3	5:B:328:GLU:CB	1.54	1.37
10:I:25:LEU:HA	10:I:26:LEU:CB	1.50	1.36
4:A:973:ILE:HG23	4:A:974:ASP:CA	1.56	1.35
5:B:227:LYS:CA	5:B:228:LYS:HB2	1.55	1.34
4:A:289:ILE:HG23	4:A:290:GLU:CB	1.57	1.34
5:B:327:ARG:CB	5:B:328:GLU:HB2	1.58	1.32
5:B:227:LYS:HA	5:B:228:LYS:CB	1.56	1.30
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	1.66	1.30
4:A:701:LEU:HA	4:A:702:LEU:CB	1.47	1.29
9:H:109:LYS:CG	9:H:110:ASP:HB2	1.62	1.29
4:A:282:ASN:HB3	4:A:283:GLY:CA	1.60	1.28
4:A:1167:GLU:CB	4:A:1168:GLU:HA	1.58	1.28
4:A:1066:VAL:O	4:A:1069:ALA:HB3	1.34	1.27
9:H:111:LEU:HB2	9:H:112:ILE:CG2	1.66	1.26
5:B:868:MET:N	5:B:869:SER:HB3	1.49	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1019:SER:HB2	5:B:1020:ARG:CB	1.66	1.24
4:A:286:HIS:ND1	4:A:289:ILE:HD12	1.50	1.23
4:A:712:GLU:N	4:A:713:SER:HB2	1.53	1.22
5:B:877:PRO:CA	5:B:878:GLN:HB3	1.70	1.21
10:I:103:CYS:HB3	10:I:106:CYS:O	1.38	1.21
4:A:1083:THR:H	4:A:1084:PHE:C	1.48	1.21
4:A:1159:ARG:HB2	4:A:1161:THR:N	1.54	1.21
5:B:877:PRO:HA	5:B:878:GLN:CB	1.68	1.21
4:A:1083:THR:OG1	4:A:1084:PHE:HB3	1.36	1.20
5:B:705:MET:HB3	5:B:706:GLN:HB2	1.20	1.18
9:H:111:LEU:O	9:H:111:LEU:HD23	1.40	1.18
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.19	1.17
11:J:43:ARG:CG	11:J:46:CYS:SG	2.33	1.16
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.26	1.15
4:A:1159:ARG:HA	4:A:1160:SER:O	1.44	1.15
4:A:287:HIS:HA	4:A:289:ILE:HB	1.21	1.15
4:A:287:HIS:CA	4:A:289:ILE:HB	1.76	1.14
4:A:286:HIS:CG	4:A:287:HIS:HB3	1.83	1.14
10:I:3:THR:HA	10:I:4:PHE:CG	1.83	1.14
4:A:709:THR:HG22	4:A:710:LEU:HD23	1.27	1.13
4:A:286:HIS:CE1	4:A:287:HIS:HB2	1.84	1.13
5:B:573:GLN:O	5:B:575:PRO:HD3	1.46	1.13
10:I:45:ARG:HA	10:I:46:HIS:CB	1.77	1.13
8:F:99:LEU:O	8:F:99:LEU:HD13	1.47	1.12
9:H:111:LEU:CB	9:H:112:ILE:HG22	1.79	1.12
4:A:1071:SER:N	4:A:1072:ILE:HB	1.64	1.12
9:H:111:LEU:HB3	9:H:128:ASN:HB2	1.13	1.12
4:A:284:ALA:H	4:A:285:PRO:CD	1.64	1.11
4:A:1152:ILE:HA	4:A:1153:TYR:HB2	1.18	1.11
13:L:42:ARG:HB2	13:L:43:THR:HB	1.15	1.11
10:I:25:LEU:CA	10:I:26:LEU:HB2	1.77	1.11
5:B:1019:SER:H	5:B:1020:ARG:HB3	1.07	1.10
10:I:25:LEU:HA	10:I:26:LEU:HB2	1.13	1.10
4:A:1226:VAL:HB	4:A:1228:TRP:CH2	1.87	1.09
4:A:287:HIS:HA	4:A:289:ILE:CG2	1.80	1.08
4:A:1162:VAL:C	4:A:1163:ILE:HG12	1.74	1.08
10:I:45:ARG:CA	10:I:46:HIS:HB2	1.81	1.08
4:A:768:GLN:HE22	4:A:1087:ALA:HB1	1.14	1.08
10:I:20:LYS:HA	10:I:21:GLU:O	1.51	1.08
4:A:381:THR:CG2	4:A:382:PRO:HD2	1.84	1.08
5:B:571:PRO:HB2	5:B:572:HIS:HA	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:137:GLN:HG2	9:H:138:GLU:H	1.00	1.08
9:H:84:ALA:HA	9:H:85:GLY:C	1.77	1.08
4:A:1162:VAL:HA	4:A:1163:ILE:O	1.55	1.07
4:A:1091:SER:HB3	4:A:1093:LYS:C	1.79	1.07
5:B:882:THR:HB	5:B:883:LEU:HA	1.28	1.07
5:B:293:PRO:HA	5:B:294:ASP:HB2	1.30	1.07
4:A:1156:PRO:HB2	4:A:1159:ARG:H	1.15	1.06
5:B:1019:SER:HB2	5:B:1020:ARG:HB2	1.07	1.06
4:A:701:LEU:HA	4:A:702:LEU:HB3	1.10	1.06
4:A:67:CYS:HB2	4:A:70:CYS:HB2	1.38	1.06
4:A:381:THR:HG22	4:A:382:PRO:HD2	1.06	1.06
4:A:701:LEU:HA	4:A:702:LEU:HB2	1.31	1.06
9:H:111:LEU:HA	9:H:112:ILE:CB	1.85	1.06
4:A:712:GLU:H	4:A:713:SER:HB2	0.89	1.05
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	0.90	1.05
4:A:57:ARG:HB3	4:A:68:GLN:HB3	1.39	1.05
4:A:1083:THR:N	4:A:1084:PHE:O	1.90	1.04
4:A:1083:THR:HG23	4:A:1084:PHE:HD2	1.19	1.04
4:A:1091:SER:HB3	4:A:1093:LYS:O	1.57	1.04
4:A:282:ASN:HB3	4:A:283:GLY:HA2	1.31	1.04
4:A:286:HIS:CE1	4:A:289:ILE:HD12	1.92	1.04
4:A:701:LEU:CA	4:A:702:LEU:CB	2.32	1.04
4:A:286:HIS:CD2	4:A:287:HIS:CB	2.40	1.04
4:A:1200:ALA:N	4:A:1201:ALA:HB3	1.72	1.04
9:H:109:LYS:CG	9:H:110:ASP:CB	2.35	1.04
4:A:712:GLU:H	4:A:713:SER:CB	1.71	1.03
5:B:350:GLN:HB3	5:B:351:TYR:HB2	1.39	1.03
4:A:526:ASP:HB2	5:B:835:GLN:NE2	1.74	1.03
5:B:611:PRO:HB3	5:B:685:LEU:HD21	1.41	1.03
9:H:109:LYS:HB3	9:H:110:ASP:HB2	1.40	1.03
9:H:111:LEU:CA	9:H:112:ILE:HB	1.89	1.03
4:A:702:LEU:HG	4:A:704:ALA:H	1.21	1.02
9:H:111:LEU:HD12	9:H:128:ASN:H	1.23	1.02
4:A:973:ILE:CB	4:A:974:ASP:HA	1.84	1.02
13:L:55:ILE:O	13:L:56:LEU:HB2	1.58	1.02
9:H:87:ARG:HH11	9:H:87:ARG:HG3	1.23	1.01
9:H:109:LYS:HG3	9:H:110:ASP:CG	1.84	1.01
10:I:25:LEU:HA	10:I:26:LEU:HB3	1.40	1.01
5:B:1019:SER:N	5:B:1020:ARG:HB3	1.77	1.00
9:H:111:LEU:HA	9:H:112:ILE:HB	1.00	1.00
5:B:230:ALA:C	5:B:232:SER:HB3	1.87	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:42:LEU:HD22	10:I:43:VAL:H	1.24	1.00
4:A:287:HIS:CA	4:A:289:ILE:CB	2.35	1.00
9:H:109:LYS:HG3	9:H:110:ASP:CB	1.90	1.00
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.44	0.99
4:A:282:ASN:HB3	4:A:283:GLY:HA3	1.44	0.99
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.92	0.99
4:A:1159:ARG:HA	4:A:1160:SER:C	1.86	0.99
10:I:2:THR:O	10:I:3:THR:OG1	1.80	0.99
4:A:1085:HIS:HB3	4:A:1086:PHE:CD2	1.97	0.99
9:H:89:LEU:O	9:H:89:LEU:HD22	1.63	0.99
4:A:1159:ARG:HB3	4:A:1161:THR:HA	1.45	0.98
4:A:108:MET:HE3	4:A:167:CYS:HB2	1.45	0.98
4:A:1071:SER:H	4:A:1072:ILE:HB	0.83	0.98
5:B:383:ASN:O	5:B:387:LEU:HD23	1.63	0.98
4:A:701:LEU:CA	4:A:702:LEU:HB3	1.89	0.98
5:B:1175:LEU:HB2	5:B:1176:ASN:HA	1.45	0.98
9:H:137:GLN:HG2	9:H:138:GLU:N	1.77	0.98
4:A:975:HIS:O	4:A:977:LYS:HB2	1.63	0.98
5:B:709:ASP:H	5:B:710:LEU:HB2	1.23	0.98
5:B:231:PRO:N	5:B:232:SER:HB3	1.78	0.97
4:A:284:ALA:H	4:A:285:PRO:HD3	1.26	0.97
9:H:129:TYR:O	9:H:130:ARG:HG2	1.64	0.97
5:B:955:THR:HG22	5:B:956:THR:H	1.26	0.97
5:B:1019:SER:H	5:B:1020:ARG:CB	1.77	0.97
5:B:635:ARG:HB2	5:B:636:PRO:CD	1.94	0.97
5:B:1175:LEU:HA	5:B:1177:HIS:HD2	1.30	0.96
4:A:702:LEU:HG	4:A:704:ALA:N	1.78	0.96
5:B:1019:SER:CB	5:B:1020:ARG:CB	2.30	0.96
5:B:571:PRO:HD2	5:B:572:HIS:CD2	2.00	0.96
5:B:709:ASP:N	5:B:710:LEU:HB2	1.78	0.96
8:F:99:LEU:HD13	8:F:99:LEU:C	1.90	0.96
10:I:79:HIS:CA	10:I:80:SER:HB3	1.93	0.96
4:A:286:HIS:CE1	4:A:287:HIS:CB	2.47	0.96
4:A:1159:ARG:CA	4:A:1160:SER:C	2.36	0.96
5:B:571:PRO:HD2	5:B:572:HIS:CG	2.00	0.95
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.49	0.95
4:A:278:THR:O	4:A:279:LEU:HB2	1.67	0.95
4:A:1083:THR:N	4:A:1084:PHE:C	2.24	0.95
4:A:1226:VAL:CG1	4:A:1228:TRP:CZ3	2.49	0.95
4:A:287:HIS:H	4:A:289:ILE:H	1.13	0.95
10:I:25:LEU:CA	10:I:26:LEU:CB	2.37	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:853:ASP:OD2	4:A:855:THR:HG22	1.64	0.95
5:B:1019:SER:CA	5:B:1020:ARG:HB2	1.92	0.94
5:B:705:MET:HB3	5:B:706:GLN:CB	1.97	0.94
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.48	0.94
4:A:972:HIS:HB2	4:A:974:ASP:OD1	1.67	0.94
5:B:766:ARG:HH21	5:B:1020:ARG:HA	1.30	0.94
4:A:107:CYS:SG	4:A:108:MET:HB2	2.07	0.94
4:A:287:HIS:HA	4:A:289:ILE:CA	1.97	0.94
4:A:503:GLN:C	4:A:504:LEU:HD12	1.91	0.94
4:A:67:CYS:CB	4:A:70:CYS:HB2	1.97	0.94
4:A:282:ASN:CB	4:A:283:GLY:CA	2.41	0.94
5:B:868:MET:H	5:B:869:SER:HB3	1.31	0.94
7:E:18:THR:HG21	7:E:140:LEU:HD13	1.47	0.94
4:A:1071:SER:H	4:A:1072:ILE:CB	1.78	0.93
5:B:1175:LEU:HA	5:B:1177:HIS:CD2	2.04	0.93
4:A:287:HIS:N	4:A:289:ILE:H	1.65	0.93
10:I:42:LEU:HD22	10:I:43:VAL:N	1.84	0.93
4:A:108:MET:HG2	4:A:169:ASN:HD21	1.32	0.92
4:A:754:SER:H	4:A:757:ASN:HD22	1.13	0.92
9:H:85:GLY:HA2	9:H:86:ASP:HB2	1.48	0.92
4:A:286:HIS:ND1	4:A:289:ILE:CD1	2.32	0.92
13:L:42:ARG:CB	13:L:43:THR:CB	2.46	0.92
5:B:868:MET:N	5:B:869:SER:CB	2.31	0.92
9:H:111:LEU:HB2	9:H:112:ILE:HG22	0.92	0.92
4:A:1152:ILE:CA	4:A:1153:TYR:HB2	1.98	0.91
5:B:1019:SER:CA	5:B:1020:ARG:CB	2.47	0.91
9:H:87:ARG:HH11	9:H:87:ARG:CG	1.82	0.91
10:I:80:SER:HB2	10:I:105:SER:OG	1.70	0.91
9:H:111:LEU:HD12	9:H:128:ASN:N	1.83	0.91
4:A:1162:VAL:O	4:A:1163:ILE:HG12	1.70	0.91
4:A:1072:ILE:HG22	4:A:1073:GLY:N	1.84	0.91
9:H:111:LEU:CB	9:H:128:ASN:HB2	2.01	0.91
4:A:287:HIS:CB	4:A:289:ILE:HB	2.01	0.90
4:A:768:GLN:OE1	4:A:768:GLN:HA	1.72	0.90
5:B:744:HIS:CG	5:B:745:PRO:HD2	2.07	0.90
4:A:282:ASN:CB	4:A:283:GLY:HA3	1.97	0.90
4:A:286:HIS:NE2	4:A:287:HIS:CB	2.34	0.90
5:B:709:ASP:CA	5:B:710:LEU:HB2	2.01	0.90
5:B:868:MET:H	5:B:869:SER:C	1.80	0.90
4:A:1091:SER:CB	4:A:1093:LYS:C	2.44	0.90
9:H:128:ASN:HA	9:H:130:ARG:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1239:ARG:HD3	4:A:1241:ARG:HH12	1.35	0.89
4:A:289:ILE:HG21	4:A:290:GLU:HB3	1.53	0.89
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.37	0.89
4:A:1159:ARG:CB	4:A:1161:THR:HA	2.02	0.89
5:B:709:ASP:HB3	5:B:710:LEU:HD12	1.53	0.89
4:A:1098:VAL:N	4:A:1099:PRO:HD2	1.87	0.89
5:B:868:MET:H	5:B:869:SER:CB	1.86	0.89
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.37	0.89
6:C:58:LEU:HD11	11:J:2:ILE:HD12	1.55	0.88
4:A:802:ASN:HD21	5:B:729:ILE:H	1.19	0.88
5:B:572:HIS:H	5:B:573:GLN:HB3	1.39	0.88
10:I:79:HIS:HA	10:I:80:SER:HB3	1.52	0.88
4:A:699:ALA:H	4:A:700:ASN:HA	1.38	0.88
4:A:702:LEU:HD21	4:A:704:ALA:HB2	1.56	0.88
9:H:81:PRO:HB2	9:H:82:PRO:CD	2.04	0.88
4:A:1167:GLU:CB	4:A:1168:GLU:CA	2.34	0.88
4:A:289:ILE:CG2	4:A:290:GLU:CB	2.33	0.87
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.53	0.87
9:H:129:TYR:HB2	9:H:130:ARG:O	1.74	0.87
4:A:707:GLY:O	4:A:708:MET:SD	2.33	0.87
4:A:1069:ALA:O	4:A:1071:SER:HB2	1.75	0.87
5:B:883:LEU:HD13	5:B:883:LEU:H	1.38	0.87
5:B:1019:SER:N	5:B:1020:ARG:CB	2.36	0.87
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.05	0.86
5:B:868:MET:CA	5:B:869:SER:HB3	2.05	0.86
4:A:973:ILE:HG23	4:A:974:ASP:CB	2.05	0.86
10:I:78:CYS:SG	10:I:80:SER:CB	2.63	0.86
4:A:287:HIS:HA	4:A:289:ILE:HG22	1.56	0.86
4:A:1159:ARG:HB2	4:A:1160:SER:C	2.01	0.86
9:H:89:LEU:HD22	9:H:89:LEU:C	2.01	0.86
4:A:1155:ASP:HB2	4:A:1192:LEU:HD23	1.57	0.86
4:A:702:LEU:HD11	4:A:704:ALA:HB2	1.56	0.86
10:I:42:LEU:CD2	10:I:43:VAL:H	1.89	0.86
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	1.58	0.86
4:A:287:HIS:CA	4:A:289:ILE:N	2.38	0.85
10:I:78:CYS:SG	10:I:80:SER:HB3	2.16	0.85
5:B:1177:HIS:HA	5:B:1178:ASN:CG	2.01	0.85
4:A:1083:THR:HG23	4:A:1084:PHE:CD2	2.11	0.85
4:A:1159:ARG:HB2	4:A:1161:THR:CA	2.05	0.85
4:A:286:HIS:CG	4:A:287:HIS:CB	2.56	0.85
4:A:696:GLU:O	4:A:700:ASN:HA	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1162:VAL:C	4:A:1163:ILE:CG1	2.49	0.85
5:B:1176:ASN:O	5:B:1177:HIS:CG	2.30	0.85
10:I:43:VAL:HB	10:I:44:TYR:HA	1.59	0.85
4:A:286:HIS:NE2	4:A:287:HIS:HB3	1.91	0.85
4:A:973:ILE:HG12	4:A:974:ASP:C	2.01	0.85
4:A:1159:ARG:CB	4:A:1160:SER:C	2.50	0.85
4:A:1159:ARG:CB	4:A:1161:THR:N	2.37	0.85
9:H:109:LYS:CG	9:H:110:ASP:CG	2.49	0.85
4:A:57:ARG:CB	4:A:68:GLN:HB3	2.06	0.84
4:A:827:THR:OG1	4:A:1083:THR:HG21	1.76	0.84
5:B:879:ARG:O	5:B:880:THR:HG22	1.77	0.84
4:A:1162:VAL:HG22	4:A:1163:ILE:N	1.91	0.84
4:A:1226:VAL:HG12	4:A:1228:TRP:CZ3	2.13	0.84
10:I:3:THR:N	10:I:4:PHE:HB3	1.92	0.84
4:A:284:ALA:N	4:A:285:PRO:CD	2.38	0.84
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.59	0.84
5:B:1163:CYS:HB3	5:B:1167:GLY:N	1.91	0.84
10:I:79:HIS:HA	10:I:80:SER:CB	2.08	0.84
9:H:111:LEU:CB	9:H:112:ILE:CG2	2.49	0.83
4:A:1096:SER:N	4:A:1097:GLY:HA3	1.93	0.83
4:A:707:GLY:HA2	4:A:709:THR:H	1.42	0.83
4:A:1077:THR:O	4:A:1081:LEU:HB3	1.77	0.83
9:H:109:LYS:CB	9:H:110:ASP:CB	2.50	0.83
4:A:503:GLN:HB3	4:A:504:LEU:CD1	2.07	0.83
4:A:630:ILE:H	4:A:630:ILE:HD12	1.42	0.83
5:B:711:GLU:H	5:B:712:PRO:CD	1.92	0.83
4:A:287:HIS:HA	4:A:289:ILE:N	1.92	0.83
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	1.84	0.83
4:A:1083:THR:OG1	4:A:1084:PHE:CB	2.23	0.83
5:B:709:ASP:H	5:B:710:LEU:CB	1.91	0.83
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.61	0.83
4:A:287:HIS:O	4:A:287:HIS:CG	2.32	0.83
4:A:1162:VAL:HG23	4:A:1163:ILE:C	2.04	0.83
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.60	0.83
4:A:1050:GLU:O	4:A:1054:LEU:HD13	1.79	0.82
4:A:699:ALA:N	4:A:700:ASN:HA	1.88	0.82
5:B:225:VAL:HG11	5:B:388:CYS:HB3	1.62	0.82
5:B:868:MET:CB	5:B:869:SER:CB	2.58	0.82
5:B:886:LYS:HG2	5:B:940:PRO:HG3	1.61	0.82
4:A:754:SER:H	4:A:757:ASN:ND2	1.75	0.82
5:B:708:GLU:O	5:B:708:GLU:HG2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:45:ARG:HA	10:I:46:HIS:HB2	0.88	0.82
10:I:3:THR:CA	10:I:4:PHE:HB3	2.09	0.82
4:A:973:ILE:HG23	4:A:974:ASP:HA	0.82	0.81
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.61	0.81
4:A:768:GLN:NE2	4:A:1087:ALA:HB1	1.95	0.81
4:A:1082:ASN:HB3	4:A:1084:PHE:O	1.80	0.81
4:A:1167:GLU:HB2	4:A:1168:GLU:C	2.04	0.81
4:A:1436:ILE:HG22	4:A:1437:GLY:N	1.96	0.81
7:E:137:GLU:C	7:E:139:ALA:HB3	2.05	0.81
4:A:1083:THR:C	4:A:1084:PHE:O	2.22	0.81
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.45	0.81
4:A:1197:LEU:HB2	4:A:1198:ASP:O	1.80	0.81
4:A:1069:ALA:O	4:A:1071:SER:CB	2.28	0.81
4:A:704:ALA:HB1	4:A:710:LEU:HD21	1.62	0.81
6:C:67:LEU:O	6:C:70:ILE:HG22	1.81	0.81
9:H:129:TYR:N	9:H:129:TYR:HD2	1.78	0.81
10:I:75:CYS:SG	10:I:110:PHE:CE2	2.74	0.81
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.62	0.81
5:B:878:GLN:HG3	5:B:881:ASN:HB2	1.61	0.81
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.62	0.80
5:B:705:MET:CB	5:B:706:GLN:HB2	2.07	0.80
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.62	0.80
4:A:1096:SER:OG	4:A:1097:GLY:HA2	1.80	0.80
9:H:109:LYS:HG3	9:H:110:ASP:HB2	1.46	0.80
4:A:1160:SER:HB2	4:A:1162:VAL:HG12	1.61	0.80
4:A:702:LEU:CG	4:A:704:ALA:HB2	2.10	0.80
5:B:865:LYS:HG3	5:B:866:TYR:H	1.43	0.80
5:B:230:ALA:H	5:B:231:PRO:CD	1.95	0.80
5:B:230:ALA:N	5:B:231:PRO:CD	2.45	0.80
6:C:32:SER:O	6:C:36:VAL:HG23	1.81	0.80
5:B:635:ARG:CB	5:B:636:PRO:HD2	2.09	0.80
5:B:778:MET:HE1	5:B:1094:ARG:HH11	1.47	0.80
4:A:1089:VAL:N	4:A:1090:ALA:HA	1.97	0.80
4:A:1156:PRO:HB2	4:A:1159:ARG:N	1.95	0.79
11:J:43:ARG:CD	11:J:46:CYS:SG	2.70	0.79
5:B:183:GLU:N	5:B:184:ALA:HB3	1.98	0.79
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.65	0.79
4:A:108:MET:HE2	4:A:169:ASN:OD1	1.82	0.79
10:I:3:THR:HA	10:I:4:PHE:CB	2.11	0.79
2:T:19:DT:H2'	2:T:20:DC:H6	1.48	0.79
5:B:327:ARG:O	5:B:330:ALA:HB3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:287:HIS:N	4:A:289:ILE:N	2.31	0.79
4:A:701:LEU:HD23	4:A:701:LEU:H	1.48	0.79
4:A:768:GLN:HG3	4:A:816:HIS:HA	1.65	0.79
10:I:75:CYS:SG	10:I:108:HIS:CD2	2.76	0.78
4:A:675:THR:HG21	4:A:736:ASN:HD21	1.46	0.78
7:E:18:THR:CG2	7:E:140:LEU:HD13	2.13	0.78
9:H:131:ASN:O	9:H:132:LEU:HB3	1.81	0.78
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.62	0.78
4:A:1084:PHE:HA	4:A:1085:HIS:C	2.08	0.78
4:A:1156:PRO:HD2	4:A:1163:ILE:HD13	1.66	0.78
4:A:1159:ARG:CB	4:A:1161:THR:CA	2.60	0.78
10:I:75:CYS:SG	10:I:108:HIS:NE2	2.56	0.78
4:A:1191:TRP:CA	4:A:1192:LEU:CB	2.17	0.78
10:I:20:LYS:HG2	10:I:24:ARG:H	1.48	0.78
4:A:702:LEU:HD21	4:A:704:ALA:CB	2.13	0.78
4:A:1158:PRO:HA	4:A:1159:ARG:HG3	1.66	0.78
4:A:1162:VAL:CA	4:A:1163:ILE:O	2.32	0.78
4:A:108:MET:CE	4:A:167:CYS:HB2	2.13	0.78
4:A:702:LEU:CD2	4:A:704:ALA:HB2	2.14	0.78
8:F:99:LEU:C	8:F:99:LEU:CD1	2.57	0.78
4:A:973:ILE:HD11	4:A:977:LYS:O	1.83	0.77
4:A:1074:GLU:HB3	4:A:1075:PRO:CD	2.14	0.77
4:A:1200:ALA:H	4:A:1201:ALA:HB3	1.47	0.77
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.47	0.77
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.65	0.77
9:H:137:GLN:CG	9:H:138:GLU:H	1.89	0.77
10:I:107:SER:OG	10:I:108:HIS:HB2	1.85	0.77
13:L:42:ARG:CB	13:L:43:THR:HB	2.06	0.77
5:B:1175:LEU:HB2	5:B:1177:HIS:O	1.84	0.77
5:B:549:THR:HG22	5:B:550:ASP:H	1.50	0.77
5:B:868:MET:CB	5:B:869:SER:HB3	2.13	0.77
5:B:1177:HIS:HA	5:B:1178:ASN:OD1	1.83	0.77
8:F:99:LEU:HD21	8:F:103:MET:HE3	1.65	0.77
10:I:78:CYS:O	10:I:79:HIS:CG	2.38	0.77
4:A:702:LEU:CD1	4:A:704:ALA:HB2	2.14	0.77
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.15	0.77
4:A:1152:ILE:HG22	4:A:1153:TYR:O	1.84	0.77
5:B:636:PRO:CB	5:B:637:LEU:HA	2.15	0.77
10:I:103:CYS:SG	10:I:106:CYS:N	2.57	0.77
5:B:1175:LEU:HG	5:B:1176:ASN:OD1	1.85	0.77
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1085:HIS:H	4:A:1085:HIS:CD2	2.02	0.76
5:B:230:ALA:N	5:B:231:PRO:HD2	1.99	0.76
5:B:1019:SER:HB3	5:B:1020:ARG:HB2	1.65	0.76
5:B:1156:ASP:HB3	5:B:1198:TYR:H	1.49	0.76
9:H:129:TYR:N	9:H:129:TYR:CD2	2.51	0.76
9:H:111:LEU:O	9:H:111:LEU:CD2	2.30	0.76
6:C:142:VAL:HG13	11:J:15:GLY:HA3	1.66	0.76
10:I:3:THR:H	10:I:4:PHE:HB3	1.49	0.76
10:I:21:GLU:O	10:I:22:ASN:HB3	1.85	0.76
4:A:320:ARG:HB2	4:A:321:PRO:HA	1.67	0.76
4:A:710:LEU:HG	4:A:710:LEU:O	1.85	0.76
4:A:1157:ASP:OD2	4:A:1188:GLN:HB3	1.85	0.76
9:H:85:GLY:HA2	9:H:86:ASP:CB	2.15	0.76
10:I:3:THR:CA	10:I:4:PHE:CB	2.62	0.76
5:B:573:GLN:O	5:B:575:PRO:CD	2.30	0.76
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.68	0.76
5:B:883:LEU:HD13	5:B:883:LEU:N	2.01	0.76
6:C:74:SER:O	6:C:77:ILE:HB	1.85	0.76
4:A:289:ILE:HG12	4:A:290:GLU:HA	1.68	0.76
4:A:1226:VAL:CG1	4:A:1228:TRP:HZ3	1.98	0.76
9:H:108:SER:HB3	9:H:111:LEU:H	1.51	0.76
5:B:705:MET:H	5:B:710:LEU:HD13	1.49	0.75
9:H:90:ALA:HB1	9:H:93:TYR:H	1.50	0.75
4:A:1071:SER:O	4:A:1075:PRO:CD	2.34	0.75
4:A:381:THR:HG22	4:A:382:PRO:CD	2.02	0.75
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.51	0.75
5:B:882:THR:CB	5:B:883:LEU:HA	2.02	0.75
4:A:287:HIS:CA	4:A:289:ILE:HG22	2.17	0.75
9:H:77:ARG:HG3	9:H:77:ARG:HH11	1.52	0.74
10:I:43:VAL:CB	10:I:44:TYR:HA	2.16	0.74
4:A:1200:ALA:HA	4:A:1201:ALA:C	2.12	0.74
11:J:43:ARG:HD2	11:J:46:CYS:SG	2.27	0.74
10:I:5:ARG:HG2	10:I:6:PHE:H	1.53	0.74
4:A:289:ILE:HG23	4:A:290:GLU:HB3	0.75	0.74
4:A:304:MET:SD	5:B:1210:MET:HG3	2.26	0.74
4:A:1068:ALA:O	4:A:1072:ILE:HG13	1.86	0.74
5:B:709:ASP:CB	5:B:710:LEU:HB2	2.17	0.74
13:L:42:ARG:HB2	13:L:43:THR:CA	2.12	0.74
5:B:711:GLU:H	5:B:712:PRO:HD3	1.52	0.74
4:A:249:SER:HA	4:A:259:GLU:HA	1.68	0.73
4:A:523:ILE:HD13	4:A:622:VAL:HG22	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:868:MET:H	5:B:869:SER:CA	1.99	0.73
13:L:42:ARG:HB2	13:L:43:THR:OG1	1.87	0.73
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.70	0.73
4:A:973:ILE:CG1	4:A:974:ASP:HA	2.18	0.73
5:B:230:ALA:H	5:B:231:PRO:HD2	1.51	0.73
9:H:107:VAL:CG1	9:H:108:SER:N	2.51	0.73
4:A:95:PHE:HE2	4:A:1414:ALA:HB2	1.53	0.73
4:A:280:GLU:O	4:A:281:HIS:HB2	1.88	0.73
4:A:287:HIS:CA	4:A:289:ILE:CG2	2.62	0.73
4:A:1156:PRO:HD2	4:A:1163:ILE:CD1	2.18	0.73
4:A:1236:LEU:HA	4:A:1237:ILE:HB	1.69	0.73
10:I:25:LEU:HG	10:I:25:LEU:O	1.88	0.73
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.21	0.73
10:I:4:PHE:CD1	10:I:4:PHE:C	2.64	0.73
13:L:42:ARG:CB	13:L:43:THR:OG1	2.37	0.73
4:A:701:LEU:CA	4:A:702:LEU:HB2	2.09	0.72
5:B:1163:CYS:HB3	5:B:1167:GLY:H	1.52	0.72
9:H:85:GLY:CA	9:H:86:ASP:HB2	2.17	0.72
5:B:571:PRO:CB	5:B:572:HIS:HA	2.15	0.72
5:B:1175:LEU:CB	5:B:1177:HIS:O	2.37	0.72
4:A:168:GLY:O	4:A:169:ASN:O	2.07	0.72
4:A:1157:ASP:H	4:A:1159:ARG:N	1.87	0.72
10:I:78:CYS:C	10:I:79:HIS:CG	2.68	0.72
4:A:380:VAL:HG21	4:A:427:GLN:O	1.89	0.72
5:B:868:MET:CA	5:B:869:SER:CB	2.67	0.72
9:H:109:LYS:HB3	9:H:110:ASP:CB	2.18	0.72
5:B:327:ARG:HB3	5:B:328:GLU:CA	2.19	0.72
4:A:1197:LEU:CB	4:A:1198:ASP:O	2.38	0.72
5:B:1175:LEU:CB	5:B:1176:ASN:HA	2.14	0.72
4:A:1075:PRO:O	4:A:1079:MET:N	2.22	0.72
5:B:256:VAL:HG11	5:B:382:ILE:CD1	2.20	0.72
5:B:706:GLN:HB3	5:B:709:ASP:HB2	1.71	0.72
5:B:744:HIS:ND1	5:B:745:PRO:HD2	2.04	0.72
4:A:286:HIS:ND1	4:A:287:HIS:HB2	2.05	0.72
4:A:567:LYS:CB	4:A:568:PRO:CD	2.67	0.72
5:B:35:SER:HA	5:B:811:TYR:HE2	1.54	0.72
10:I:4:PHE:C	10:I:4:PHE:HD1	1.97	0.72
4:A:70:CYS:SG	4:A:77:CYS:HB2	2.30	0.71
4:A:1167:GLU:HB2	4:A:1168:GLU:HA	0.75	0.71
4:A:278:THR:O	4:A:279:LEU:CB	2.38	0.71
4:A:503:GLN:CB	4:A:504:LEU:CD1	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:109:LYS:HG2	9:H:110:ASP:OD2	1.90	0.71
4:A:1097:GLY:H	4:A:1100:ARG:HB2	1.54	0.71
4:A:1226:VAL:HG11	4:A:1228:TRP:HZ3	1.56	0.71
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.54	0.71
4:A:1091:SER:CB	4:A:1094:VAL:N	2.54	0.71
9:H:83:GLN:O	9:H:83:GLN:HG3	1.90	0.71
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.08	0.71
4:A:1085:HIS:HB3	4:A:1086:PHE:CG	2.24	0.71
7:E:138:ALA:N	7:E:139:ALA:HB3	2.05	0.71
4:A:289:ILE:HG23	4:A:290:GLU:CA	2.19	0.71
4:A:1089:VAL:HG13	4:A:1090:ALA:N	2.06	0.71
5:B:496:ARG:HB3	5:B:539:LEU:HD12	1.72	0.71
10:I:80:SER:HB2	10:I:105:SER:HG	1.52	0.71
4:A:1161:THR:O	4:A:1163:ILE:CG1	2.39	0.71
4:A:1171:GLN:C	4:A:1173:HIS:N	2.49	0.71
4:A:875:ALA:HB2	4:A:1366:ARG:HD3	1.72	0.70
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.72	0.70
4:A:55:ASP:O	4:A:58:LEU:N	2.24	0.70
4:A:704:ALA:HB1	4:A:710:LEU:CD2	2.21	0.70
4:A:1421:CYS:HA	4:A:1426:GLU:HG2	1.73	0.70
5:B:877:PRO:HA	5:B:878:GLN:HB3	0.80	0.70
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.20	0.70
4:A:1154:TYR:O	4:A:1192:LEU:HD21	1.91	0.70
9:H:107:VAL:HG12	9:H:108:SER:H	1.56	0.70
4:A:289:ILE:HG23	4:A:290:GLU:N	2.06	0.70
4:A:1072:ILE:HG22	4:A:1073:GLY:H	1.56	0.70
4:A:1162:VAL:CG2	4:A:1163:ILE:N	2.55	0.70
5:B:880:THR:HG23	5:B:880:THR:O	1.92	0.70
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.24	0.69
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.05	0.69
9:H:139:ASN:O	9:H:140:ALA:HB2	1.92	0.69
4:A:596:THR:C	4:A:598:LEU:H	1.99	0.69
5:B:868:MET:HB2	5:B:869:SER:HB3	1.74	0.69
6:C:66:ARG:NH2	11:J:3:VAL:O	2.24	0.69
9:H:105:GLU:O	9:H:106:GLU:HB2	1.92	0.69
4:A:768:GLN:HE21	4:A:816:HIS:CE1	2.09	0.69
4:A:1116:LEU:HD13	4:A:1329:THR:HG23	1.73	0.69
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.58	0.69
4:A:380:VAL:HG22	4:A:430:TRP:H	1.58	0.69
4:A:973:ILE:CB	4:A:974:ASP:CA	2.68	0.69
4:A:1063:MET:SD	4:A:1436:ILE:HG23	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.75	0.69
5:B:709:ASP:HB3	5:B:710:LEU:CD1	2.20	0.69
4:A:265:LYS:HZ1	4:A:323:LYS:HE2	1.58	0.69
5:B:955:THR:HG23	13:L:54:ARG:HB3	1.74	0.69
5:B:350:GLN:HB3	5:B:351:TYR:CB	2.21	0.69
5:B:572:HIS:H	5:B:573:GLN:CB	2.05	0.69
10:I:78:CYS:O	10:I:79:HIS:CD2	2.46	0.69
4:A:1096:SER:H	4:A:1097:GLY:HA3	1.55	0.69
5:B:1176:ASN:C	5:B:1177:HIS:CG	2.71	0.69
4:A:1054:LEU:C	4:A:1054:LEU:CD2	2.65	0.69
4:A:1162:VAL:HG23	4:A:1163:ILE:O	1.92	0.69
4:A:1438:THR:HG22	8:F:92:ARG:HB2	1.74	0.69
4:A:972:HIS:CD2	4:A:972:HIS:N	2.61	0.68
4:A:973:ILE:CG1	4:A:974:ASP:CA	2.70	0.68
4:A:1155:ASP:OD1	4:A:1157:ASP:HB2	1.93	0.68
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.73	0.68
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.28	0.68
9:H:107:VAL:HG12	9:H:111:LEU:O	1.93	0.68
4:A:249:SER:HB3	4:A:259:GLU:HG2	1.74	0.68
4:A:973:ILE:HG12	4:A:974:ASP:CA	2.22	0.68
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.28	0.68
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.75	0.68
4:A:1098:VAL:N	4:A:1099:PRO:CD	2.54	0.68
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	2.08	0.68
5:B:589:VAL:HG12	5:B:590:HIS:N	2.08	0.68
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.74	0.68
4:A:289:ILE:HG12	4:A:290:GLU:CA	2.22	0.68
4:A:1161:THR:O	4:A:1163:ILE:HG13	1.94	0.68
9:H:112:ILE:CG2	9:H:127:GLY:O	2.41	0.68
4:A:855:THR:CG2	4:A:857:ARG:HE	2.07	0.68
5:B:589:VAL:HG12	5:B:590:HIS:H	1.58	0.68
4:A:290:GLU:OE2	4:A:291:GLU:N	2.25	0.68
4:A:1200:ALA:HB2	4:A:1203:ASN:HB2	1.75	0.68
5:B:390:LEU:C	5:B:391:ASP:CG	2.62	0.68
9:H:126:GLU:HG2	9:H:127:GLY:H	1.58	0.68
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.76	0.68
4:A:1069:ALA:HB1	4:A:1070:GLN:HA	1.75	0.68
9:H:107:VAL:HG12	9:H:108:SER:N	2.09	0.68
4:A:1319:VAL:O	4:A:1322:ILE:HD13	1.94	0.68
4:A:312:PRO:O	4:A:313:GLN:HB2	1.93	0.67
4:A:972:HIS:CD2	4:A:972:HIS:H	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1318:THR:HB	7:E:141:VAL:HG11	1.76	0.67
9:H:111:LEU:CA	9:H:112:ILE:CB	2.55	0.67
4:A:503:GLN:C	4:A:504:LEU:CD1	2.67	0.67
4:A:1084:PHE:HA	4:A:1085:HIS:O	1.94	0.67
10:I:21:GLU:O	10:I:22:ASN:CB	2.40	0.67
4:A:1071:SER:O	4:A:1075:PRO:HD2	1.93	0.67
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.30	0.67
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.24	0.67
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.76	0.67
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.76	0.67
4:A:712:GLU:N	4:A:713:SER:CB	2.43	0.67
4:A:1159:ARG:CZ	4:A:1159:ARG:O	2.42	0.67
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.59	0.67
9:H:87:ARG:CG	9:H:87:ARG:NH1	2.50	0.67
5:B:183:GLU:CA	5:B:184:ALA:HB3	2.24	0.67
7:E:18:THR:HG21	7:E:140:LEU:CD1	2.23	0.67
5:B:572:HIS:N	5:B:573:GLN:C	2.53	0.67
5:B:1001:PHE:HE1	6:C:178:PHE:HB3	1.60	0.67
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.75	0.67
9:H:129:TYR:HD2	9:H:129:TYR:H	1.40	0.67
4:A:351:THR:HG22	4:A:352:VAL:N	2.08	0.67
4:A:1104:ILE:HG22	4:A:1105:LEU:HD12	1.76	0.67
5:B:709:ASP:HB3	5:B:710:LEU:HB2	1.75	0.67
5:B:1017:ILE:H	5:B:1018:PRO:HD2	1.59	0.67
4:A:287:HIS:HB2	4:A:289:ILE:HB	1.76	0.66
4:A:380:VAL:HG23	4:A:429:GLY:H	1.60	0.66
4:A:605:MET:HE3	4:A:606:LEU:H	1.60	0.66
4:A:768:GLN:NE2	4:A:816:HIS:ND1	2.34	0.66
4:A:1080:THR:C	4:A:1082:ASN:H	2.03	0.66
5:B:474:SER:HB2	5:B:476:ARG:HG3	1.77	0.66
5:B:882:THR:HB	5:B:883:LEU:CA	2.17	0.66
7:E:127:ILE:HD11	7:E:132:ILE:HD11	1.76	0.66
5:B:983:ARG:HD2	5:B:1091:TYR:CD2	2.26	0.66
10:I:25:LEU:N	10:I:26:LEU:HB2	2.09	0.66
4:A:404:TYR:HA	4:A:413:ILE:O	1.95	0.66
4:A:1226:VAL:HB	4:A:1228:TRP:CZ3	2.29	0.66
4:A:332:LYS:H	4:A:337:ARG:HB2	1.60	0.66
4:A:1078:GLN:C	4:A:1080:THR:O	2.38	0.66
7:E:138:ALA:CA	7:E:139:ALA:HB3	2.25	0.66
5:B:868:MET:CB	5:B:869:SER:HB2	2.24	0.66
9:H:88:SER:O	9:H:89:LEU:HD12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:1:MET:O	11:J:2:ILE:HB	1.94	0.66
4:A:525:GLN:HA	5:B:1015:HIS:CE1	2.31	0.66
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	1.77	0.66
5:B:571:PRO:HB2	5:B:572:HIS:CA	2.18	0.66
5:B:325:GLN:O	5:B:326:ASP:HB2	1.95	0.66
5:B:567:GLU:H	5:B:567:GLU:CD	2.03	0.66
4:A:814:PHE:HB2	5:B:519:TRP:HZ3	1.60	0.66
5:B:706:GLN:CB	5:B:710:LEU:HD12	2.25	0.66
9:H:5:LEU:HB2	9:H:60:ALA:H	1.61	0.66
4:A:380:VAL:CG2	4:A:430:TRP:H	2.07	0.65
4:A:1070:GLN:O	4:A:1073:GLY:C	2.39	0.65
5:B:512:ARG:HB3	5:B:534:GLY:HA3	1.77	0.65
5:B:1004:GLU:O	6:C:177:GLU:HG2	1.97	0.65
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.77	0.65
4:A:1155:ASP:CB	4:A:1192:LEU:HD23	2.26	0.65
5:B:846:ILE:HG23	5:B:974:PRO:HG2	1.78	0.65
4:A:10:PRO:HG2	5:B:1192:TYR:HA	1.79	0.65
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.26	0.65
4:A:456:MET:HB2	4:A:478:TYR:OH	1.96	0.65
4:A:1392:SER:O	4:A:1393:ASN:C	2.40	0.65
5:B:868:MET:HB2	5:B:869:SER:CB	2.26	0.65
10:I:103:CYS:CB	10:I:106:CYS:O	2.32	0.65
4:A:286:HIS:ND1	4:A:287:HIS:CB	2.59	0.65
4:A:287:HIS:C	4:A:289:ILE:HG22	2.21	0.65
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.62	0.65
10:I:78:CYS:SG	10:I:79:HIS:N	2.70	0.65
4:A:1153:TYR:HB3	4:A:1192:LEU:CD1	2.26	0.64
5:B:811:TYR:N	5:B:811:TYR:CD1	2.65	0.64
9:H:6:PHE:CZ	9:H:134:ASN:HB2	2.32	0.64
5:B:230:ALA:CA	5:B:232:SER:HB3	2.27	0.64
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.79	0.64
5:B:1177:HIS:HB2	5:B:1178:ASN:HB2	1.78	0.64
4:A:350:ARG:HD3	4:A:488:ASN:OD1	1.96	0.64
4:A:466:SER:HB3	12:K:2:ASN:HD22	1.61	0.64
9:H:109:LYS:CA	9:H:110:ASP:HB2	2.15	0.64
4:A:909:ASP:C	4:A:911:SER:H	2.03	0.64
5:B:364:ILE:O	5:B:365:THR:HB	1.96	0.64
6:C:18:VAL:HG12	6:C:20:PHE:CD2	2.32	0.64
8:F:116:ASP:OD2	8:F:117:PRO:HD2	1.98	0.64
5:B:872:GLU:HG2	5:B:916:THR:HB	1.78	0.64
5:B:1177:HIS:HA	5:B:1178:ASN:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:2:THR:C	10:I:3:THR:HG1	1.90	0.64
10:I:33:SER:HA	10:I:34:TYR:HB3	1.78	0.64
4:A:288:ALA:O	4:A:290:GLU:N	2.31	0.64
4:A:700:ASN:OD1	4:A:702:LEU:HD13	1.98	0.64
4:A:1089:VAL:H	4:A:1090:ALA:HA	1.61	0.64
4:A:1098:VAL:HG12	4:A:1099:PRO:HD3	1.79	0.64
4:A:1322:ILE:O	4:A:1324:PRO:HD3	1.98	0.64
8:F:119:ARG:HH11	8:F:119:ARG:HG3	1.63	0.64
9:H:81:PRO:HB2	9:H:82:PRO:HD3	1.79	0.64
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.33	0.64
10:I:22:ASN:O	10:I:23:ASN:HB2	1.98	0.64
5:B:1156:ASP:CB	5:B:1198:TYR:H	2.11	0.64
9:H:90:ALA:O	9:H:92:ASP:N	2.30	0.64
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.63	0.63
5:B:1033:LYS:NZ	5:B:1068:GLY:O	2.31	0.63
9:H:112:ILE:CG2	9:H:112:ILE:O	2.46	0.63
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.79	0.63
4:A:1083:THR:CA	4:A:1084:PHE:O	2.47	0.63
8:F:145:ASP:O	8:F:146:TRP:HB2	1.98	0.63
4:A:739:ASP:O	4:A:745:GLN:NE2	2.29	0.63
10:I:42:LEU:CD2	10:I:43:VAL:N	2.56	0.63
4:A:451:HIS:HB3	4:A:453:MET:N	2.13	0.63
9:H:108:SER:HB3	9:H:111:LEU:N	2.14	0.63
4:A:168:GLY:O	4:A:169:ASN:C	2.41	0.63
4:A:579:SER:OG	4:A:612:ILE:HG22	1.97	0.63
4:A:907:THR:HG22	4:A:908:LEU:N	2.13	0.63
5:B:108:VAL:HG12	5:B:109:THR:H	1.64	0.63
5:B:868:MET:N	5:B:869:SER:O	2.30	0.63
10:I:107:SER:OG	10:I:108:HIS:CB	2.47	0.63
2:T:19:DT:H2'	2:T:20:DC:C6	2.33	0.63
4:A:527:THR:O	4:A:653:VAL:HG11	1.99	0.63
4:A:1096:SER:OG	4:A:1097:GLY:CA	2.47	0.63
4:A:1147:THR:HA	4:A:1196:GLU:O	1.98	0.63
4:A:1159:ARG:CA	4:A:1160:SER:O	2.30	0.63
5:B:327:ARG:N	5:B:328:GLU:O	2.31	0.63
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.34	0.63
4:A:567:LYS:NZ	9:H:43:ASN:HB3	2.14	0.63
4:A:901:LEU:H	4:A:926:GLN:NE2	1.97	0.63
4:A:1069:ALA:C	4:A:1071:SER:N	2.57	0.63
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.81	0.63
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:131:ASN:O	9:H:132:LEU:CB	2.45	0.63
9:H:84:ALA:HA	9:H:86:ASP:N	2.13	0.62
13:L:32:ALA:H	13:L:55:ILE:HD13	1.63	0.62
4:A:1173:HIS:CG	4:A:1173:HIS:O	2.52	0.62
4:A:1364:ASN:HD22	4:A:1364:ASN:C	2.08	0.62
5:B:35:SER:O	5:B:39:ARG:HG3	1.99	0.62
5:B:864:LYS:HD3	5:B:871:THR:HG23	1.80	0.62
7:E:23:VAL:HG13	7:E:28:TYR:HD1	1.64	0.62
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.79	0.62
4:A:1213:GLY:O	4:A:1228:TRP:CZ3	2.52	0.62
5:B:709:ASP:HB3	5:B:710:LEU:CG	2.29	0.62
13:L:25:ALA:O	13:L:26:THR:C	2.42	0.62
4:A:1083:THR:OG1	4:A:1084:PHE:N	2.32	0.62
5:B:293:PRO:HA	5:B:294:ASP:CB	2.16	0.62
4:A:1064:VAL:O	4:A:1068:ALA:N	2.32	0.62
4:A:1434:ALA:O	4:A:1436:ILE:N	2.33	0.62
5:B:349:ILE:HA	5:B:352:ALA:HB2	1.81	0.62
5:B:1177:HIS:CB	5:B:1178:ASN:HB2	2.30	0.62
5:B:1177:HIS:CA	5:B:1178:ASN:CB	2.78	0.62
6:C:58:LEU:HD11	11:J:2:ILE:CD1	2.28	0.62
4:A:381:THR:C	4:A:383:TYR:H	2.07	0.62
5:B:1077:THR:HG23	5:B:1079:LYS:H	1.65	0.62
4:A:286:HIS:ND1	4:A:289:ILE:CG1	2.63	0.62
5:B:803:LEU:N	5:B:822:ASN:HD21	1.98	0.62
9:H:109:LYS:H	9:H:110:ASP:C	2.08	0.62
4:A:847:ASP:HB3	4:A:1424:VAL:HG23	1.82	0.61
5:B:256:VAL:HG11	5:B:382:ILE:HD11	1.81	0.61
5:B:955:THR:HA	13:L:46:VAL:HG11	1.81	0.61
1:R:9:G:N2	2:T:21:DC:H1'	2.14	0.61
4:A:445:ASN:HB2	4:A:454:SER:O	2.00	0.61
4:A:696:GLU:O	4:A:700:ASN:CA	2.48	0.61
5:B:878:GLN:HG3	5:B:878:GLN:O	1.98	0.61
7:E:78:LEU:HD12	7:E:107:THR:HB	1.82	0.61
9:H:109:LYS:CG	9:H:110:ASP:OD2	2.48	0.61
10:I:16:PRO:O	10:I:17:ARG:HG2	2.00	0.61
4:A:975:HIS:C	4:A:977:LYS:HB2	2.25	0.61
9:H:139:ASN:O	9:H:140:ALA:CB	2.48	0.61
4:A:33:ALA:HB3	4:A:82:GLY:HA3	1.82	0.61
4:A:108:MET:CE	4:A:169:ASN:OD1	2.48	0.61
4:A:1154:TYR:O	4:A:1192:LEU:CD2	2.48	0.61
5:B:318:VAL:HG11	10:I:13:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:347:PHE:HE2	4:A:375:THR:CG2	2.12	0.61
4:A:1071:SER:O	4:A:1075:PRO:HD3	2.00	0.61
4:A:1226:VAL:CB	4:A:1228:TRP:CZ3	2.84	0.61
5:B:34:ILE:HD13	5:B:542:MET:HE1	1.81	0.61
5:B:120:ARG:HD2	5:B:955:THR:HG21	1.82	0.61
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.82	0.61
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.35	0.61
4:A:974:ASP:HB2	4:A:975:HIS:NE2	2.15	0.61
9:H:128:ASN:CA	9:H:130:ARG:H	2.12	0.61
10:I:79:HIS:N	10:I:80:SER:HB3	2.16	0.61
5:B:231:PRO:N	5:B:232:SER:CB	2.59	0.61
5:B:370:PHE:HD2	5:B:373:ARG:HG3	1.65	0.61
5:B:709:ASP:N	5:B:710:LEU:CB	2.57	0.61
5:B:711:GLU:N	5:B:712:PRO:HD3	2.15	0.61
5:B:899:ILE:HD11	5:B:911:ILE:HA	1.82	0.61
5:B:983:ARG:HH11	5:B:1091:TYR:HB3	1.65	0.61
5:B:1017:ILE:CB	5:B:1018:PRO:HD3	2.25	0.61
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.82	0.61
4:A:675:THR:CG2	4:A:736:ASN:HD21	2.13	0.61
4:A:1030:ARG:HD3	4:A:1034:GLU:HG3	1.82	0.60
5:B:509:ALA:O	5:B:510:LYS:HG3	2.01	0.60
5:B:582:VAL:HG22	5:B:626:ILE:HB	1.83	0.60
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.66	0.60
4:A:802:ASN:ND2	5:B:729:ILE:H	1.96	0.60
4:A:1070:GLN:O	4:A:1074:GLU:N	2.34	0.60
6:C:71:PRO:HB2	6:C:133:ILE:HD12	1.83	0.60
6:C:84:ARG:HD2	12:K:11:LEU:HD11	1.82	0.60
5:B:1177:HIS:CA	5:B:1178:ASN:HB2	2.31	0.60
4:A:596:THR:O	4:A:598:LEU:N	2.33	0.60
10:I:20:LYS:CA	10:I:21:GLU:O	2.38	0.60
4:A:504:LEU:CD1	4:A:504:LEU:N	2.63	0.60
5:B:789:MET:HE3	5:B:965:LYS:HB3	1.82	0.60
6:C:142:VAL:HG11	11:J:5:VAL:HG13	1.83	0.60
4:A:1171:GLN:C	4:A:1173:HIS:H	2.08	0.60
4:A:1209:MET:HE1	4:A:1228:TRP:O	2.01	0.60
5:B:998:ASP:HB3	5:B:1076:HIS:CE1	2.37	0.60
6:C:43:THR:HG22	6:C:44:LEU:H	1.65	0.60
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.84	0.60
4:A:975:HIS:O	4:A:977:LYS:CB	2.45	0.60
4:A:1091:SER:CB	4:A:1094:VAL:H	2.15	0.60
4:A:1153:TYR:HB3	4:A:1192:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:6:PHE:HZ	9:H:134:ASN:HB2	1.65	0.60
4:A:208:LEU:C	4:A:208:LEU:CD2	2.75	0.60
4:A:286:HIS:NE2	4:A:287:HIS:CG	2.70	0.60
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.84	0.60
6:C:50:GLU:HB2	6:C:156:THR:OG1	2.02	0.60
4:A:49:LYS:NZ	4:A:60:SER:HA	2.17	0.60
4:A:1226:VAL:CB	4:A:1228:TRP:CH2	2.77	0.60
5:B:421:PHE:O	5:B:424:LEU:HD23	2.02	0.60
6:C:45:ALA:HA	6:C:72:LEU:HD13	1.83	0.60
4:A:284:ALA:N	4:A:285:PRO:HD3	2.09	0.59
4:A:1084:PHE:CD1	4:A:1085:HIS:HA	2.37	0.59
9:H:136:LYS:O	9:H:136:LYS:HG2	2.01	0.59
4:A:899:VAL:HG23	4:A:1029:ARG:HG2	1.83	0.59
5:B:363:HIS:O	5:B:364:ILE:HB	2.03	0.59
4:A:284:ALA:H	4:A:285:PRO:HD2	1.58	0.59
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.85	0.59
7:E:140:LEU:HA	7:E:141:VAL:HB	1.84	0.59
4:A:1085:HIS:H	4:A:1085:HIS:HD2	1.48	0.59
5:B:327:ARG:HB3	5:B:328:GLU:HB2	0.69	0.59
5:B:572:HIS:C	5:B:573:GLN:O	2.45	0.59
9:H:77:ARG:HH11	9:H:77:ARG:CG	2.15	0.59
9:H:96:VAL:HA	9:H:142:LEU:O	2.01	0.59
4:A:1427:ASN:HB2	4:A:1434:ALA:HB2	1.85	0.59
4:A:451:HIS:HB3	4:A:453:MET:H	1.67	0.59
4:A:1091:SER:HB2	4:A:1092:LYS:C	2.27	0.59
9:H:87:ARG:HG3	9:H:87:ARG:NH1	2.06	0.59
4:A:286:HIS:ND1	4:A:289:ILE:HB	2.17	0.59
4:A:1171:GLN:O	4:A:1173:HIS:N	2.36	0.59
5:B:955:THR:HG22	5:B:956:THR:N	2.07	0.59
10:I:5:ARG:HG2	10:I:6:PHE:N	2.17	0.59
6:C:39:ALA:HA	6:C:164:ALA:CB	2.26	0.59
5:B:567:GLU:OE1	5:B:567:GLU:N	2.31	0.58
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.68	0.58
4:A:1092:LYS:O	4:A:1093:LYS:HB2	2.02	0.58
4:A:1200:ALA:HA	4:A:1202:MET:N	2.17	0.58
5:B:636:PRO:CB	5:B:637:LEU:CA	2.81	0.58
5:B:868:MET:HB3	5:B:869:SER:HB2	1.85	0.58
4:A:972:HIS:H	4:A:972:HIS:HD2	1.50	0.58
5:B:345:LYS:HA	5:B:348:ARG:HE	1.67	0.58
5:B:1143:ALA:HB1	5:B:1146:PHE:HB3	1.84	0.58
4:A:351:THR:HB	4:A:468:PHE:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:525:GLN:HA	5:B:1015:HIS:HE1	1.67	0.58
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.85	0.58
4:A:1159:ARG:CG	4:A:1161:THR:HG23	2.33	0.58
10:I:101:PHE:N	10:I:101:PHE:CD1	2.70	0.58
5:B:706:GLN:O	5:B:710:LEU:HD13	2.04	0.58
5:B:744:HIS:HD2	5:B:746:SER:OG	1.87	0.58
5:B:361:LEU:HD11	5:B:381:MET:HE1	1.84	0.58
10:I:59:VAL:HG12	10:I:60:GLN:H	1.69	0.58
4:A:503:GLN:CB	4:A:504:LEU:HD13	2.34	0.58
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.03	0.58
6:C:73:GLN:HE21	6:C:75:MET:H	1.51	0.58
4:A:350:ARG:CD	4:A:488:ASN:OD1	2.52	0.58
4:A:405:VAL:O	4:A:413:ILE:HB	2.03	0.58
4:A:809:THR:HB	4:A:810:PRO:HD2	1.86	0.58
5:B:706:GLN:HB3	5:B:709:ASP:CB	2.33	0.58
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.39	0.58
4:A:351:THR:HB	4:A:468:PHE:HD1	1.69	0.58
4:A:819:GLY:O	4:A:822:GLU:N	2.37	0.58
5:B:706:GLN:HB2	5:B:710:LEU:HD12	1.85	0.58
5:B:810:GLU:HB2	5:B:815:ARG:HH12	1.68	0.57
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.69	0.57
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.84	0.57
7:E:138:ALA:HA	7:E:139:ALA:C	2.28	0.57
4:A:596:THR:C	4:A:598:LEU:N	2.60	0.57
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.70	0.57
10:I:27:PHE:O	10:I:35:VAL:HA	2.03	0.57
10:I:78:CYS:SG	10:I:80:SER:HB2	2.44	0.57
4:A:540:PHE:HD2	4:A:573:SER:HA	1.69	0.57
5:B:821:GLN:HE22	5:B:851:PHE:H	1.52	0.57
6:C:102:GLN:HG2	6:C:154:LYS:HD3	1.86	0.57
4:A:605:MET:HE2	4:A:607:ILE:HG13	1.85	0.57
6:C:254:LYS:HD3	12:K:38:GLU:OE2	2.04	0.57
10:I:103:CYS:CB	10:I:106:CYS:H	2.17	0.57
4:A:286:HIS:CD2	4:A:286:HIS:C	2.81	0.57
4:A:1200:ALA:HA	4:A:1203:ASN:H	1.69	0.57
5:B:706:GLN:HB3	5:B:710:LEU:HD12	1.85	0.57
4:A:709:THR:CB	4:A:710:LEU:HB3	2.29	0.57
5:B:1175:LEU:CG	5:B:1176:ASN:OD1	2.52	0.57
6:C:46:ILE:HG23	6:C:157:CYS:HB3	1.86	0.57
4:A:423:ASP:CG	4:A:424:ILE:H	2.13	0.57
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:826:ASP:HB3	4:A:830:LYS:HB2	1.87	0.57
4:A:1159:ARG:HD2	4:A:1161:THR:HG23	1.86	0.57
4:A:286:HIS:CD2	4:A:286:HIS:O	2.58	0.57
5:B:65:GLU:O	5:B:66:ASP:HB3	2.04	0.57
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.86	0.57
13:L:48:CYS:HB3	13:L:51:CYS:SG	2.45	0.57
4:A:1157:ASP:H	4:A:1159:ARG:CG	2.17	0.57
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.38	0.56
5:B:886:LYS:C	5:B:888:GLY:H	2.13	0.56
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.05	0.56
9:H:89:LEU:HD13	9:H:90:ALA:N	2.19	0.56
10:I:106:CYS:O	10:I:108:HIS:HB3	2.05	0.56
11:J:48:ARG:HE	11:J:49:MET:CE	2.17	0.56
13:L:42:ARG:HB3	13:L:43:THR:OG1	2.05	0.56
4:A:291:GLU:O	4:A:295:LEU:HB2	2.05	0.56
4:A:328:ARG:HD3	4:A:335:ARG:HH12	1.70	0.56
4:A:1153:TYR:O	4:A:1192:LEU:HG	2.04	0.56
5:B:212:LEU:HD21	5:B:461:LEU:HD11	1.87	0.56
9:H:90:ALA:C	9:H:92:ASP:N	2.63	0.56
13:L:54:ARG:O	13:L:55:ILE:C	2.46	0.56
4:A:99:ILE:HG13	4:A:234:MET:SD	2.45	0.56
4:A:907:THR:HG22	4:A:908:LEU:H	1.70	0.56
4:A:936:LEU:O	4:A:939:ASP:HB2	2.05	0.56
5:B:879:ARG:HG3	5:B:883:LEU:HG	1.88	0.56
13:L:30:ILE:HG22	13:L:31:CYS:O	2.05	0.56
4:A:370:ILE:HG23	5:B:1105:ALA:HB2	1.88	0.56
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.86	0.56
2:T:26:DG:C2	2:T:27:DA:H1'	2.40	0.56
5:B:226:PHE:HB3	5:B:228:LYS:HD3	1.88	0.56
5:B:493:SER:OG	5:B:751:VAL:HB	2.04	0.56
8:F:119:ARG:HH11	8:F:119:ARG:CG	2.17	0.56
4:A:208:LEU:O	4:A:208:LEU:HD23	2.05	0.56
4:A:1151:GLU:C	4:A:1152:ILE:HG13	2.31	0.56
5:B:593:PRO:HA	5:B:596:LEU:HB3	1.88	0.56
5:B:1019:SER:HB2	5:B:1020:ARG:HB3	1.77	0.56
7:E:5:ASN:HA	7:E:8:ASN:HB2	1.87	0.56
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.45	0.56
4:A:930:ASP:HA	4:A:933:TYR:HB3	1.87	0.56
4:A:1080:THR:O	4:A:1082:ASN:N	2.39	0.56
4:A:1236:LEU:N	4:A:1237:ILE:HA	2.21	0.56
10:I:3:THR:HA	10:I:4:PHE:CD2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:6:G:H2'	1:R:7:A:H8	1.69	0.56
1:R:10:A:O2'	4:A:485:ASP:HA	2.04	0.56
4:A:782:ARG:NH2	5:B:699:GLU:O	2.36	0.56
4:A:925:LEU:HD21	4:A:984:LYS:HE2	1.87	0.56
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.87	0.56
9:H:93:TYR:HB3	9:H:143:LEU:HB3	1.86	0.56
4:A:107:CYS:SG	4:A:108:MET:CB	2.91	0.56
4:A:332:LYS:H	4:A:337:ARG:CB	2.19	0.56
4:A:855:THR:HG21	4:A:857:ARG:HE	1.70	0.56
4:A:1094:VAL:O	4:A:1094:VAL:HG22	2.06	0.56
10:I:19:ASP:N	10:I:20:LYS:HB2	2.20	0.56
10:I:108:HIS:C	10:I:109:ILE:HG13	2.29	0.56
13:L:60:ARG:HG3	13:L:61:THR:H	1.70	0.56
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.88	0.56
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.70	0.56
5:B:1069:PHE:O	5:B:1070:GLU:HG3	2.05	0.56
4:A:347:PHE:HE2	4:A:375:THR:HG22	1.70	0.55
4:A:686:ALA:O	4:A:690:VAL:HG23	2.06	0.55
4:A:1085:HIS:CD2	4:A:1085:HIS:N	2.70	0.55
4:A:1089:VAL:HG13	4:A:1090:ALA:CA	2.36	0.55
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.88	0.55
4:A:372:LYS:O	4:A:435:HIS:CE1	2.59	0.55
4:A:503:GLN:HB3	4:A:504:LEU:HD12	1.85	0.55
5:B:370:PHE:CD2	5:B:373:ARG:HG3	2.42	0.55
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.87	0.55
7:E:173:SER:O	7:E:175:LEU:N	2.38	0.55
7:E:213:ILE:HG12	7:E:214:CYS:H	1.70	0.55
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.89	0.55
7:E:18:THR:CG2	7:E:140:LEU:CD1	2.82	0.55
12:K:36:GLU:OE2	12:K:70:ARG:HD3	2.07	0.55
2:T:24:DT:H2'	2:T:24:DT:O2	2.06	0.55
4:A:279:LEU:HB2	4:A:280:GLU:OE1	2.06	0.55
4:A:467:THR:HG21	5:B:976:ILE:HG22	1.86	0.55
5:B:1177:HIS:HA	5:B:1178:ASN:HB2	1.89	0.55
4:A:550:LEU:HD12	4:A:556:TRP:NE1	2.22	0.55
4:A:1364:ASN:O	4:A:1366:ARG:N	2.40	0.55
5:B:308:TRP:CH2	10:I:46:HIS:N	2.75	0.55
5:B:1175:LEU:CA	5:B:1177:HIS:CD2	2.86	0.55
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.71	0.55
4:A:971:PHE:O	4:A:972:HIS:C	2.50	0.55
4:A:1154:TYR:C	4:A:1192:LEU:HG	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1427:ASN:O	4:A:1432:GLN:N	2.32	0.55
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.72	0.55
4:A:108:MET:CG	4:A:109:HIS:H	2.20	0.55
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.87	0.55
4:A:1096:SER:N	4:A:1097:GLY:CA	2.69	0.55
4:A:1319:VAL:O	4:A:1322:ILE:CD1	2.54	0.55
9:H:112:ILE:O	9:H:112:ILE:HG23	2.06	0.55
4:A:331:GLY:HA2	4:A:337:ARG:HG3	1.89	0.55
5:B:524:PRO:HG3	5:B:748:ILE:HD12	1.89	0.55
5:B:837:ASP:OD2	5:B:837:ASP:N	2.39	0.55
1:R:4:G:H2'	1:R:5:A:H8	1.72	0.54
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.27	0.54
4:A:381:THR:O	4:A:383:TYR:N	2.40	0.54
4:A:1164:PRO:O	4:A:1165:GLU:C	2.50	0.54
4:A:381:THR:C	4:A:383:TYR:N	2.64	0.54
5:B:558:LEU:HB3	5:B:563:MET:SD	2.47	0.54
5:B:868:MET:N	5:B:869:SER:CA	2.67	0.54
10:I:14:LEU:HD23	10:I:27:PHE:HB3	1.88	0.54
10:I:20:LYS:CG	10:I:24:ARG:H	2.17	0.54
10:I:101:PHE:HD1	10:I:101:PHE:H	1.55	0.54
4:A:466:SER:O	5:B:1103:ILE:HD11	2.07	0.54
5:B:705:MET:N	5:B:710:LEU:HD13	2.22	0.54
8:F:111:LEU:HD12	8:F:111:LEU:H	1.72	0.54
4:A:53:LEU:O	4:A:54:ASN:OD1	2.25	0.54
4:A:320:ARG:CB	4:A:321:PRO:HA	2.37	0.54
4:A:768:GLN:NE2	4:A:816:HIS:CE1	2.74	0.54
4:A:1169:ILE:O	4:A:1169:ILE:HG13	2.07	0.54
5:B:836:GLU:C	5:B:837:ASP:OD2	2.51	0.54
5:B:957:ASN:OD1	5:B:958:GLN:N	2.40	0.54
7:E:29:PHE:O	7:E:30:ILE:HB	2.08	0.54
4:A:1091:SER:HB2	4:A:1093:LYS:C	2.30	0.54
4:A:1406:VAL:HG12	4:A:1410:PHE:CE1	2.43	0.54
5:B:1106:ARG:HH11	5:B:1126:GLY:HA2	1.72	0.54
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.72	0.54
9:H:111:LEU:CA	9:H:112:ILE:CG2	2.84	0.54
4:A:110:CYS:SG	4:A:111:GLY:N	2.81	0.54
4:A:1223:ASP:CB	4:A:1243:VAL:HB	2.38	0.54
5:B:386:LEU:O	5:B:390:LEU:HG	2.07	0.54
5:B:435:THR:O	5:B:436:VAL:C	2.51	0.54
5:B:709:ASP:HB3	5:B:710:LEU:CB	2.37	0.54
5:B:994:TYR:HB2	5:B:999:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.89	0.54
10:I:43:VAL:CG1	10:I:44:TYR:HA	2.37	0.54
4:A:973:ILE:HG12	4:A:974:ASP:HA	1.86	0.54
5:B:684:LEU:HD23	5:B:689:LEU:HD13	1.90	0.54
5:B:1017:ILE:H	5:B:1018:PRO:CD	2.20	0.54
4:A:700:ASN:O	4:A:702:LEU:N	2.41	0.54
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.40	0.54
12:K:40:HIS:HA	12:K:43:GLY:H	1.73	0.54
4:A:909:ASP:C	4:A:911:SER:N	2.66	0.54
4:A:1154:TYR:CG	4:A:1155:ASP:N	2.75	0.54
4:A:1436:ILE:CG2	4:A:1437:GLY:N	2.67	0.54
5:B:1176:ASN:O	5:B:1177:HIS:CD2	2.61	0.54
10:I:75:CYS:HG	10:I:110:PHE:HE2	1.43	0.54
4:A:284:ALA:N	4:A:285:PRO:HD2	2.20	0.53
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.88	0.53
4:A:1200:ALA:CA	4:A:1201:ALA:HB3	2.38	0.53
5:B:1166:CYS:O	5:B:1167:GLY:C	2.50	0.53
9:H:107:VAL:CG1	9:H:111:LEU:O	2.55	0.53
9:H:128:ASN:HA	9:H:130:ARG:N	2.16	0.53
10:I:86:PHE:HD1	10:I:87:GLN:O	1.91	0.53
5:B:779:GLY:O	5:B:795:ILE:HA	2.07	0.53
7:E:137:GLU:O	7:E:139:ALA:HB3	2.07	0.53
9:H:6:PHE:O	9:H:7:ASP:HB3	2.08	0.53
5:B:515:HIS:H	5:B:518:HIS:HD2	1.54	0.53
5:B:1131:GLY:O	5:B:1134:GLU:HB2	2.08	0.53
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.90	0.53
9:H:82:PRO:O	9:H:83:GLN:HB3	2.07	0.53
4:A:699:ALA:N	4:A:700:ASN:CA	2.65	0.53
4:A:1053:PHE:O	4:A:1056:SER:N	2.32	0.53
5:B:23:ALA:O	5:B:654:ARG:HD3	2.09	0.53
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.88	0.53
10:I:33:SER:HA	10:I:34:TYR:CB	2.39	0.53
4:A:826:ASP:HA	4:A:830:LYS:H	1.73	0.53
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.38	0.53
4:A:971:PHE:N	4:A:971:PHE:CD1	2.76	0.53
4:A:1263:ILE:HG22	4:A:1267:MET:HE2	1.91	0.53
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.73	0.53
10:I:19:ASP:HA	10:I:20:LYS:C	2.34	0.53
4:A:636:GLU:O	4:A:637:LYS:C	2.51	0.53
4:A:709:THR:CA	4:A:710:LEU:CB	2.30	0.53
4:A:754:SER:N	4:A:757:ASN:HD22	1.94	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:858:ASN:HD21	4:A:862:ASN:H	1.55	0.53
5:B:294:ASP:N	5:B:297:ILE:HG12	2.24	0.53
5:B:614:SER:HB3	5:B:694:ASP:OD1	2.09	0.53
5:B:998:ASP:OD2	5:B:998:ASP:N	2.41	0.53
5:B:1176:ASN:C	5:B:1177:HIS:CD2	2.87	0.53
6:C:182:PRO:HG3	6:C:206:ASN:O	2.08	0.53
4:A:590:ARG:HD2	4:A:604:GLY:HA2	1.90	0.53
4:A:915:SER:O	4:A:919:ILE:HG12	2.09	0.53
4:A:1082:ASN:N	4:A:1083:THR:HA	2.23	0.53
5:B:883:LEU:HD22	5:B:884:ARG:N	2.24	0.53
5:B:1019:SER:HB2	5:B:1020:ARG:CG	2.35	0.53
7:E:165:LEU:HD13	7:E:170:LEU:HB2	1.91	0.53
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.43	0.53
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.91	0.52
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.91	0.52
4:A:708:MET:O	4:A:710:LEU:HB2	2.10	0.52
4:A:800:VAL:HG11	4:A:808:LEU:HG	1.90	0.52
4:A:1226:VAL:O	4:A:1228:TRP:CZ2	2.62	0.52
6:C:66:ARG:HB3	6:C:66:ARG:HH11	1.73	0.52
10:I:16:PRO:C	10:I:17:ARG:HG2	2.33	0.52
4:A:54:ASN:O	4:A:55:ASP:HB2	2.09	0.52
5:B:557:PHE:O	5:B:561:TRP:HB3	2.09	0.52
5:B:709:ASP:CA	5:B:710:LEU:CB	2.83	0.52
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.91	0.52
6:C:124:LEU:C	6:C:126:GLY:H	2.17	0.52
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.55	0.52
4:A:711:ARG:HA	4:A:713:SER:HB2	1.91	0.52
4:A:1086:PHE:CD1	4:A:1086:PHE:N	2.77	0.52
4:A:1116:LEU:HD13	4:A:1329:THR:CG2	2.39	0.52
5:B:61:ASP:HA	5:B:64:CYS:HB2	1.91	0.52
4:A:855:THR:HG23	4:A:857:ARG:HE	1.72	0.52
5:B:842:ASN:HB3	5:B:845:SER:OG	2.09	0.52
9:H:126:GLU:HG2	9:H:127:GLY:N	2.22	0.52
2:T:27:DA:H2'	2:T:27:DA:N3	2.25	0.52
4:A:630:ILE:HD12	4:A:630:ILE:N	2.19	0.52
4:A:800:VAL:HG13	4:A:812:GLU:OE2	2.09	0.52
5:B:571:PRO:CD	5:B:572:HIS:CG	2.84	0.52
5:B:600:LEU:HB3	5:B:615:MET:SD	2.50	0.52
6:C:56:THR:HG21	6:C:145:CYS:SG	2.49	0.52
4:A:868:TYR:CZ	4:A:1064:VAL:HG11	2.37	0.52
4:A:909:ASP:O	4:A:911:SER:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:212:LEU:HD21	5:B:461:LEU:CD1	2.39	0.52
6:C:251:LEU:O	6:C:255:VAL:HG23	2.09	0.52
13:L:27:LEU:HD23	13:L:27:LEU:N	2.24	0.52
4:A:115:LEU:HD11	4:A:145:LYS:HD2	1.91	0.52
4:A:304:MET:SD	5:B:1210:MET:HA	2.49	0.52
4:A:407:ARG:HG2	4:A:430:TRP:CH2	2.45	0.52
4:A:702:LEU:CD2	4:A:704:ALA:CB	2.83	0.52
4:A:1054:LEU:C	4:A:1054:LEU:HD23	2.33	0.52
4:A:1097:GLY:C	4:A:1099:PRO:HD2	2.34	0.52
4:A:1147:THR:HG23	4:A:1196:GLU:H	1.74	0.52
4:A:1153:TYR:HB3	4:A:1192:LEU:HD11	1.92	0.52
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.10	0.52
5:B:764:SER:N	5:B:765:PRO:HD2	2.25	0.52
4:A:287:HIS:O	4:A:287:HIS:CD2	2.63	0.52
5:B:706:GLN:HB2	5:B:710:LEU:CD1	2.39	0.52
10:I:17:ARG:O	10:I:25:LEU:HD12	2.10	0.52
4:A:575:LYS:NZ	4:A:615:GLY:H	2.07	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.10	0.52
5:B:270:LYS:HA	5:B:281:PRO:HA	1.91	0.52
4:A:523:ILE:HG22	4:A:528:LEU:HB2	1.92	0.52
4:A:702:LEU:CG	4:A:704:ALA:H	2.10	0.52
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.91	0.52
5:B:299:GLU:OE1	5:B:572:HIS:CE1	2.63	0.52
7:E:140:LEU:HA	7:E:141:VAL:C	2.35	0.52
4:A:374:LEU:O	4:A:436:ILE:HG13	2.10	0.51
4:A:384:ASN:O	4:A:388:LEU:HB2	2.10	0.51
4:A:1086:PHE:O	5:B:765:PRO:HG3	2.10	0.51
4:A:1162:VAL:CG2	4:A:1163:ILE:C	2.79	0.51
5:B:811:TYR:H	5:B:811:TYR:HD1	1.58	0.51
5:B:979:LYS:HA	5:B:989:THR:HG22	1.92	0.51
10:I:20:LYS:HA	10:I:21:GLU:C	2.31	0.51
4:A:1436:ILE:HD13	5:B:1139:ILE:HG23	1.92	0.51
5:B:118:ARG:NH2	5:B:194:GLU:OE1	2.41	0.51
5:B:361:LEU:O	5:B:363:HIS:O	2.27	0.51
9:H:105:GLU:O	9:H:106:GLU:CB	2.57	0.51
4:A:38:PRO:HG3	4:A:270:LEU:HB3	1.92	0.51
4:A:961:ARG:CG	4:A:961:ARG:NH1	2.67	0.51
5:B:294:ASP:H	5:B:297:ILE:HG12	1.76	0.51
6:C:86:CYS:SG	6:C:87:PHE:N	2.83	0.51
8:F:145:ASP:O	8:F:146:TRP:CB	2.58	0.51
4:A:90:VAL:HG13	4:A:297:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.10	0.51
5:B:351:TYR:H	5:B:354:ASP:HB2	1.74	0.51
5:B:879:ARG:HD3	5:B:885:MET:SD	2.49	0.51
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.40	0.51
10:I:106:CYS:HB2	10:I:107:SER:OG	2.11	0.51
4:A:249:SER:HB3	4:A:259:GLU:CG	2.41	0.51
4:A:286:HIS:CG	4:A:289:ILE:HB	2.46	0.51
4:A:1066:VAL:O	4:A:1069:ALA:CB	2.30	0.51
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.98	0.51
6:C:241:ASP:O	6:C:245:VAL:HG23	2.10	0.51
11:J:16:ASP:OD1	11:J:17:LYS:HG3	2.11	0.51
4:A:38:PRO:CB	4:A:39:GLU:HA	2.39	0.51
4:A:701:LEU:H	4:A:701:LEU:CD2	2.22	0.51
4:A:702:LEU:HG	4:A:704:ALA:CA	2.41	0.51
4:A:988:LEU:O	4:A:988:LEU:HD23	2.11	0.51
4:A:1054:LEU:C	4:A:1054:LEU:HD22	2.36	0.51
5:B:1033:LYS:HG3	5:B:1089:PRO:HD3	1.91	0.51
10:I:17:ARG:HA	10:I:18:GLU:HB3	1.92	0.51
4:A:380:VAL:HG22	4:A:430:TRP:N	2.26	0.51
4:A:744:LYS:HE2	4:A:748:MET:HE3	1.92	0.51
5:B:327:ARG:O	5:B:330:ALA:CB	2.55	0.51
5:B:842:ASN:O	5:B:845:SER:N	2.44	0.51
4:A:973:ILE:N	4:A:974:ASP:OD2	2.44	0.51
4:A:1162:VAL:HG22	4:A:1163:ILE:H	1.69	0.51
5:B:291:ILE:HG22	5:B:293:PRO:HD2	1.91	0.51
5:B:1013:ASN:C	5:B:1015:HIS:H	2.19	0.51
5:B:1148:LYS:O	5:B:1152:MET:HB2	2.11	0.51
6:C:107:SER:OG	6:C:111:THR:OG1	2.28	0.51
8:F:99:LEU:HD21	8:F:103:MET:CE	2.38	0.51
9:H:137:GLN:CG	9:H:138:GLU:N	2.57	0.51
4:A:1064:VAL:O	4:A:1068:ALA:CB	2.58	0.51
5:B:553:PRO:HA	5:B:556:THR:HG22	1.93	0.51
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.76	0.51
8:F:72:LYS:O	8:F:73:ALA:HB2	2.10	0.51
13:L:55:ILE:O	13:L:56:LEU:CB	2.42	0.51
4:A:663:SER:HB2	5:B:827:ILE:O	2.11	0.51
5:B:994:TYR:HB2	5:B:999:MET:CE	2.41	0.51
1:R:4:G:H2'	1:R:5:A:C8	2.46	0.50
4:A:49:LYS:HZ1	4:A:61:ILE:HG12	1.75	0.50
4:A:986:ILE:O	4:A:990:VAL:HG23	2.10	0.50
4:A:1155:ASP:OD1	4:A:1157:ASP:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:327:ARG:C	5:B:330:ALA:H	2.18	0.50
6:C:35:ARG:HH12	12:K:41:THR:N	2.10	0.50
9:H:5:LEU:HD12	9:H:59:ILE:HG22	1.93	0.50
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.76	0.50
4:A:338:GLY:O	5:B:1129:ARG:NH1	2.43	0.50
4:A:344:ARG:HB3	5:B:1118:PRO:HD2	1.93	0.50
4:A:782:ARG:HB3	4:A:789:LYS:HA	1.93	0.50
4:A:1071:SER:N	4:A:1072:ILE:CB	2.53	0.50
4:A:1075:PRO:HB2	4:A:1079:MET:HG3	1.93	0.50
4:A:1392:SER:O	4:A:1394:THR:N	2.44	0.50
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.47	0.50
11:J:10:CYS:SG	11:J:11:GLY:N	2.79	0.50
4:A:699:ALA:HB3	4:A:700:ASN:HA	1.93	0.50
4:A:781:ASP:O	4:A:790:ASP:N	2.35	0.50
5:B:515:HIS:HD2	5:B:517:THR:H	1.58	0.50
5:B:878:GLN:HG3	5:B:881:ASN:CB	2.39	0.50
10:I:18:GLU:C	10:I:20:LYS:HB2	2.36	0.50
4:A:43:GLU:O	4:A:43:GLU:HG2	2.12	0.50
4:A:55:ASP:O	4:A:57:ARG:C	2.53	0.50
4:A:69:THR:HG22	4:A:71:GLN:HE22	1.77	0.50
5:B:642:ASP:HA	5:B:649:LYS:HA	1.93	0.50
5:B:1156:ASP:HB2	5:B:1197:PRO:HA	1.93	0.50
10:I:2:THR:HG23	10:I:3:THR:H	1.76	0.50
4:A:777:PHE:CD2	4:A:782:ARG:C	2.89	0.50
4:A:1155:ASP:OD1	4:A:1156:PRO:O	2.30	0.50
4:A:1160:SER:HB2	4:A:1162:VAL:CG1	2.38	0.50
4:A:1226:VAL:HB	4:A:1228:TRP:HH2	1.65	0.50
5:B:483:LEU:CD2	5:B:484:ASN:H	2.24	0.50
5:B:976:ILE:O	5:B:990:ILE:HB	2.12	0.50
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.92	0.50
4:A:1200:ALA:HB2	4:A:1203:ASN:CB	2.39	0.50
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.93	0.50
9:H:95:TYR:HE2	9:H:97:MET:CG	2.25	0.50
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.47	0.50
4:A:413:ILE:O	4:A:413:ILE:HG22	2.11	0.50
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.42	0.50
4:A:1089:VAL:CG1	4:A:1090:ALA:CA	2.89	0.50
4:A:1391:ARG:O	4:A:1393:ASN:N	2.45	0.50
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.26	0.50
5:B:1177:HIS:CA	5:B:1178:ASN:CG	2.80	0.50
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1080:THR:HG23	4:A:1081:LEU:N	2.26	0.50
5:B:476:ARG:O	5:B:478:GLY:N	2.44	0.50
5:B:1135:ARG:HG2	5:B:1139:ILE:HD11	1.94	0.50
7:E:100:ILE:HG23	7:E:105:PHE:HB2	1.93	0.50
11:J:9:SER:OG	11:J:45:CYS:HB2	2.12	0.50
4:A:290:GLU:OE2	4:A:291:GLU:HG3	2.11	0.50
4:A:567:LYS:HZ3	9:H:43:ASN:HB3	1.76	0.50
4:A:841:LEU:HD13	4:A:1072:ILE:CG2	2.42	0.50
4:A:1398:MET:HB2	4:A:1425:SER:HB2	1.93	0.50
5:B:108:VAL:HG12	5:B:109:THR:N	2.27	0.50
5:B:571:PRO:HD2	5:B:572:HIS:CB	2.42	0.50
5:B:977:GLY:HA3	5:B:1099:VAL:CG1	2.42	0.50
5:B:995:ARG:HB3	5:B:997:GLU:OE2	2.12	0.50
1:R:9:G:H22	2:T:21:DC:H1'	1.77	0.49
4:A:567:LYS:HE2	9:H:95:TYR:CZ	2.47	0.49
4:A:709:THR:HG22	4:A:710:LEU:CD2	2.19	0.49
4:A:1089:VAL:CG1	4:A:1090:ALA:N	2.75	0.49
4:A:1157:ASP:N	4:A:1159:ARG:CG	2.75	0.49
4:A:1394:THR:HG22	4:A:1398:MET:HE3	1.94	0.49
5:B:256:VAL:HG11	5:B:382:ILE:HD12	1.94	0.49
5:B:879:ARG:O	5:B:880:THR:CG2	2.53	0.49
4:A:1054:LEU:HD13	4:A:1054:LEU:H	1.77	0.49
5:B:391:ASP:CA	5:B:392:ARG:HB2	2.43	0.49
7:E:213:ILE:HG12	7:E:214:CYS:N	2.27	0.49
13:L:54:ARG:C	13:L:55:ILE:HG13	2.36	0.49
4:A:972:HIS:N	4:A:972:HIS:HD2	2.09	0.49
7:E:173:SER:C	7:E:175:LEU:H	2.19	0.49
4:A:534:LEU:O	4:A:574:GLY:HA3	2.12	0.49
4:A:719:VAL:O	4:A:723:ASN:ND2	2.45	0.49
4:A:943:LEU:C	4:A:945:GLU:H	2.19	0.49
4:A:1356:ILE:O	4:A:1361:SER:HB2	2.12	0.49
5:B:35:SER:HA	5:B:811:TYR:CE2	2.43	0.49
7:E:140:LEU:HA	7:E:142:VAL:N	2.27	0.49
4:A:638:GLY:H	4:A:641:VAL:HB	1.78	0.49
4:A:830:LYS:HZ3	4:A:1094:VAL:HG13	1.76	0.49
4:A:1084:PHE:CA	4:A:1085:HIS:C	2.82	0.49
4:A:1098:VAL:H	4:A:1099:PRO:HD2	1.75	0.49
4:A:1191:TRP:HA	4:A:1192:LEU:HB3	1.69	0.49
4:A:1278:ASN:O	4:A:1310:GLY:HA3	2.12	0.49
5:B:864:LYS:HB2	5:B:871:THR:HA	1.93	0.49
4:A:446:ARG:NH2	4:A:485:ASP:OD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1066:VAL:O	4:A:1070:GLN:OE1	2.31	0.49
4:A:1084:PHE:HD1	4:A:1086:PHE:HA	1.77	0.49
5:B:571:PRO:O	5:B:574:SER:O	2.31	0.49
4:A:445:ASN:CB	4:A:455:MET:HG2	2.42	0.49
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.28	0.49
5:B:292:ILE:H	5:B:293:PRO:CD	2.25	0.49
5:B:1019:SER:H	5:B:1020:ARG:CA	2.24	0.49
7:E:28:TYR:HA	7:E:64:PRO:HA	1.94	0.49
10:I:43:VAL:HG12	10:I:45:ARG:H	1.78	0.49
10:I:52:ILE:HG13	10:I:53:GLY:N	2.27	0.49
10:I:71:SER:OG	10:I:101:PHE:HE2	1.96	0.49
4:A:774:ARG:O	4:A:775:ILE:C	2.55	0.49
4:A:827:THR:HG1	4:A:1083:THR:HG21	1.75	0.49
4:A:845:LEU:O	4:A:848:ILE:HG12	2.13	0.49
4:A:1075:PRO:O	4:A:1076:ALA:C	2.55	0.49
5:B:294:ASP:HB3	10:I:12:ASN:HA	1.94	0.49
5:B:376:PHE:CE2	5:B:569:TYR:CD2	2.96	0.49
5:B:704:ALA:HB1	5:B:710:LEU:HD22	1.93	0.49
10:I:19:ASP:N	10:I:20:LYS:CB	2.76	0.49
4:A:219:PHE:O	4:A:220:THR:C	2.56	0.49
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.95	0.49
4:A:503:GLN:HB2	4:A:504:LEU:HD13	1.95	0.49
4:A:658:LEU:HD21	5:B:1076:HIS:HD2	1.78	0.49
4:A:702:LEU:CG	4:A:704:ALA:CB	2.88	0.49
4:A:706:HIS:HD2	4:A:1283:VAL:HG13	1.77	0.49
5:B:574:SER:HB2	5:B:591:ARG:HG2	1.95	0.49
5:B:865:LYS:HG3	5:B:866:TYR:N	2.19	0.49
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.48	0.49
4:A:1318:THR:CB	7:E:141:VAL:HG11	2.43	0.49
4:A:1414:ALA:C	4:A:1416:ALA:H	2.20	0.49
5:B:882:THR:CB	5:B:883:LEU:CA	2.84	0.49
4:A:265:LYS:HZ3	4:A:313:GLN:HE22	1.61	0.48
4:A:384:ASN:OD1	4:A:384:ASN:C	2.56	0.48
4:A:696:GLU:O	4:A:700:ASN:O	2.31	0.48
5:B:942:ARG:HB2	5:B:945:GLU:HB2	1.94	0.48
2:T:17:DG:H5''	2:T:18:DC:OP1	2.13	0.48
4:A:206:GLU:O	4:A:210:ILE:HG12	2.13	0.48
4:A:453:MET:C	4:A:455:MET:H	2.21	0.48
4:A:503:GLN:O	4:A:509:LEU:HD13	2.13	0.48
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.95	0.48
4:A:1057:VAL:HG12	4:A:1058:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:391:ASP:HA	5:B:392:ARG:HB2	1.93	0.48
9:H:90:ALA:HB1	9:H:93:TYR:O	2.13	0.48
4:A:1207:LEU:HD22	4:A:1212:VAL:HG23	1.93	0.48
5:B:483:LEU:HD22	5:B:484:ASN:H	1.79	0.48
4:A:288:ALA:O	4:A:289:ILE:C	2.57	0.48
4:A:1167:GLU:OE1	4:A:1170:ILE:HG22	2.13	0.48
5:B:705:MET:HB2	5:B:710:LEU:HD11	1.95	0.48
5:B:744:HIS:CD2	5:B:746:SER:OG	2.67	0.48
5:B:1020:ARG:O	5:B:1022:THR:HG22	2.14	0.48
7:E:139:ALA:O	7:E:141:VAL:HB	2.13	0.48
9:H:6:PHE:CE1	9:H:131:ASN:ND2	2.80	0.48
4:A:78:PRO:O	5:B:1205:GLN:NE2	2.44	0.48
4:A:208:LEU:C	4:A:208:LEU:HD23	2.39	0.48
4:A:387:ARG:O	4:A:391:LEU:HD23	2.13	0.48
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.95	0.48
4:A:1070:GLN:O	4:A:1073:GLY:N	2.46	0.48
5:B:784:ASN:ND2	5:B:788:ARG:HD2	2.29	0.48
5:B:886:LYS:O	5:B:888:GLY:N	2.32	0.48
5:B:1202:LEU:HD13	5:B:1206:GLU:HG3	1.95	0.48
9:H:111:LEU:CD2	9:H:111:LEU:N	2.76	0.48
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.94	0.48
5:B:101:MET:HE3	5:B:169:ARG:HH12	1.77	0.48
5:B:267:ARG:HD2	5:B:313:MET:HE1	1.95	0.48
5:B:1106:ARG:HG3	5:B:1107:ALA:N	2.29	0.48
8:F:109:VAL:HG12	8:F:110:ASP:N	2.28	0.48
8:F:116:ASP:C	8:F:118:LEU:H	2.22	0.48
10:I:3:THR:HA	10:I:4:PHE:CD1	2.43	0.48
12:K:7:PHE:C	12:K:9:LEU:H	2.21	0.48
8:F:119:ARG:CG	8:F:119:ARG:NH1	2.76	0.48
9:H:129:TYR:C	9:H:130:ARG:HG2	2.35	0.48
10:I:43:VAL:HG12	10:I:45:ARG:N	2.29	0.48
4:A:265:LYS:NZ	4:A:313:GLN:HE22	2.11	0.48
4:A:1162:VAL:CG2	4:A:1163:ILE:O	2.62	0.48
4:A:1407:GLU:HA	4:A:1410:PHE:HB2	1.96	0.48
5:B:878:GLN:O	5:B:881:ASN:HB2	2.14	0.48
5:B:1176:ASN:O	5:B:1177:HIS:ND1	2.47	0.48
12:K:12:LEU:H	12:K:12:LEU:HD12	1.77	0.48
5:B:868:MET:N	5:B:869:SER:C	2.61	0.48
5:B:956:THR:HA	5:B:961:LEU:O	2.14	0.48
5:B:1175:LEU:CA	5:B:1177:HIS:HD2	2.14	0.48
4:A:701:LEU:HD23	4:A:701:LEU:N	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:707:GLY:CA	4:A:709:THR:H	2.19	0.48
4:A:802:ASN:ND2	5:B:728:ARG:HB2	2.29	0.48
5:B:509:ALA:C	5:B:510:LYS:HG3	2.38	0.48
5:B:648:HIS:CG	5:B:649:LYS:H	2.32	0.48
7:E:173:SER:C	7:E:175:LEU:N	2.72	0.48
10:I:43:VAL:HG12	10:I:44:TYR:HA	1.96	0.48
4:A:545:GLN:HB3	4:A:549:MET:HE3	1.95	0.47
4:A:1159:ARG:HG2	4:A:1161:THR:HG23	1.96	0.47
5:B:327:ARG:N	5:B:328:GLU:C	2.72	0.47
5:B:882:THR:CG2	5:B:935:ARG:HA	2.44	0.47
10:I:20:LYS:HG3	10:I:23:ASN:H	1.79	0.47
4:A:591:PHE:HA	4:A:595:THR:HG21	1.96	0.47
4:A:700:ASN:O	4:A:702:LEU:CA	2.62	0.47
5:B:515:HIS:H	5:B:518:HIS:CD2	2.31	0.47
9:H:111:LEU:CA	9:H:112:ILE:HG22	2.39	0.47
4:A:1078:GLN:HA	4:A:1080:THR:O	2.14	0.47
5:B:684:LEU:HA	5:B:689:LEU:HD12	1.96	0.47
5:B:849:GLY:O	5:B:850:LEU:C	2.57	0.47
4:A:3:GLY:HA2	4:A:4:GLN:HA	1.61	0.47
4:A:347:PHE:CE2	4:A:375:THR:HG22	2.48	0.47
4:A:351:THR:CG2	4:A:352:VAL:N	2.77	0.47
4:A:452:LYS:HB3	5:B:1140:ALA:HB3	1.97	0.47
4:A:830:LYS:NZ	4:A:1094:VAL:HG13	2.29	0.47
4:A:833:GLU:O	4:A:837:ILE:HG12	2.14	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.49	0.47
4:A:1078:GLN:CA	4:A:1080:THR:O	2.63	0.47
4:A:1282:VAL:HA	4:A:1307:GLU:O	2.14	0.47
5:B:571:PRO:O	5:B:574:SER:C	2.57	0.47
5:B:955:THR:CG2	5:B:956:THR:H	2.09	0.47
6:C:66:ARG:HB3	6:C:66:ARG:NH1	2.30	0.47
9:H:5:LEU:HB3	9:H:6:PHE:CD2	2.50	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.96	0.47
4:A:1069:ALA:O	4:A:1071:SER:OG	2.33	0.47
5:B:711:GLU:N	5:B:712:PRO:CD	2.63	0.47
4:A:185:TRP:H	4:A:199:LEU:HD13	1.80	0.47
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.50	0.47
4:A:588:LEU:HD13	4:A:632:VAL:HG21	1.97	0.47
4:A:699:ALA:CB	4:A:700:ASN:HA	2.45	0.47
4:A:709:THR:HA	4:A:710:LEU:HB3	0.57	0.47
4:A:1364:ASN:HD22	4:A:1366:ARG:H	1.62	0.47
5:B:871:THR:HG22	5:B:872:GLU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:289:ILE:CG2	4:A:290:GLU:N	2.77	0.47
4:A:1223:ASP:O	4:A:1224:LEU:HB2	2.15	0.47
4:A:1239:ARG:HD3	4:A:1241:ARG:NH1	2.17	0.47
5:B:183:GLU:CA	5:B:184:ALA:CB	2.90	0.47
5:B:211:VAL:CG2	5:B:483:LEU:HG	2.45	0.47
5:B:331:LEU:H	5:B:331:LEU:HD12	1.80	0.47
5:B:579:ARG:HA	5:B:589:VAL:HA	1.96	0.47
5:B:709:ASP:CB	5:B:710:LEU:HD12	2.37	0.47
5:B:765:PRO:O	5:B:769:TYR:HD1	1.96	0.47
5:B:781:PHE:H	5:B:781:PHE:HD2	1.62	0.47
6:C:3:GLU:HB3	12:K:104:ASN:ND2	2.28	0.47
9:H:111:LEU:N	9:H:111:LEU:HD22	2.29	0.47
10:I:15:TYR:HA	10:I:16:PRO:HD3	1.69	0.47
4:A:447:GLN:HA	4:A:448:PRO:C	2.40	0.47
4:A:712:GLU:H	4:A:713:SER:CA	2.27	0.47
4:A:933:TYR:O	4:A:937:VAL:HG23	2.15	0.47
4:A:1064:VAL:O	4:A:1068:ALA:HB2	2.15	0.47
4:A:1154:TYR:O	4:A:1192:LEU:HG	2.15	0.47
4:A:1157:ASP:N	4:A:1159:ARG:N	2.60	0.47
5:B:801:LYS:O	11:J:52:THR:HG22	2.15	0.47
5:B:1017:ILE:N	5:B:1018:PRO:CD	2.78	0.47
9:H:89:LEU:O	9:H:89:LEU:CD2	2.48	0.47
4:A:350:ARG:HH11	4:A:488:ASN:HD21	1.63	0.47
4:A:1083:THR:CB	4:A:1084:PHE:HB3	2.39	0.47
4:A:1169:ILE:O	4:A:1171:GLN:O	2.33	0.47
5:B:459:TYR:C	5:B:459:TYR:CD2	2.93	0.47
5:B:745:PRO:C	5:B:747:MET:H	2.23	0.47
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.50	0.47
7:E:198:ILE:HB	7:E:210:SER:HB3	1.96	0.47
4:A:1211:GLN:HA	4:A:1214:GLU:HG2	1.96	0.47
5:B:866:TYR:CD1	5:B:867:GLY:N	2.83	0.47
5:B:883:LEU:O	5:B:884:ARG:C	2.58	0.47
9:H:23:VAL:HG11	9:H:121:LEU:HD22	1.97	0.47
4:A:265:LYS:NZ	4:A:323:LYS:HE2	2.28	0.46
4:A:1089:VAL:HG13	4:A:1090:ALA:C	2.40	0.46
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.50	0.46
8:F:92:ARG:HG3	8:F:92:ARG:O	2.13	0.46
12:K:37:LYS:O	12:K:38:GLU:HG2	2.16	0.46
4:A:582:ILE:CG2	4:A:610:GLY:HA2	2.45	0.46
4:A:599:SER:HB3	4:A:603:ASN:H	1.81	0.46
4:A:711:ARG:C	4:A:713:SER:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:754:SER:N	4:A:757:ASN:ND2	2.56	0.46
4:A:1159:ARG:CD	4:A:1161:THR:HG23	2.46	0.46
4:A:1192:LEU:H	4:A:1242:VAL:HG13	1.81	0.46
11:J:48:ARG:HE	11:J:49:MET:HE2	1.79	0.46
4:A:645:LEU:O	4:A:646:PHE:C	2.58	0.46
5:B:239:GLU:HG3	5:B:255:GLN:HG2	1.95	0.46
5:B:570:VAL:HB	5:B:572:HIS:HB2	1.97	0.46
7:E:23:VAL:CG1	7:E:28:TYR:HD1	2.27	0.46
4:A:269:ILE:HD11	4:A:300:VAL:HG23	1.98	0.46
4:A:1284:MET:H	4:A:1284:MET:HG3	1.52	0.46
5:B:487:THR:HG22	5:B:489:SER:H	1.80	0.46
5:B:701:ILE:HD11	5:B:703:ILE:HD11	1.96	0.46
5:B:806:THR:H	5:B:809:MET:HE3	1.81	0.46
5:B:1065:GLN:OE1	5:B:1069:PHE:HD1	1.99	0.46
6:C:234:SER:HB3	6:C:240:VAL:HG13	1.96	0.46
9:H:102:TYR:N	9:H:102:TYR:CD2	2.82	0.46
4:A:54:ASN:OD1	4:A:54:ASN:O	2.33	0.46
4:A:279:LEU:CB	4:A:280:GLU:OE1	2.63	0.46
4:A:1071:SER:HB2	4:A:1072:ILE:HG12	1.98	0.46
4:A:1153:TYR:O	4:A:1192:LEU:CG	2.62	0.46
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.81	0.46
5:B:574:SER:CB	5:B:591:ARG:HG2	2.46	0.46
5:B:744:HIS:CE1	5:B:745:PRO:HD2	2.50	0.46
5:B:784:ASN:HD21	5:B:788:ARG:HD2	1.81	0.46
5:B:882:THR:HG21	5:B:935:ARG:HA	1.97	0.46
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.50	0.46
9:H:135:LEU:C	9:H:137:GLN:H	2.24	0.46
4:A:375:THR:HA	4:A:434:ARG:O	2.15	0.46
4:A:973:ILE:N	4:A:974:ASP:CG	2.73	0.46
4:A:1152:ILE:CA	4:A:1153:TYR:CB	2.81	0.46
4:A:1173:HIS:O	4:A:1175:SER:N	2.47	0.46
4:A:1197:LEU:HD21	4:A:1238:ILE:HG13	1.97	0.46
5:B:102:VAL:HG23	5:B:112:LEU:HD22	1.97	0.46
5:B:282:ILE:HD13	5:B:382:ILE:HG13	1.97	0.46
5:B:1001:PHE:HE1	6:C:178:PHE:CB	2.27	0.46
5:B:1082:MET:HG2	6:C:188:HIS:O	2.15	0.46
10:I:17:ARG:CA	10:I:18:GLU:CB	2.93	0.46
4:A:337:ARG:HD2	5:B:1132:GLU:OE1	2.15	0.46
4:A:899:VAL:CG2	4:A:1029:ARG:HG2	2.46	0.46
5:B:313:MET:HE2	5:B:386:LEU:HD22	1.96	0.46
5:B:466:TRP:HB2	5:B:479:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:848:ARG:NH1	11:J:8:PHE:O	2.49	0.46
5:B:883:LEU:N	5:B:883:LEU:CD1	2.73	0.46
5:B:1017:ILE:CB	5:B:1018:PRO:CD	2.92	0.46
7:E:69:ILE:HD13	7:E:73:PRO:HA	1.96	0.46
10:I:4:PHE:HD1	10:I:5:ARG:HA	1.80	0.46
4:A:873:MET:HE3	4:A:957:PRO:HG2	1.98	0.46
5:B:293:PRO:C	5:B:297:ILE:HG12	2.40	0.46
9:H:112:ILE:HG23	9:H:127:GLY:O	2.15	0.46
4:A:108:MET:HG2	4:A:169:ASN:ND2	2.13	0.46
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.51	0.46
4:A:843:LYS:HE2	5:B:1135:ARG:HH22	1.81	0.46
4:A:1080:THR:C	4:A:1082:ASN:N	2.64	0.46
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.98	0.46
5:B:616:ILE:HG13	5:B:697:GLU:HA	1.98	0.46
6:C:80:LEU:HD22	6:C:129:ILE:HD11	1.98	0.46
4:A:50:ILE:HD13	4:A:50:ILE:H	1.80	0.46
4:A:87:ALA:H	4:A:273:ASN:HD21	1.63	0.46
4:A:278:THR:O	4:A:279:LEU:HD23	2.16	0.46
4:A:416:ARG:HG3	4:A:417:TYR:CD1	2.51	0.46
4:A:456:MET:HE1	4:A:477:PRO:HG2	1.98	0.46
4:A:1364:ASN:ND2	4:A:1364:ASN:C	2.72	0.46
4:A:699:ALA:HB3	4:A:700:ASN:CA	2.47	0.45
4:A:1293:SER:O	4:A:1295:THR:N	2.49	0.45
5:B:589:VAL:CG1	5:B:590:HIS:N	2.77	0.45
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.97	0.45
5:B:945:GLU:O	5:B:946:ASN:HB3	2.16	0.45
8:F:127:GLU:O	8:F:129:LYS:N	2.49	0.45
4:A:706:HIS:HE2	4:A:1283:VAL:HA	1.80	0.45
4:A:814:PHE:O	4:A:817:ALA:HB3	2.17	0.45
4:A:830:LYS:HZ3	4:A:1095:THR:HG22	1.80	0.45
5:B:65:GLU:O	5:B:66:ASP:CB	2.65	0.45
5:B:821:GLN:NE2	5:B:851:PHE:H	2.12	0.45
5:B:1143:ALA:HB1	5:B:1146:PHE:CB	2.44	0.45
6:C:51:VAL:HA	6:C:155:LEU:HD23	1.98	0.45
6:C:57:VAL:HG11	11:J:60:PHE:HD1	1.80	0.45
6:C:258:ILE:H	6:C:258:ILE:HG13	1.58	0.45
7:E:9:ILE:HD13	7:E:53:PRO:HG2	1.98	0.45
14:T:3000:GTP:HN22	4:A:448:PRO:HG3	1.81	0.45
4:A:47:ARG:NH2	5:B:919:SER:O	2.49	0.45
4:A:92:HIS:HD2	4:A:236:LEU:HD21	1.81	0.45
4:A:623:GLY:C	4:A:625:SER:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:693:VAL:HG11	4:A:717:ASN:OD1	2.16	0.45
4:A:907:THR:CG2	4:A:908:LEU:N	2.80	0.45
5:B:477:ALA:O	5:B:478:GLY:C	2.60	0.45
6:C:18:VAL:HG12	6:C:20:PHE:CE2	2.52	0.45
12:K:82:ASP:HA	12:K:83:PRO:HD3	1.82	0.45
4:A:560:ILE:H	4:A:560:ILE:HG12	1.56	0.45
4:A:634:THR:HA	4:A:638:GLY:O	2.15	0.45
4:A:800:VAL:HG13	4:A:812:GLU:CD	2.41	0.45
4:A:868:TYR:HE2	4:A:1366:ARG:HE	1.63	0.45
5:B:711:GLU:HG2	5:B:712:PRO:HD3	1.97	0.45
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.97	0.45
6:C:48:SER:HB3	6:C:158:VAL:HB	1.99	0.45
8:F:99:LEU:CD2	8:F:103:MET:HE3	2.42	0.45
10:I:17:ARG:CA	10:I:18:GLU:HB3	2.46	0.45
10:I:17:ARG:HB2	10:I:26:LEU:HD12	1.97	0.45
10:I:103:CYS:HB3	10:I:106:CYS:H	1.82	0.45
2:T:13:DA:N6	3:N:2:DT:C4	2.85	0.45
4:A:663:SER:CB	5:B:827:ILE:O	2.65	0.45
4:A:675:THR:HG21	4:A:736:ASN:ND2	2.23	0.45
9:H:7:ASP:HA	9:H:57:VAL:O	2.17	0.45
10:I:111:THR:HG22	10:I:113:ASP:H	1.82	0.45
1:R:2:U:H2'	1:R:3:C:C6	2.51	0.45
4:A:546:VAL:O	4:A:550:LEU:HD23	2.17	0.45
4:A:947:PHE:CE2	4:A:954:TRP:CE2	3.05	0.45
4:A:969:GLN:HA	4:A:972:HIS:HB3	1.99	0.45
4:A:1116:LEU:HD13	4:A:1329:THR:CB	2.45	0.45
4:A:1154:TYR:O	4:A:1192:LEU:CG	2.64	0.45
5:B:408:LEU:HD23	5:B:545:ILE:HG21	1.98	0.45
7:E:195:VAL:HA	7:E:212:ARG:O	2.16	0.45
9:H:111:LEU:HD23	9:H:111:LEU:C	2.17	0.45
4:A:289:ILE:HG12	4:A:290:GLU:CB	2.46	0.45
4:A:601:LYS:HB2	4:A:603:ASN:ND2	2.31	0.45
4:A:678:GLU:O	4:A:682:THR:OG1	2.26	0.45
4:A:1011:GLN:O	4:A:1015:VAL:HG23	2.16	0.45
4:A:1127:ASP:HB3	4:A:1130:GLN:HB2	1.99	0.45
5:B:589:VAL:CG1	5:B:590:HIS:H	2.28	0.45
10:I:45:ARG:CA	10:I:46:HIS:CB	2.59	0.45
4:A:777:PHE:CE2	4:A:782:ARG:HA	2.52	0.45
4:A:817:ALA:O	4:A:818:MET:C	2.59	0.45
5:B:365:THR:HG21	5:B:370:PHE:CG	2.52	0.45
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:18:GLU:HA	10:I:18:GLU:OE2	2.15	0.45
4:A:302:THR:HG23	4:A:306:ASN:HB3	1.98	0.45
4:A:710:LEU:HA	4:A:712:GLU:N	2.32	0.45
4:A:815:PHE:O	4:A:818:MET:HB2	2.16	0.45
4:A:960:ILE:HG13	4:A:1049:ILE:HD11	1.99	0.45
4:A:974:ASP:HB2	4:A:975:HIS:CD2	2.51	0.45
5:B:168:GLY:H	5:B:450:ALA:HB1	1.82	0.45
5:B:179:CYS:SG	5:B:180:TYR:N	2.90	0.45
5:B:326:ASP:HB3	5:B:328:GLU:O	2.17	0.45
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.80	0.45
5:B:390:LEU:O	5:B:391:ASP:CG	2.60	0.45
5:B:797:TYR:HB2	5:B:852:ARG:O	2.17	0.45
5:B:911:ILE:HD11	5:B:941:LEU:HG	1.99	0.45
5:B:913:GLY:HA2	5:B:938:SER:HB3	1.98	0.45
9:H:89:LEU:C	9:H:89:LEU:HD13	2.42	0.45
9:H:111:LEU:HB2	9:H:112:ILE:HG21	1.83	0.45
10:I:78:CYS:C	10:I:79:HIS:ND1	2.75	0.45
4:A:683:ILE:HG22	4:A:687:LYS:HG3	1.98	0.45
4:A:702:LEU:HD21	4:A:704:ALA:HB3	1.97	0.44
5:B:350:GLN:H	5:B:351:TYR:C	2.25	0.44
5:B:843:GLN:HB3	5:B:995:ARG:HG3	1.99	0.44
6:C:134:ILE:HD12	6:C:141:GLY:H	1.81	0.44
1:R:3:C:H2'	1:R:4:G:C8	2.53	0.44
4:A:814:PHE:CE1	5:B:524:PRO:HB3	2.52	0.44
4:A:819:GLY:O	4:A:820:GLY:C	2.61	0.44
4:A:1236:LEU:CA	4:A:1237:ILE:HB	2.41	0.44
4:A:1261:LYS:C	4:A:1263:ILE:H	2.25	0.44
5:B:67:SER:HB2	5:B:92:PHE:H	1.81	0.44
5:B:327:ARG:HD3	5:B:327:ARG:HA	1.46	0.44
5:B:822:ASN:O	11:J:48:ARG:NH1	2.50	0.44
10:I:114:GLN:HA	10:I:115:LYS:HA	1.83	0.44
12:K:20:LYS:HB3	12:K:34:THR:HB	2.00	0.44
4:A:353:ILE:HD13	4:A:487:MET:SD	2.58	0.44
4:A:482:PHE:C	4:A:484:GLY:H	2.26	0.44
4:A:534:LEU:HD21	4:A:578:LEU:HB2	1.99	0.44
4:A:701:LEU:O	4:A:701:LEU:HG	2.18	0.44
4:A:1072:ILE:CG2	4:A:1073:GLY:N	2.56	0.44
5:B:549:THR:HG22	5:B:550:ASP:N	2.25	0.44
6:C:250:THR:HA	6:C:253:LYS:HB2	1.99	0.44
7:E:153:HIS:CE1	7:E:184:VAL:HG11	2.52	0.44
4:A:630:ILE:H	4:A:630:ILE:CD1	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:639:PRO:HG2	4:A:640:GLN:H	1.83	0.44
4:A:1211:GLN:OE1	4:A:1274:ARG:NH2	2.51	0.44
5:B:123:THR:HG22	5:B:125:SER:HB3	1.99	0.44
5:B:515:HIS:CD2	5:B:517:THR:H	2.34	0.44
5:B:898:LEU:H	5:B:898:LEU:HG	1.49	0.44
5:B:1030:LEU:HD11	5:B:1068:GLY:CA	2.47	0.44
7:E:124:VAL:HB	7:E:125:PRO:HD3	2.00	0.44
7:E:202:SER:OG	7:E:204:THR:HG22	2.18	0.44
10:I:4:PHE:CD1	10:I:5:ARG:HA	2.53	0.44
14:T:3000:GTP:O2A	14:T:3000:GTP:H4'	2.18	0.44
4:A:802:ASN:HD21	5:B:729:ILE:N	2.01	0.44
4:A:1011:GLN:NE2	4:A:1015:VAL:CG2	2.81	0.44
4:A:1158:PRO:C	4:A:1159:ARG:O	2.61	0.44
5:B:225:VAL:HG11	5:B:388:CYS:CB	2.42	0.44
5:B:572:HIS:H	5:B:573:GLN:CA	2.29	0.44
4:A:148:CYS:H	4:A:170:THR:HG22	1.83	0.44
4:A:802:ASN:HD21	5:B:728:ARG:HB2	1.82	0.44
4:A:1191:TRP:CB	4:A:1192:LEU:CB	2.93	0.44
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.98	0.44
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.83	0.44
4:A:538:ASP:HB2	9:H:20:TYR:HD2	1.83	0.44
4:A:670:ILE:HD13	4:A:805:LEU:HD21	1.99	0.44
4:A:834:THR:HG23	4:A:835:GLY:N	2.32	0.44
4:A:1143:LEU:HD13	4:A:1273:LEU:HD21	2.00	0.44
4:A:1427:ASN:HD22	4:A:1427:ASN:H	1.65	0.44
5:B:276:ILE:HD12	5:B:351:TYR:HE2	1.83	0.44
5:B:424:LEU:HD22	5:B:453:ILE:HD11	2.00	0.44
5:B:882:THR:HG21	5:B:936:ASP:H	1.82	0.44
14:T:3000:GTP:O2G	14:T:3000:GTP:O1A	2.35	0.44
4:A:253:ASN:O	4:A:254:GLU:CB	2.66	0.44
4:A:538:ASP:HB2	9:H:20:TYR:CD2	2.53	0.44
4:A:705:LYS:O	4:A:709:THR:HG23	2.18	0.44
4:A:814:PHE:HB2	5:B:519:TRP:CZ3	2.46	0.44
4:A:974:ASP:HB2	4:A:975:HIS:CE1	2.52	0.44
4:A:1153:TYR:CB	4:A:1192:LEU:HD12	2.46	0.44
5:B:836:GLU:HG3	5:B:837:ASP:OD2	2.17	0.44
9:H:95:TYR:HE2	9:H:97:MET:SD	2.41	0.44
12:K:40:HIS:HB3	12:K:61:TYR:CE1	2.53	0.44
12:K:82:ASP:OD2	12:K:84:LYS:HB2	2.18	0.44
4:A:56:PRO:HA	4:A:57:ARG:HA	1.73	0.43
4:A:313:GLN:HB2	4:A:322:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:525:GLN:O	4:A:526:ASP:C	2.60	0.43
4:A:636:GLU:O	4:A:637:LYS:O	2.36	0.43
4:A:1116:LEU:HB3	4:A:1308:THR:HB	1.99	0.43
5:B:488:TYR:C	5:B:490:SER:H	2.25	0.43
6:C:166:GLU:O	6:C:167:HIS:HB2	2.17	0.43
4:A:108:MET:HG3	4:A:167:CYS:SG	2.58	0.43
4:A:151:ASP:OD2	4:A:163:SER:HA	2.17	0.43
4:A:767:GLN:OE1	4:A:799:PHE:HB2	2.17	0.43
5:B:278:GLN:HG2	5:B:279:ASP:H	1.82	0.43
5:B:331:LEU:HB3	5:B:352:ALA:HB1	2.00	0.43
5:B:637:LEU:HD13	5:B:740:HIS:HB2	2.00	0.43
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.53	0.43
6:C:169:LYS:HE2	6:C:170:TRP:CE2	2.52	0.43
7:E:23:VAL:HG13	7:E:28:TYR:CD1	2.48	0.43
4:A:68:GLN:O	4:A:68:GLN:HG2	2.18	0.43
4:A:286:HIS:ND1	4:A:289:ILE:CB	2.81	0.43
4:A:899:VAL:HG22	4:A:1029:ARG:HE	1.82	0.43
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.99	0.43
4:A:1104:ILE:HG13	4:A:1332:PHE:CE2	2.54	0.43
4:A:1116:LEU:HD12	4:A:1117:THR:H	1.83	0.43
5:B:487:THR:HG22	5:B:488:TYR:N	2.33	0.43
7:E:22:MET:HG3	7:E:187:TYR:CD1	2.53	0.43
7:E:147:HIS:HD2	7:E:149:LEU:H	1.65	0.43
10:I:75:CYS:SG	10:I:110:PHE:HE2	2.35	0.43
5:B:363:HIS:C	5:B:365:THR:H	2.27	0.43
5:B:705:MET:H	5:B:710:LEU:CD1	2.24	0.43
5:B:996:ARG:HG3	5:B:1007:VAL:HG11	1.99	0.43
6:C:124:LEU:O	6:C:125:MET:HB2	2.18	0.43
10:I:17:ARG:HA	10:I:18:GLU:CB	2.48	0.43
10:I:103:CYS:O	10:I:106:CYS:O	2.35	0.43
4:A:57:ARG:HD3	4:A:68:GLN:HB2	1.99	0.43
4:A:224:PHE:CZ	4:A:231:PRO:HG3	2.53	0.43
4:A:312:PRO:O	4:A:313:GLN:CB	2.65	0.43
5:B:202:TYR:CD1	5:B:209:GLU:HB3	2.53	0.43
5:B:273:LEU:HD23	5:B:274:PRO:HD2	2.00	0.43
5:B:977:GLY:HA3	5:B:1099:VAL:HG13	2.00	0.43
8:F:95:GLY:O	8:F:98:ALA:HB3	2.19	0.43
13:L:48:CYS:CB	13:L:51:CYS:SG	3.05	0.43
4:A:903:ASN:O	4:A:907:THR:OG1	2.37	0.43
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	2.00	0.43
5:B:345:LYS:N	5:B:347:LYS:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:578:THR:HG23	5:B:622:LYS:C	2.44	0.43
5:B:620:ARG:NH2	10:I:68:LEU:HD21	2.33	0.43
5:B:1016:ALA:C	5:B:1020:ARG:HG2	2.43	0.43
6:C:173:ALA:O	6:C:174:ALA:HB3	2.18	0.43
2:T:15:DA:H2''	2:T:16:DC:O5'	2.19	0.43
5:B:411:PRO:HA	5:B:414:ALA:HB3	2.01	0.43
10:I:75:CYS:O	10:I:78:CYS:O	2.37	0.43
4:A:347:PHE:H	5:B:1107:ALA:HA	1.82	0.43
4:A:474:VAL:O	4:A:474:VAL:HG13	2.18	0.43
4:A:1072:ILE:CG2	4:A:1073:GLY:H	2.21	0.43
4:A:1077:THR:O	4:A:1080:THR:O	2.37	0.43
4:A:1365:TYR:O	4:A:1366:ARG:C	2.60	0.43
5:B:1194:ILE:H	5:B:1194:ILE:HD13	1.83	0.43
8:F:114:GLU:OE2	8:F:119:ARG:HG2	2.18	0.43
9:H:77:ARG:CG	9:H:77:ARG:NH1	2.77	0.43
4:A:108:MET:CG	4:A:109:HIS:N	2.82	0.43
4:A:573:SER:O	4:A:576:GLN:HB2	2.18	0.43
4:A:647:GLY:O	4:A:651:LYS:HG3	2.19	0.43
4:A:702:LEU:HG	4:A:704:ALA:CB	2.49	0.43
4:A:1005:GLU:O	4:A:1009:ASN:ND2	2.51	0.43
4:A:1116:LEU:HD12	4:A:1117:THR:N	2.34	0.43
4:A:1391:ARG:O	4:A:1392:SER:C	2.61	0.43
5:B:204:ILE:N	5:B:204:ILE:HD12	2.33	0.43
5:B:1019:SER:N	5:B:1020:ARG:CA	2.80	0.43
7:E:138:ALA:CA	7:E:139:ALA:CB	2.93	0.43
7:E:176:PRO:O	7:E:212:ARG:HA	2.18	0.43
4:A:8:SER:O	4:A:10:PRO:HD3	2.18	0.43
4:A:634:THR:O	4:A:638:GLY:O	2.37	0.43
4:A:943:LEU:C	4:A:945:GLU:N	2.77	0.43
4:A:1170:ILE:HA	4:A:1171:GLN:C	2.42	0.43
4:A:1364:ASN:O	4:A:1365:TYR:C	2.61	0.43
5:B:942:ARG:O	5:B:944:THR:N	2.52	0.43
10:I:22:ASN:O	10:I:23:ASN:CB	2.65	0.43
6:C:258:ILE:HD11	12:K:42:LEU:HD21	2.01	0.42
12:K:36:GLU:O	12:K:37:LYS:C	2.62	0.42
4:A:1223:ASP:HB3	4:A:1243:VAL:HB	2.00	0.42
5:B:458:LYS:O	5:B:459:TYR:C	2.62	0.42
6:C:67:LEU:HD13	6:C:157:CYS:SG	2.60	0.42
4:A:382:PRO:HB3	4:A:428:TYR:CE2	2.54	0.42
4:A:992:ASP:O	4:A:995:GLU:HB2	2.20	0.42
4:A:1015:VAL:O	4:A:1016:THR:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1226:VAL:HG11	4:A:1228:TRP:CZ3	2.34	0.42
5:B:228:LYS:N	5:B:228:LYS:HD2	2.32	0.42
6:C:77:ILE:HD13	6:C:80:LEU:HB3	2.01	0.42
6:C:146:LYS:HB3	11:J:61:LEU:HD11	2.02	0.42
6:C:248:ILE:H	6:C:248:ILE:HG13	1.68	0.42
4:A:351:THR:HG22	4:A:352:VAL:H	1.83	0.42
4:A:407:ARG:HD3	4:A:411:ASP:HB2	2.01	0.42
4:A:495:GLU:HB3	8:F:98:ALA:HB1	2.02	0.42
4:A:913:LEU:HD23	4:A:1032:LEU:HD13	2.01	0.42
4:A:1070:GLN:O	4:A:1073:GLY:CA	2.67	0.42
4:A:1171:GLN:O	4:A:1172:LEU:C	2.63	0.42
5:B:531:GLN:HE21	5:B:531:GLN:HB2	1.67	0.42
5:B:637:LEU:HB2	5:B:741:CYS:O	2.19	0.42
7:E:141:VAL:HG12	7:E:142:VAL:HG23	2.01	0.42
8:F:116:ASP:C	8:F:118:LEU:N	2.77	0.42
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.84	0.42
4:A:374:LEU:HB3	4:A:436:ILE:HD11	2.00	0.42
4:A:565:ILE:CG2	4:A:567:LYS:HG2	2.49	0.42
4:A:702:LEU:HD11	4:A:704:ALA:CB	2.40	0.42
5:B:308:TRP:HH2	10:I:46:HIS:N	2.15	0.42
5:B:485:ARG:CZ	5:B:782:LEU:HD11	2.49	0.42
5:B:556:THR:O	5:B:560:GLU:HB2	2.19	0.42
5:B:648:HIS:CD2	5:B:649:LYS:H	2.37	0.42
5:B:840:ILE:HD12	5:B:1011:ILE:HB	2.00	0.42
8:F:81:THR:HG21	8:F:136:ARG:HD3	2.02	0.42
9:H:5:LEU:HD13	9:H:6:PHE:CE2	2.54	0.42
9:H:6:PHE:HD2	9:H:59:ILE:HB	1.84	0.42
9:H:22:LYS:HG2	9:H:45:GLU:CD	2.45	0.42
10:I:25:LEU:O	10:I:25:LEU:CG	2.64	0.42
4:A:313:GLN:HE21	4:A:322:VAL:HG11	1.84	0.42
4:A:848:ILE:HB	4:A:1065:GLY:HA3	2.02	0.42
4:A:1017:LEU:HB2	7:E:206:GLY:H	1.84	0.42
4:A:1130:GLN:HA	4:A:1133:LEU:HD12	2.01	0.42
4:A:1152:ILE:HD12	10:I:44:TYR:H	1.85	0.42
5:B:572:HIS:N	5:B:573:GLN:CA	2.83	0.42
9:H:90:ALA:CB	9:H:93:TYR:H	2.25	0.42
2:T:6:DG:H2"	2:T:7:DA:C8	2.55	0.42
4:A:863:VAL:HG11	4:A:866:PHE:CE2	2.54	0.42
4:A:951:GLU:HA	4:A:951:GLU:OE2	2.20	0.42
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.50	0.42
4:A:1069:ALA:HB3	4:A:1070:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1345:ARG:HG2	4:A:1376:THR:HG21	2.02	0.42
5:B:408:LEU:O	5:B:409:ALA:C	2.62	0.42
7:E:47:CYS:HA	7:E:53:PRO:HA	2.02	0.42
8:F:97:ARG:NH1	8:F:100:GLN:OE1	2.46	0.42
10:I:103:CYS:HB2	10:I:108:HIS:CD2	2.55	0.42
2:T:9:DA:H61	3:N:6:DT:H3	1.67	0.42
4:A:356:ASP:HB2	4:A:469:ARG:HH11	1.85	0.42
4:A:456:MET:HE3	4:A:478:TYR:CZ	2.54	0.42
4:A:867:ILE:O	4:A:868:TYR:C	2.62	0.42
5:B:62:ILE:HG23	5:B:418:LYS:HG2	2.01	0.42
5:B:258:LEU:HD11	5:B:267:ARG:HD2	2.02	0.42
5:B:380:TYR:O	5:B:380:TYR:CG	2.73	0.42
5:B:510:LYS:HA	5:B:511:PRO:HD3	1.40	0.42
5:B:1012:ILE:H	5:B:1012:ILE:HG13	1.74	0.42
5:B:1045:SER:HA	5:B:1046:PRO:HD3	1.87	0.42
9:H:23:VAL:HA	9:H:43:ASN:HA	2.01	0.42
13:L:55:ILE:HB	13:L:56:LEU:H	1.56	0.42
4:A:49:LYS:HZ3	4:A:60:SER:HA	1.85	0.42
4:A:116:ASP:HB2	4:A:118:HIS:HD2	1.85	0.42
4:A:266:LEU:O	4:A:269:ILE:HG22	2.20	0.42
4:A:587:HIS:CE1	4:A:609:ASP:H	2.37	0.42
4:A:754:SER:O	4:A:757:ASN:HB2	2.20	0.42
4:A:1189:SER:HB2	4:A:1243:VAL:HA	2.02	0.42
4:A:1236:LEU:N	4:A:1237:ILE:CA	2.83	0.42
4:A:1440:ALA:HB3	4:A:1441:PHE:CD2	2.54	0.42
5:B:295:GLY:HA2	10:I:6:PHE:CZ	2.54	0.42
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.47	0.42
7:E:192:ARG:HG3	7:E:192:ARG:O	2.18	0.42
9:H:6:PHE:CD1	9:H:131:ASN:ND2	2.88	0.42
1:R:6:G:H2'	1:R:7:A:C8	2.54	0.42
4:A:858:ASN:HD22	4:A:858:ASN:H	1.68	0.42
4:A:1061:GLY:O	4:A:1062:GLU:C	2.63	0.42
4:A:1069:ALA:O	4:A:1071:SER:N	2.53	0.42
5:B:219:ALA:HB2	5:B:405:ARG:HG2	2.01	0.42
5:B:748:ILE:HG13	5:B:749:LEU:N	2.33	0.42
5:B:1051:THR:HB	5:B:1054:GLY:N	2.34	0.42
4:A:308:ILE:H	4:A:308:ILE:HG13	1.59	0.41
4:A:336:ILE:CG2	4:A:1401:SER:HB3	2.50	0.41
4:A:381:THR:HG23	8:F:104:ASN:HB3	2.01	0.41
4:A:504:LEU:HD11	8:F:91:ALA:HB2	2.02	0.41
4:A:1084:PHE:CA	4:A:1085:HIS:O	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1345:ARG:HD2	4:A:1372:VAL:HG12	2.01	0.41
5:B:331:LEU:HD12	5:B:331:LEU:N	2.35	0.41
5:B:463:THR:HB	5:B:465:ASN:H	1.85	0.41
5:B:571:PRO:CB	5:B:572:HIS:CA	2.90	0.41
5:B:766:ARG:NH2	5:B:1020:ARG:HD2	2.35	0.41
5:B:806:THR:O	5:B:807:ARG:C	2.63	0.41
5:B:1103:ILE:O	5:B:1103:ILE:HG22	2.20	0.41
5:B:1138:MET:HA	5:B:1138:MET:HE3	2.01	0.41
6:C:249:ASP:O	6:C:253:LYS:N	2.47	0.41
10:I:4:PHE:HD1	10:I:5:ARG:CA	2.32	0.41
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.85	0.41
4:A:116:ASP:C	4:A:118:HIS:H	2.27	0.41
4:A:601:LYS:HB2	4:A:603:ASN:HD21	1.84	0.41
4:A:711:ARG:CA	4:A:713:SER:HB2	2.49	0.41
5:B:37:PHE:C	5:B:39:ARG:H	2.28	0.41
5:B:918:ILE:HD13	5:B:918:ILE:HA	1.91	0.41
9:H:84:ALA:CA	9:H:85:GLY:C	2.66	0.41
14:T:3000:GTP:O1A	14:T:3000:GTP:PG	2.78	0.41
4:A:907:THR:CG2	4:A:908:LEU:H	2.32	0.41
5:B:213:ILE:HD12	5:B:497:ARG:HB3	2.02	0.41
7:E:150:VAL:HA	7:E:151:PRO:HD3	1.86	0.41
10:I:26:LEU:HD22	10:I:35:VAL:HG11	2.02	0.41
12:K:40:HIS:HB3	12:K:61:TYR:HE1	1.84	0.41
4:A:53:LEU:O	4:A:54:ASN:CG	2.64	0.41
4:A:380:VAL:CG2	4:A:427:GLN:O	2.64	0.41
4:A:834:THR:HG23	4:A:835:GLY:H	1.85	0.41
4:A:1091:SER:CB	4:A:1092:LYS:C	2.92	0.41
5:B:121:ASN:N	5:B:121:ASN:HD22	2.17	0.41
5:B:308:TRP:HH2	10:I:46:HIS:H	1.65	0.41
5:B:801:LYS:O	11:J:52:THR:CG2	2.69	0.41
7:E:18:THR:HB	7:E:140:LEU:HD12	2.03	0.41
11:J:3:VAL:CG2	11:J:18:TRP:CG	3.03	0.41
4:A:4:GLN:HG2	4:A:5:GLN:HG3	2.01	0.41
4:A:575:LYS:HD3	4:A:612:ILE:HD11	2.03	0.41
4:A:675:THR:HA	4:A:678:GLU:HB2	2.02	0.41
4:A:814:PHE:HE1	5:B:524:PRO:HB3	1.86	0.41
4:A:860:LEU:HD13	4:A:1393:ASN:OD1	2.21	0.41
5:B:120:ARG:HA	5:B:963:PHE:CE2	2.56	0.41
5:B:582:VAL:HA	5:B:626:ILE:O	2.21	0.41
4:A:993:LEU:HA	4:A:996:ASN:HD21	1.85	0.41
8:F:72:LYS:O	8:F:73:ALA:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:83:PRO:HB3	8:F:146:TRP:CH2	2.55	0.41
9:H:109:LYS:HG2	9:H:110:ASP:CB	2.42	0.41
10:I:5:ARG:CG	10:I:6:PHE:H	2.22	0.41
13:L:60:ARG:HG3	13:L:61:THR:N	2.34	0.41
4:A:768:GLN:HE22	4:A:1087:ALA:CB	2.05	0.41
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.21	0.41
4:A:1041:ALA:O	4:A:1045:VAL:HG23	2.20	0.41
4:A:1112:LYS:O	4:A:1114:PRO:HD3	2.21	0.41
5:B:772:ALA:O	5:B:776:GLN:NE2	2.52	0.41
5:B:863:GLU:OE2	5:B:873:THR:HA	2.21	0.41
5:B:879:ARG:O	5:B:880:THR:CB	2.69	0.41
5:B:978:ASP:CB	5:B:980:PHE:HE1	2.33	0.41
5:B:980:PHE:CD1	5:B:980:PHE:N	2.89	0.41
5:B:1039:GLY:O	11:J:51:LEU:HD11	2.20	0.41
5:B:1068:GLY:HA3	5:B:1086:PHE:CE1	2.55	0.41
6:C:127:ARG:HG3	6:C:129:ILE:HG22	2.03	0.41
7:E:147:HIS:CD2	7:E:149:LEU:H	2.38	0.41
9:H:135:LEU:C	9:H:137:GLN:N	2.79	0.41
10:I:43:VAL:CB	10:I:44:TYR:CA	2.96	0.41
4:A:208:LEU:CD2	4:A:208:LEU:O	2.68	0.41
4:A:499:ALA:O	4:A:503:GLN:HB2	2.21	0.41
4:A:642:CYS:O	4:A:645:LEU:HB3	2.20	0.41
4:A:741:ASN:HD22	4:A:743:VAL:H	1.68	0.41
4:A:1143:LEU:HA	4:A:1146:VAL:CG2	2.51	0.41
4:A:1173:HIS:C	4:A:1175:SER:H	2.29	0.41
4:A:1271:ILE:HD13	4:A:1271:ILE:HA	1.84	0.41
5:B:327:ARG:O	5:B:330:ALA:N	2.46	0.41
5:B:755:ILE:HD12	5:B:814:PHE:CD1	2.56	0.41
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.86	0.41
6:C:3:GLU:HG3	6:C:4:GLU:H	1.86	0.41
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.78	0.41
8:F:85:MET:HE1	8:F:93:ILE:HG21	2.03	0.41
8:F:145:ASP:O	8:F:146:TRP:CD1	2.74	0.41
4:A:40:THR:O	4:A:50:ILE:HD12	2.19	0.41
4:A:287:HIS:N	4:A:289:ILE:CA	2.83	0.41
4:A:443:LEU:HD23	4:A:444:PHE:N	2.36	0.41
4:A:513:SER:C	4:A:515:GLN:H	2.29	0.41
4:A:525:GLN:NE2	5:B:836:GLU:OE1	2.53	0.41
4:A:575:LYS:HD2	9:H:120:GLY:HA3	2.02	0.41
4:A:830:LYS:NZ	4:A:1095:THR:HG22	2.35	0.41
4:A:834:THR:HG21	4:A:1077:THR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:858:ASN:HD22	4:A:858:ASN:C	2.28	0.41
4:A:956:LEU:HA	4:A:957:PRO:HD3	1.88	0.41
4:A:1050:GLU:O	4:A:1054:LEU:CD1	2.61	0.41
5:B:230:ALA:H	5:B:231:PRO:HD3	1.82	0.41
5:B:291:ILE:H	5:B:291:ILE:HD12	1.86	0.41
5:B:575:PRO:C	5:B:577:ALA:H	2.28	0.41
5:B:578:THR:HA	5:B:622:LYS:HB3	2.03	0.41
5:B:792:MET:HA	5:B:856:PHE:O	2.20	0.41
5:B:806:THR:HG22	5:B:1046:PRO:HD3	2.02	0.41
5:B:890:TYR:CD1	5:B:910:VAL:HG21	2.56	0.41
5:B:986:GLN:HE22	5:B:1022:THR:HG21	1.86	0.41
5:B:1171:VAL:HG11	5:B:1191:ILE:HG12	2.03	0.41
6:C:77:ILE:HD12	6:C:161:LYS:HE3	2.03	0.41
7:E:43:LYS:O	7:E:47:CYS:HB3	2.20	0.41
7:E:178:ILE:HG22	7:E:214:CYS:HA	2.03	0.41
9:H:6:PHE:HZ	9:H:134:ASN:CB	2.30	0.41
9:H:93:TYR:CB	9:H:143:LEU:HB3	2.50	0.41
10:I:55:THR:HG22	10:I:55:THR:O	2.21	0.41
10:I:101:PHE:HB2	10:I:110:PHE:CZ	2.56	0.41
4:A:58:LEU:HD22	4:A:244:PRO:HD2	2.03	0.41
4:A:448:PRO:HB2	4:A:450:LEU:HD23	2.03	0.41
4:A:452:LYS:HB3	5:B:1140:ALA:CB	2.51	0.41
4:A:873:MET:HE2	4:A:873:MET:HB2	1.96	0.41
8:F:147:SER:O	8:F:151:LEU:HD12	2.20	0.41
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.56	0.41
10:I:21:GLU:HG2	10:I:22:ASN:N	2.36	0.41
4:A:503:GLN:O	4:A:504:LEU:HD12	2.17	0.40
4:A:1154:TYR:HD2	4:A:1191:TRP:NE1	2.18	0.40
7:E:12:LEU:HD12	7:E:12:LEU:HA	1.95	0.40
4:A:43:GLU:CD	4:A:46:THR:HB	2.46	0.40
4:A:230:ARG:HB3	4:A:232:GLU:HG2	2.04	0.40
4:A:457:ALA:HB3	4:A:506:ALA:CA	2.51	0.40
4:A:826:ASP:CB	4:A:830:LYS:HB2	2.50	0.40
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.57	0.40
5:B:292:ILE:N	5:B:293:PRO:CD	2.83	0.40
5:B:526:GLU:HG3	5:B:771:SER:HB3	2.04	0.40
5:B:886:LYS:C	5:B:888:GLY:N	2.78	0.40
7:E:111:VAL:HG12	7:E:137:GLU:HG2	2.03	0.40
8:F:82:THR:O	8:F:136:ARG:NH2	2.53	0.40
4:A:62:ASP:O	4:A:63:ARG:C	2.65	0.40
4:A:108:MET:SD	4:A:167:CYS:CB	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:254:GLU:HA	4:A:255:SER:HA	1.84	0.40
4:A:363:GLN:O	4:A:458:HIS:ND1	2.54	0.40
4:A:700:ASN:C	4:A:702:LEU:HB2	2.46	0.40
5:B:518:HIS:O	5:B:519:TRP:C	2.63	0.40
4:A:321:PRO:HB2	4:A:322:VAL:H	1.68	0.40
4:A:341:MET:HE3	4:A:341:MET:HB3	1.82	0.40
4:A:535:THR:O	4:A:536:LEU:C	2.63	0.40
4:A:698:GLN:HG2	10:I:97:MET:SD	2.62	0.40
4:A:1054:LEU:HD22	4:A:1055:ARG:N	2.36	0.40
4:A:1074:GLU:H	4:A:1075:PRO:HD2	1.87	0.40
5:B:952:VAL:HG22	5:B:966:VAL:HG22	2.02	0.40
5:B:1020:ARG:O	5:B:1021:MET:C	2.64	0.40
5:B:1138:MET:HG3	5:B:1146:PHE:CE2	2.56	0.40
6:C:49:VAL:HG23	13:L:69:ALA:HB2	2.04	0.40
6:C:183:TRP:NE1	6:C:207:CYS:SG	2.95	0.40
10:I:37:GLU:H	10:I:37:GLU:HG3	1.68	0.40
10:I:76:PRO:HD3	10:I:110:PHE:CD1	2.56	0.40
10:I:118:ARG:C	10:I:120:GLN:H	2.30	0.40
1:R:3:C:H2'	1:R:4:G:H8	1.85	0.40
4:A:465:TYR:CD2	5:B:976:ILE:HG13	2.57	0.40
4:A:718:VAL:HA	4:A:721:PHE:HB2	2.02	0.40
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.56	0.40
4:A:745:GLN:H	4:A:745:GLN:HG2	1.66	0.40
4:A:1323:ASP:C	4:A:1325:THR:H	2.30	0.40
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.56	0.40
5:B:1006:ILE:HD11	11:J:43:ARG:HB2	2.03	0.40
7:E:59:SER:OG	7:E:81:GLU:HG3	2.21	0.40
13:L:27:LEU:HD23	13:L:27:LEU:H	1.86	0.40
13:L:28:LYS:HB2	13:L:39:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1384/1733 (80%)	1048 (76%)	236 (17%)	100 (7%)	1	13
5	B	1074/1224 (88%)	863 (80%)	152 (14%)	59 (6%)	1	17
6	C	264/318 (83%)	220 (83%)	37 (14%)	7 (3%)	4	28
7	E	185/215 (86%)	149 (80%)	29 (16%)	7 (4%)	2	22
8	F	81/155 (52%)	67 (83%)	8 (10%)	6 (7%)	1	13
9	H	129/146 (88%)	86 (67%)	25 (19%)	18 (14%)	0	3
10	I	117/122 (96%)	70 (60%)	33 (28%)	14 (12%)	0	4
11	J	63/70 (90%)	52 (82%)	8 (13%)	3 (5%)	2	19
12	K	112/120 (93%)	99 (88%)	13 (12%)	0	100	100
13	L	44/70 (63%)	28 (64%)	11 (25%)	5 (11%)	0	5
All	All	3453/4173 (83%)	2682 (78%)	552 (16%)	219 (6%)	1	15

All (219) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	63	ARG
4	A	66	LYS
4	A	108	MET
4	A	169	ASN
4	A	250	ILE
4	A	282	ASN
4	A	284	ALA
4	A	287	HIS
4	A	289	ILE
4	A	313	GLN
4	A	543	LEU
4	A	567	LYS
4	A	702	LEU
4	A	713	SER
4	A	1069	ALA
4	A	1084	PHE
4	A	1085	HIS
4	A	1153	TYR
4	A	1157	ASP
4	A	1159	ARG
4	A	1165	GLU
4	A	1172	LEU
4	A	1191	TRP

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Mol	Chain	Res	Type
4	A	1192	LEU
4	A	1365	TYR
4	A	1392	SER
5	B	184	ALA
5	B	231	PRO
5	B	232	SER
5	B	326	ASP
5	B	477	ALA
5	B	511	PRO
5	B	573	GLN
5	B	636	PRO
5	B	705	MET
5	B	710	LEU
5	B	711	GLU
5	B	878	GLN
5	B	882	THR
5	B	1020	ARG
5	B	1178	ASN
7	E	130	ALA
8	F	73	ALA
8	F	104	ASN
8	F	128	LYS
9	H	77	ARG
9	H	82	PRO
9	H	89	LEU
9	H	91	ASP
9	H	106	GLU
9	H	107	VAL
9	H	110	ASP
9	H	140	ALA
10	I	4	PHE
10	I	18	GLU
10	I	22	ASN
10	I	23	ASN
10	I	26	LEU
10	I	46	HIS
10	I	80	SER
4	A	8	SER
4	A	44	THR
4	A	58	LEU
4	A	214	ILE
4	A	220	THR

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Mol	Chain	Res	Type
4	A	223	GLY
4	A	279	LEU
4	A	281	HIS
4	A	423	ASP
4	A	597	LEU
4	A	637	LYS
4	A	701	LEU
4	A	710	LEU
4	A	846	GLU
4	A	896	ARG
4	A	958	VAL
4	A	969	GLN
4	A	998	LEU
4	A	1070	GLN
4	A	1086	PHE
4	A	1127	ASP
4	A	1198	ASP
4	A	1206	ASP
4	A	1237	ILE
4	A	1393	ASN
5	B	66	ASP
5	B	100	PRO
5	B	183	GLU
5	B	327	ARG
5	B	365	THR
5	B	409	ALA
5	B	410	GLY
5	B	478	GLY
5	B	635	ARG
5	B	708	GLU
5	B	731	VAL
5	B	865	LYS
5	B	943	SER
6	C	174	ALA
7	E	30	ILE
7	E	139	ALA
7	E	141	VAL
8	F	145	ASP
8	F	146	TRP
9	H	85	GLY
9	H	105	GLU
10	I	25	LEU

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Mol	Chain	Res	Type
10	I	78	CYS
11	J	6	ARG
11	J	10	CYS
13	L	26	THR
13	L	35	SER
13	L	55	ILE
13	L	56	LEU
4	A	71	GLN
4	A	72	GLU
4	A	248	PRO
4	A	418	SER
4	A	424	ILE
4	A	591	PHE
4	A	639	PRO
4	A	703	THR
4	A	704	ALA
4	A	922	ASP
4	A	1016	THR
4	A	1072	ILE
4	A	1074	GLU
4	A	1081	LEU
4	A	1128	GLN
4	A	1160	SER
4	A	1167	GLU
4	A	1435	PRO
4	A	1436	ILE
5	B	274	PRO
5	B	275	TYR
5	B	277	LYS
5	B	483	LEU
5	B	531	GLN
5	B	836	GLU
5	B	869	SER
5	B	1046	PRO
6	C	90	ASP
6	C	184	ASN
8	F	113	GLY
9	H	81	PRO
9	H	84	ALA
9	H	112	ILE
4	A	87	ALA
4	A	254	GLU

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Mol	Chain	Res	Type
4	A	312	PRO
4	A	332	LYS
4	A	382	PRO
4	A	404	TYR
4	A	465	TYR
4	A	910	PRO
4	A	1082	ASN
4	A	1224	LEU
4	A	1388	GLY
5	B	276	ILE
5	B	301	ILE
5	B	482	VAL
5	B	706	GLN
5	B	887	HIS
5	B	974	PRO
5	B	1155	SER
9	H	83	GLN
9	H	90	ALA
9	H	139	ASN
10	I	19	ASP
10	I	20	LYS
11	J	2	ILE
13	L	43	THR
4	A	517	ASN
4	A	624	SER
4	A	674	PRO
4	A	903	ASN
4	A	1076	ALA
4	A	1200	ALA
5	B	233	PRO
5	B	328	GLU
5	B	712	PRO
5	B	870	ILE
5	B	894	ASP
5	B	1017	ILE
5	B	1097	HIS
6	C	110	THR
6	C	142	VAL
7	E	36	GLU
9	H	23	VAL
9	H	61	SER
10	I	47	GLU

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Mol	Chain	Res	Type
10	I	88	SER
10	I	118	ARG
4	A	10	PRO
4	A	52	GLY
4	A	130	ASP
4	A	321	PRO
4	A	1163	ILE
4	A	1262	LYS
5	B	648	HIS
5	B	792	MET
6	C	214	ASN
7	E	29	PHE
5	B	707	PRO
4	A	1156	PRO
4	A	1294	PRO
5	B	436	VAL
5	B	592	ASN
7	E	76	GLY
4	A	1094	VAL
5	B	290	GLY
5	B	292	ILE
6	C	6	PRO
4	A	1107	VAL
5	B	230	ALA
4	A	775	ILE
5	B	1214	PRO
4	A	1158	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1218/1520 (80%)	1023 (84%)	195 (16%)	2	14
5	B	951/1061 (90%)	810 (85%)	141 (15%)	3	16
6	C	234/274 (85%)	208 (89%)	26 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	177/197 (90%)	154 (87%)	23 (13%)	4	19
8	F	73/137 (53%)	63 (86%)	10 (14%)	3	17
9	H	117/128 (91%)	93 (80%)	24 (20%)	1	8
10	I	113/116 (97%)	83 (74%)	30 (26%)	0	4
11	J	60/65 (92%)	53 (88%)	7 (12%)	5	21
12	K	99/102 (97%)	89 (90%)	10 (10%)	7	26
13	L	40/57 (70%)	34 (85%)	6 (15%)	3	16
All	All	3082/3657 (84%)	2610 (85%)	472 (15%)	3	15

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	VAL
4	A	8	SER
4	A	13	THR
4	A	28	ARG
4	A	40	THR
4	A	41	MET
4	A	45	GLN
4	A	49	LYS
4	A	50	ILE
4	A	53	LEU
4	A	63	ARG
4	A	65	LEU
4	A	66	LYS
4	A	68	GLN
4	A	69	THR
4	A	77	CYS
4	A	80	HIS
4	A	84	ILE
4	A	90	VAL
4	A	100	LYS
4	A	108	MET
4	A	122	MET
4	A	133	LYS
4	A	199	LEU
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	251	SER

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Mol	Chain	Res	Type
4	A	256	GLN
4	A	260	ASP
4	A	269	ILE
4	A	270	LEU
4	A	271	LYS
4	A	274	ILE
4	A	280	GLU
4	A	286	HIS
4	A	287	HIS
4	A	290	GLU
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	332	LYS
4	A	341	MET
4	A	344	ARG
4	A	354	SER
4	A	373	THR
4	A	379	VAL
4	A	381	THR
4	A	391	LEU
4	A	413	ILE
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	463	ILE
4	A	474	VAL
4	A	503	GLN
4	A	504	LEU
4	A	509	LEU
4	A	513	SER
4	A	531	ILE
4	A	541	ILE
4	A	560	ILE
4	A	566	ILE
4	A	576	GLN
4	A	596	THR

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Mol	Chain	Res	Type
4	A	618	GLU
4	A	635	ARG
4	A	660	ASN
4	A	666	ILE
4	A	675	THR
4	A	680	THR
4	A	687	LYS
4	A	696	GLU
4	A	703	THR
4	A	706	HIS
4	A	708	MET
4	A	710	LEU
4	A	716	ASP
4	A	721	PHE
4	A	724	GLU
4	A	728	LYS
4	A	738	LYS
4	A	740	LEU
4	A	741	ASN
4	A	770	VAL
4	A	783	THR
4	A	826	ASP
4	A	856	THR
4	A	858	ASN
4	A	867	ILE
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	929	LEU
4	A	930	ASP
4	A	961	ARG
4	A	971	PHE
4	A	972	HIS
4	A	973	ILE
4	A	975	HIS
4	A	976	THR
4	A	994	GLN
4	A	996	ASN
4	A	998	LEU

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Mol	Chain	Res	Type
4	A	1000	LEU
4	A	1005	GLU
4	A	1015	VAL
4	A	1017	LEU
4	A	1020	CYS
4	A	1022	LEU
4	A	1030	ARG
4	A	1035	TYR
4	A	1038	THR
4	A	1048	ASN
4	A	1049	ILE
4	A	1054	LEU
4	A	1058	VAL
4	A	1070	GLN
4	A	1078	GLN
4	A	1079	MET
4	A	1082	ASN
4	A	1085	HIS
4	A	1086	PHE
4	A	1098	VAL
4	A	1101	LEU
4	A	1104	ILE
4	A	1109	LYS
4	A	1112	LYS
4	A	1113	THR
4	A	1118	VAL
4	A	1128	GLN
4	A	1141	THR
4	A	1142	THR
4	A	1152	ILE
4	A	1155	ASP
4	A	1159	ARG
4	A	1161	THR
4	A	1163	ILE
4	A	1165	GLU
4	A	1166	ASP
4	A	1168	GLU
4	A	1170	ILE
4	A	1172	LEU
4	A	1187	GLN
4	A	1192	LEU
4	A	1194	ARG

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Mol	Chain	Res	Type
4	A	1197	LEU
4	A	1198	ASP
4	A	1203	ASN
4	A	1212	VAL
4	A	1215	ARG
4	A	1219	THR
4	A	1224	LEU
4	A	1226	VAL
4	A	1227	ILE
4	A	1228	TRP
4	A	1239	ARG
4	A	1242	VAL
4	A	1262	LYS
4	A	1266	THR
4	A	1271	ILE
4	A	1281	ARG
4	A	1284	MET
4	A	1288	ASP
4	A	1295	THR
4	A	1314	SER
4	A	1322	ILE
4	A	1329	THR
4	A	1333	ILE
4	A	1336	MET
4	A	1345	ARG
4	A	1358	SER
4	A	1359	ASP
4	A	1364	ASN
4	A	1366	ARG
4	A	1371	LEU
4	A	1376	THR
4	A	1385	THR
4	A	1390	ASN
4	A	1391	ARG
4	A	1394	THR
4	A	1398	MET
4	A	1407	GLU
4	A	1418	LEU
4	A	1426	GLU
4	A	1427	ASN
4	A	1445	ILE
5	B	28	GLU

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Mol	Chain	Res	Type
5	B	44	VAL
5	B	63	ILE
5	B	68	THR
5	B	90	ILE
5	B	91	SER
5	B	94	LYS
5	B	102	VAL
5	B	108	VAL
5	B	121	ASN
5	B	167	ILE
5	B	192	LEU
5	B	194	GLU
5	B	234	ILE
5	B	251	ILE
5	B	268	THR
5	B	272	THR
5	B	273	LEU
5	B	276	ILE
5	B	277	LYS
5	B	279	ASP
5	B	283	VAL
5	B	291	ILE
5	B	292	ILE
5	B	294	ASP
5	B	297	ILE
5	B	299	GLU
5	B	304	ASP
5	B	305	VAL
5	B	320	ASP
5	B	322	PHE
5	B	324	ILE
5	B	325	GLN
5	B	327	ARG
5	B	329	THR
5	B	334	ILE
5	B	346	GLU
5	B	347	LYS
5	B	351	TYR
5	B	361	LEU
5	B	390	LEU
5	B	391	ASP
5	B	398	ARG

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Mol	Chain	Res	Type
5	B	425	THR
5	B	428	ILE
5	B	463	THR
5	B	473	MET
5	B	479	VAL
5	B	483	LEU
5	B	485	ARG
5	B	502	ILE
5	B	522	VAL
5	B	527	THR
5	B	531	GLN
5	B	537	LYS
5	B	547	VAL
5	B	561	TRP
5	B	567	GLU
5	B	570	VAL
5	B	572	HIS
5	B	573	GLN
5	B	574	SER
5	B	576	ASP
5	B	598	GLU
5	B	603	LEU
5	B	604	ARG
5	B	618	ASP
5	B	637	LEU
5	B	645	SER
5	B	650	GLU
5	B	653	VAL
5	B	655	LYS
5	B	680	THR
5	B	701	ILE
5	B	708	GLU
5	B	723	VAL
5	B	740	HIS
5	B	754	SER
5	B	764	SER
5	B	778	MET
5	B	783	THR
5	B	787	VAL
5	B	790	ASP
5	B	791	THR
5	B	796	LEU

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Mol	Chain	Res	Type
5	B	806	THR
5	B	811	TYR
5	B	812	LEU
5	B	837	ASP
5	B	844	SER
5	B	850	LEU
5	B	861	ASP
5	B	864	LYS
5	B	866	TYR
5	B	880	THR
5	B	883	LEU
5	B	898	LEU
5	B	916	THR
5	B	918	ILE
5	B	941	LEU
5	B	943	SER
5	B	944	THR
5	B	953	LEU
5	B	956	THR
5	B	970	THR
5	B	971	THR
5	B	975	GLN
5	B	976	ILE
5	B	997	GLU
5	B	998	ASP
5	B	999	MET
5	B	1002	THR
5	B	1012	ILE
5	B	1051	THR
5	B	1052	VAL
5	B	1060	ARG
5	B	1065	GLN
5	B	1071	VAL
5	B	1082	MET
5	B	1085	ILE
5	B	1090	THR
5	B	1099	VAL
5	B	1103	ILE
5	B	1108	ARG
5	B	1113	VAL
5	B	1115	THR
5	B	1124	ARG

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Mol	Chain	Res	Type
5	B	1151	LEU
5	B	1156	ASP
5	B	1159	ARG
5	B	1160	VAL
5	B	1170	THR
5	B	1179	GLN
5	B	1183	LYS
5	B	1185	CYS
5	B	1189	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1220	ARG
5	B	1222	ARG
6	C	8	VAL
6	C	27	LEU
6	C	38	ILE
6	C	41	ILE
6	C	44	LEU
6	C	49	VAL
6	C	53	THR
6	C	55	THR
6	C	56	THR
6	C	57	VAL
6	C	72	LEU
6	C	77	ILE
6	C	83	SER
6	C	106	GLU
6	C	120	ILE
6	C	124	LEU
6	C	163	ILE
6	C	197	SER
6	C	199	LYS
6	C	208	GLU
6	C	221	TYR
6	C	235	VAL
6	C	240	VAL
6	C	250	THR
6	C	258	ILE
6	C	264	GLN
7	E	3	GLN
7	E	8	ASN

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Mol	Chain	Res	Type
7	E	16	PHE
7	E	29	PHE
7	E	69	ILE
7	E	71	LYS
7	E	78	LEU
7	E	80	VAL
7	E	98	ILE
7	E	104	ASN
7	E	107	THR
7	E	111	VAL
7	E	122	LYS
7	E	123	LEU
7	E	127	ILE
7	E	132	ILE
7	E	134	THR
7	E	140	LEU
7	E	142	VAL
7	E	169	ARG
7	E	184	VAL
7	E	190	LEU
7	E	196	VAL
8	F	92	ARG
8	F	97	ARG
8	F	99	LEU
8	F	107	VAL
8	F	111	LEU
8	F	119	ARG
8	F	123	LYS
8	F	148	VAL
8	F	151	LEU
8	F	154	ASP
9	H	4	THR
9	H	32	THR
9	H	33	GLN
9	H	39	THR
9	H	56	THR
9	H	77	ARG
9	H	83	GLN
9	H	86	ASP
9	H	87	ARG
9	H	88	SER
9	H	89	LEU

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Mol	Chain	Res	Type
9	H	92	ASP
9	H	94	ASP
9	H	102	TYR
9	H	106	GLU
9	H	107	VAL
9	H	109	LYS
9	H	111	LEU
9	H	112	ILE
9	H	129	TYR
9	H	130	ARG
9	H	133	ASN
9	H	136	LYS
9	H	139	ASN
10	I	2	THR
10	I	4	PHE
10	I	13	MET
10	I	17	ARG
10	I	20	LYS
10	I	21	GLU
10	I	25	LEU
10	I	26	LEU
10	I	28	GLU
10	I	29	CYS
10	I	32	CYS
10	I	37	GLU
10	I	42	LEU
10	I	43	VAL
10	I	45	ARG
10	I	50	THR
10	I	52	ILE
10	I	59	VAL
10	I	60	GLN
10	I	78	CYS
10	I	79	HIS
10	I	84	VAL
10	I	94	ASP
10	I	101	PHE
10	I	104	LEU
10	I	105	SER
10	I	106	CYS
10	I	109	ILE
10	I	111	THR

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Mol	Chain	Res	Type
10	I	119	THR
11	J	5	VAL
11	J	7	CYS
11	J	9	SER
11	J	22	LEU
11	J	34	THR
11	J	46	CYS
11	J	52	THR
12	K	11	LEU
12	K	12	LEU
12	K	40	HIS
12	K	41	THR
12	K	46	ILE
12	K	47	ARG
12	K	50	LEU
12	K	51	LEU
12	K	63	VAL
12	K	114	LEU
13	L	31	CYS
13	L	33	GLU
13	L	43	THR
13	L	44	ASP
13	L	55	ILE
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	45	GLN
4	A	68	GLN
4	A	71	GLN
4	A	83	HIS
4	A	118	HIS
4	A	171	GLN
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	479	ASN

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Mol	Chain	Res	Type
4	A	510	GLN
4	A	517	ASN
4	A	587	HIS
4	A	603	ASN
4	A	654	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	760	GLN
4	A	802	ASN
4	A	838	GLN
4	A	858	ASN
4	A	926	GLN
4	A	965	GLN
4	A	968	GLN
4	A	969	GLN
4	A	972	HIS
4	A	996	ASN
4	A	1004	ASN
4	A	1033	GLN
4	A	1078	GLN
4	A	1085	HIS
4	A	1110	ASN
4	A	1124	HIS
4	A	1128	GLN
4	A	1140	HIS
4	A	1188	GLN
4	A	1222	ASN
4	A	1364	ASN
4	A	1378	GLN
4	A	1390	ASN
4	A	1427	ASN
5	B	121	ASN
5	B	215	GLN
5	B	255	GLN
5	B	465	ASN
5	B	515	HIS
5	B	531	GLN
5	B	740	HIS
5	B	744	HIS
5	B	762	ASN
5	B	770	GLN

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Mol	Chain	Res	Type
5	B	822	ASN
5	B	842	ASN
5	B	878	GLN
5	B	986	GLN
5	B	1015	HIS
5	B	1084	GLN
5	B	1177	HIS
5	B	1178	ASN
5	B	1179	GLN
5	B	1211	ASN
6	C	73	GLN
6	C	224	GLN
6	C	231	ASN
6	C	252	GLN
7	E	8	ASN
7	E	61	GLN
7	E	101	GLN
7	E	104	ASN
7	E	147	HIS
9	H	33	GLN
9	H	133	ASN
9	H	137	GLN
10	I	60	GLN
10	I	83	ASN
10	I	90	GLN

5.3.3 RNA ⓘ

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

There are no RNA backbone outliers to report.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	GTP	T	3000	16	33,34,34	0.91	2 (6%)	50,54,54	1.58	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	GTP	T	3000	16	-	9/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	GTP	C2-N3	2.61	1.39	1.33
14	T	3000	GTP	PA-O3A	2.03	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	GTP	C5-C4-N3	-5.43	119.75	128.39
14	T	3000	GTP	C2-N3-C4	4.38	119.85	112.30
14	T	3000	GTP	N9-C4-N3	3.35	132.66	125.95
14	T	3000	GTP	C2-N1-C6	-3.17	119.37	125.11
14	T	3000	GTP	C5-C6-N1	2.47	119.55	113.25
14	T	3000	GTP	C3'-C2'-C1'	2.28	105.78	101.46
14	T	3000	GTP	C8-N7-C5	2.22	108.21	104.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

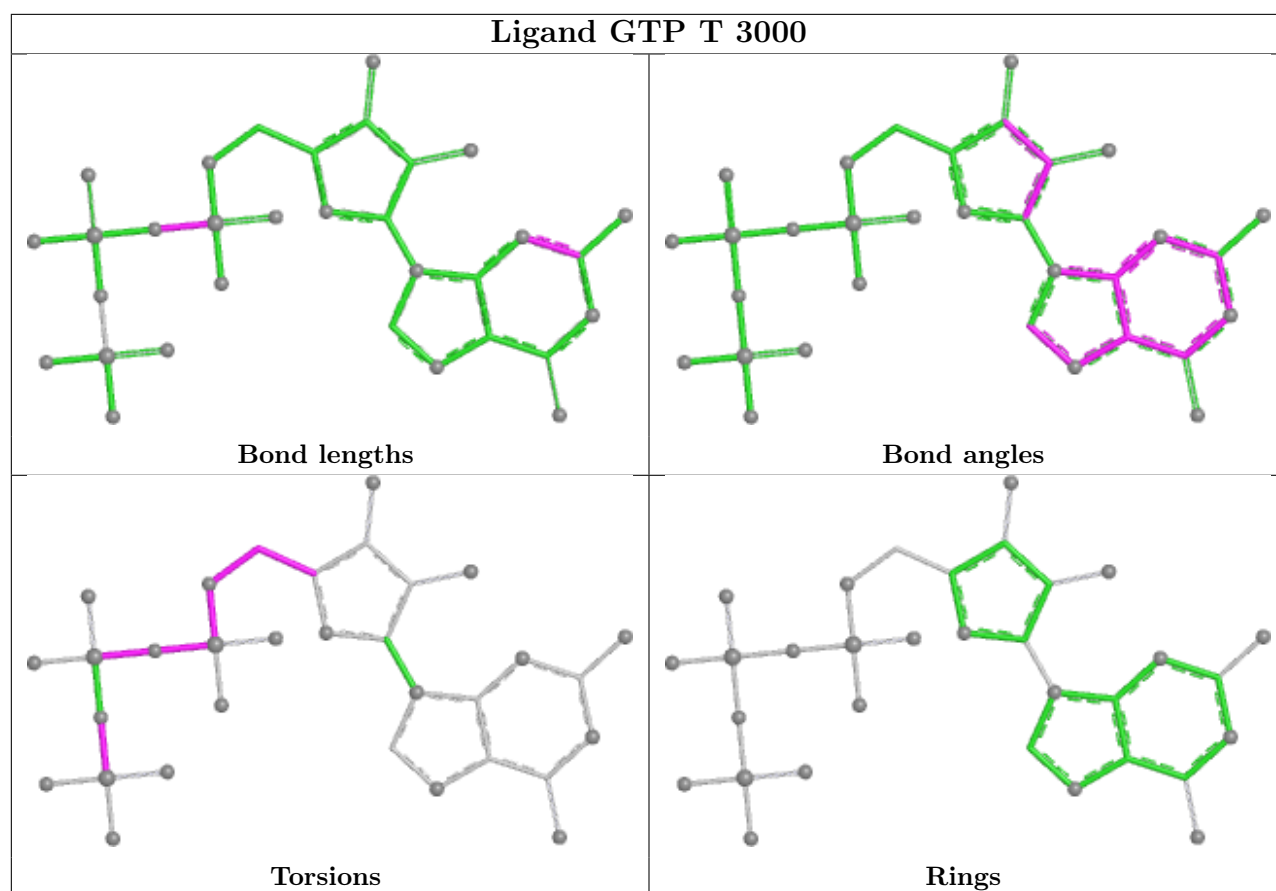
Mol	Chain	Res	Type	Atoms
14	T	3000	GTP	PB-O3B-PG-O2G
14	T	3000	GTP	PB-O3B-PG-O3G
14	T	3000	GTP	C5'-O5'-PA-O3A
14	T	3000	GTP	C5'-O5'-PA-O1A
14	T	3000	GTP	C4'-C5'-O5'-PA
14	T	3000	GTP	PB-O3A-PA-O5'
14	T	3000	GTP	O4'-C4'-C5'-O5'
14	T	3000	GTP	C3'-C4'-C5'-O5'
14	T	3000	GTP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	3000	GTP	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	10/10 (100%)	-0.14	0 100 100	88, 113, 158, 169	0
2	T	28/28 (100%)	0.27	0 100 100	88, 190, 261, 264	0
3	N	14/14 (100%)	0.60	1 (7%) 22 20	251, 259, 268, 269	0
4	A	1398/1733 (80%)	0.07	12 (0%) 81 62	76, 118, 174, 192	0
5	B	1096/1224 (89%)	0.11	16 (1%) 72 51	86, 115, 155, 171	0
6	C	266/318 (83%)	-0.17	0 100 100	93, 115, 146, 151	0
7	E	193/215 (89%)	0.05	4 (2%) 63 45	94, 131, 165, 172	0
8	F	83/155 (53%)	0.08	1 (1%) 76 56	106, 123, 135, 139	0
9	H	133/146 (91%)	0.17	2 (1%) 72 51	118, 140, 172, 175	0
10	I	119/122 (97%)	0.49	3 (2%) 58 41	131, 150, 166, 169	0
11	J	65/70 (92%)	-0.08	0 100 100	101, 113, 134, 138	0
12	K	114/120 (95%)	-0.24	0 100 100	98, 116, 132, 132	0
13	L	46/70 (65%)	0.60	3 (6%) 25 22	134, 176, 186, 188	0
All	All	3565/4225 (84%)	0.08	42 (1%) 76 56	76, 119, 170, 269	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	388	CYS	3.8
5	B	335	GLY	3.7
7	E	110	PHE	3.7
13	L	32	ALA	3.6
13	L	25	ALA	3.4
7	E	16	PHE	3.1
5	B	643	ASP	3.1
4	A	1176	LEU	3.0
4	A	147	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
13	L	28	LYS	2.9
5	B	611	PRO	2.9
4	A	596	THR	2.8
9	H	63	LEU	2.8
5	B	886	LYS	2.7
4	A	1378	GLN	2.7
7	E	96	PHE	2.6
5	B	407	ASP	2.6
5	B	816	GLU	2.6
4	A	185	TRP	2.5
7	E	98	ILE	2.5
3	N	1	DC	2.4
4	A	847	ASP	2.4
5	B	1154	ALA	2.3
4	A	2	VAL	2.3
4	A	72	GLU	2.3
5	B	387	LEU	2.3
5	B	433	GLN	2.2
4	A	1243	VAL	2.2
5	B	883	LEU	2.2
5	B	732	SER	2.2
5	B	869	SER	2.2
4	A	161	LEU	2.1
8	F	137	TYR	2.1
5	B	356	LEU	2.1
5	B	1016	ALA	2.1
10	I	59	VAL	2.1
4	A	701	LEU	2.1
10	I	79	HIS	2.1
9	H	79	TRP	2.0
10	I	77	LYS	2.0
4	A	150	THR	2.0
5	B	936	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

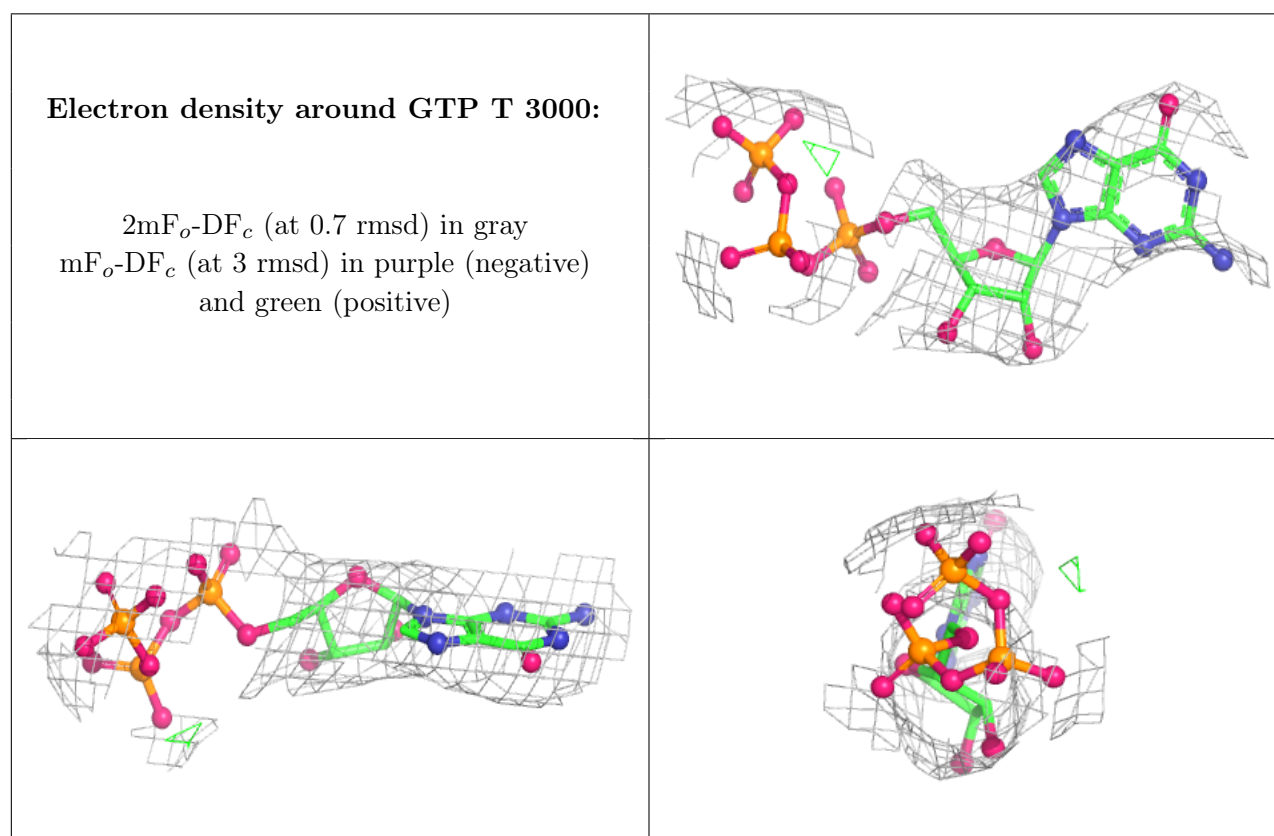
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	MG	A	2002	1/1	0.92	0.08	100,100,100,100	0
15	ZN	I	204	1/1	0.93	0.12	164,164,164,164	0
14	GTP	T	3000	32/32	0.95	0.09	105,109,114,114	0
15	ZN	L	105	1/1	0.95	0.05	175,175,175,175	0
15	ZN	B	1307	1/1	0.95	0.05	149,149,149,149	0
16	MG	A	2001	1/1	0.96	0.08	96,96,96,96	0
15	ZN	A	1734	1/1	0.96	0.06	178,178,178,178	0
15	ZN	A	1735	1/1	0.97	0.04	170,170,170,170	0
15	ZN	I	203	1/1	0.97	0.09	133,133,133,133	0
15	ZN	J	101	1/1	0.98	0.04	106,106,106,106	0
15	ZN	C	319	1/1	1.00	0.02	112,112,112,112	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.