



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 09:57 AM EDT

PDB ID : 8UKQ / pdb_00008ukq
Title : RNA polymerase II elongation complex with Fapy-dG lesion in apo state
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

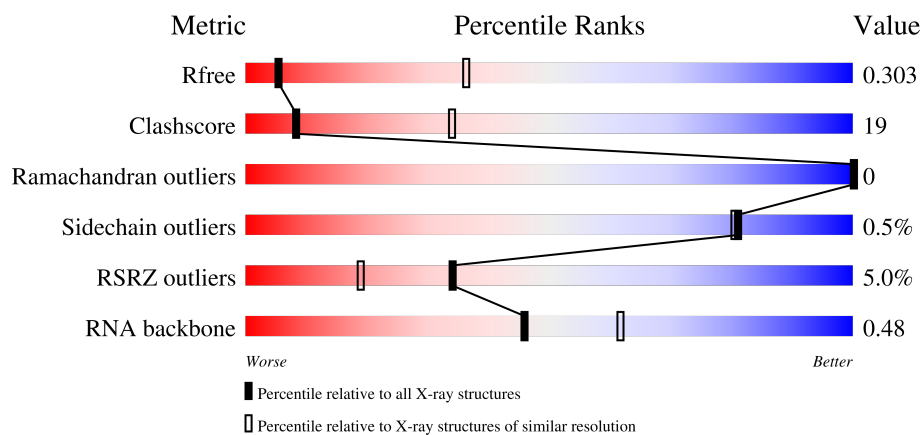
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	9	
2	T	29	
3	N	18	
4	A	1733	

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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 15 unique types of molecules in this entry. The entry contains 28981 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 RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 2 is a DNA chain called tsDNA with FapydG lesion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	0	0
			481	230	76	151	24			

- Molecule 3 is a DNA chain called ntsDNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	13	Total	C	N	O	P	0	0	0
			275	128	61	73	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10828	6831	1896	2041	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1126	Total	C	N	O	S	0	0	0
			8874	5616	1555	1650	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

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 subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

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

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

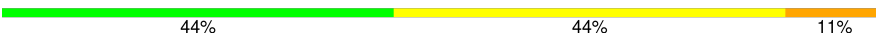
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

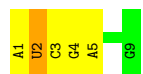
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots [i](#)

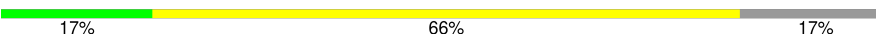
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: RNA

Chain R: 

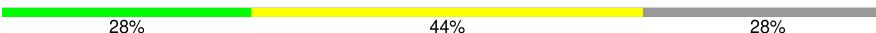


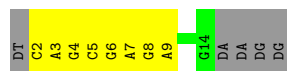
- Molecule 2: tsDNA with FapydG lesion

Chain T: 



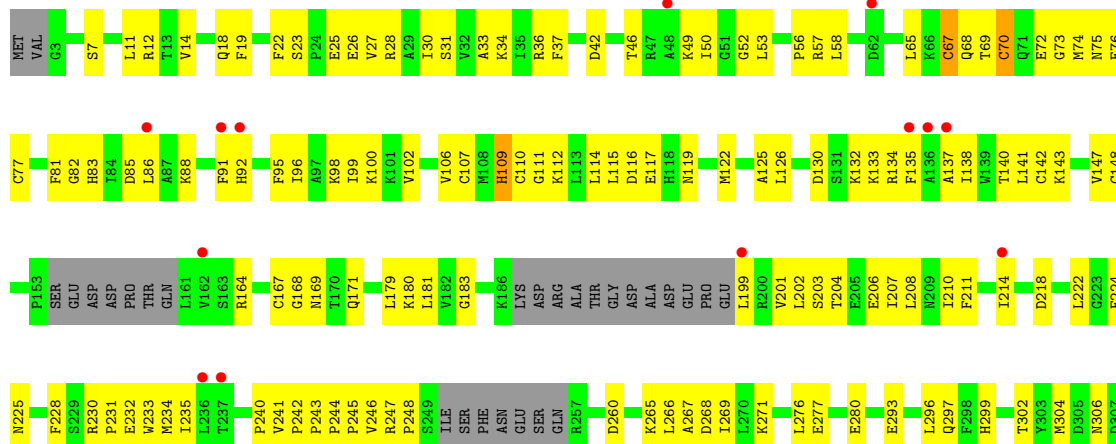
- Molecule 3: ntsDNA

Chain N: 

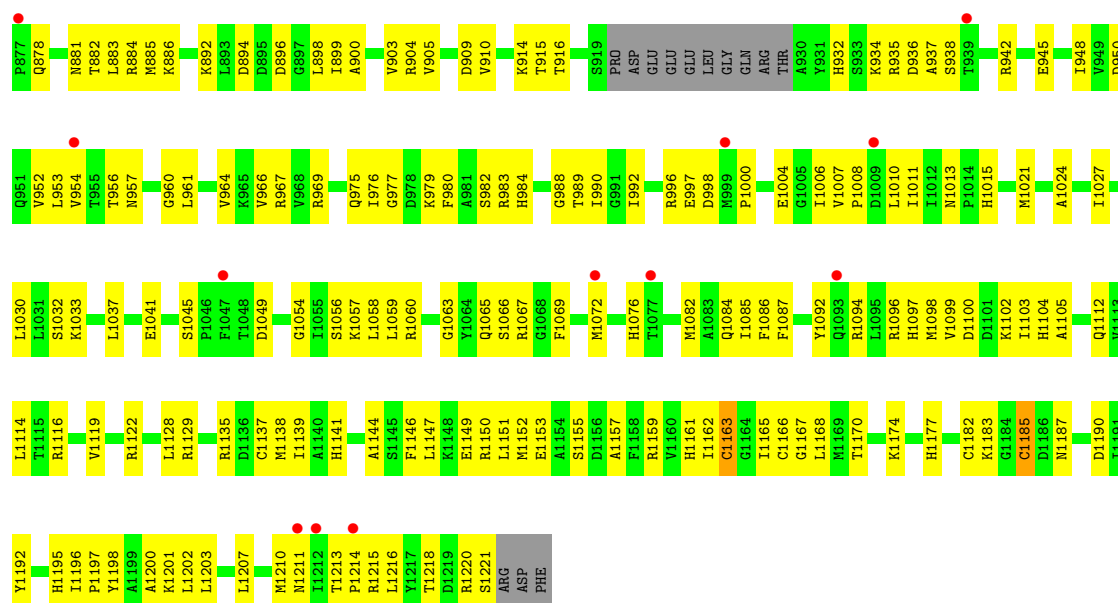


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

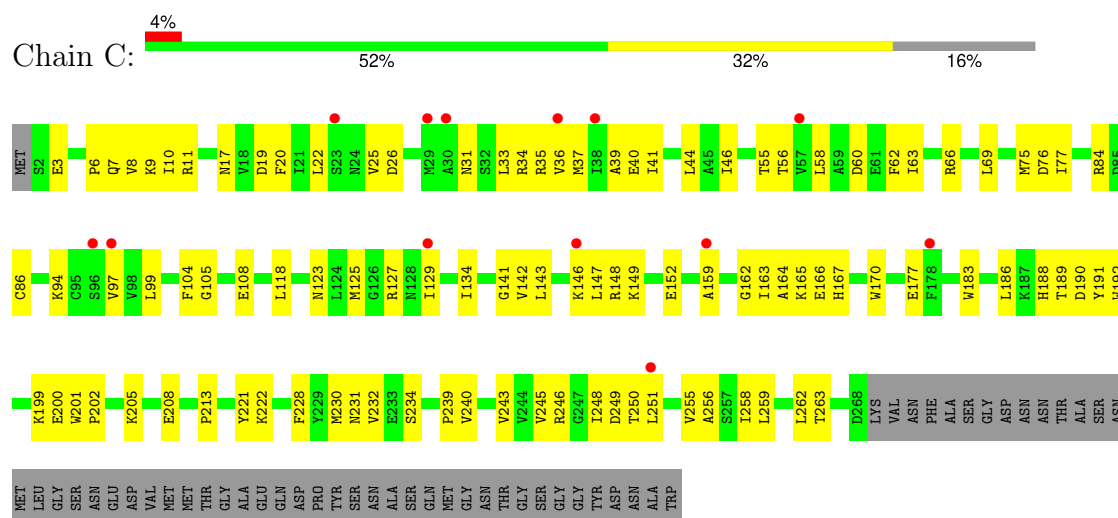
Chain A: 



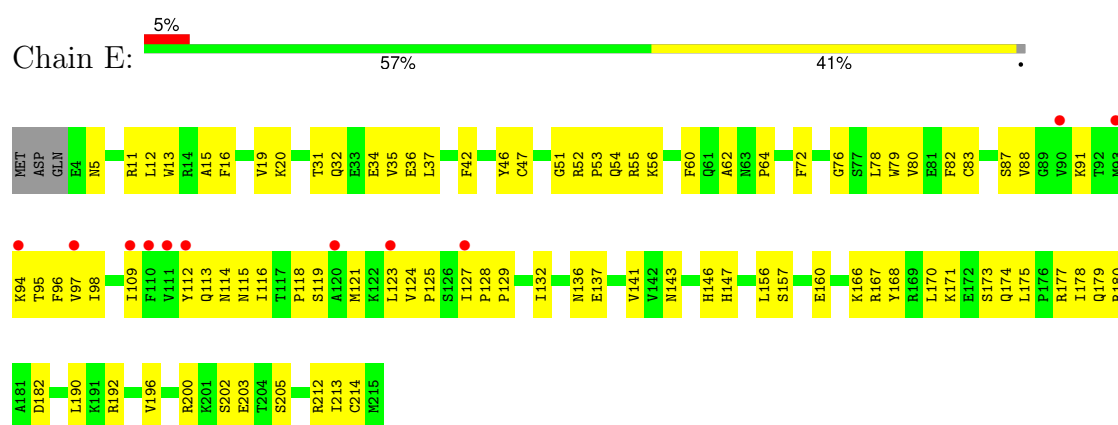
M1444	N1364	R1274	R1199	L1104	R1025	L936	L845	K752	L658	S573	R498	H399	I308
I1445	Y1365	E1277	M1202	L1105	L1026	D939	H851	T756	H659	G574	A499	L415	Q311
D1446	R1366	N1278	M1202	M1111	T1028	K941	T856	Q760	F662	Q576	E500	R420	P312
GLU	H1367	V1282	D1206	P1114	R1029	F942	R857	W61	T664	L577	A506	D423	Q316
SER	M1283	T1208	T1208	S1115	V1031	L943	N858	W65	G665	S579	V507	L424	R320
LEU	M1284	M1209	M1209	V1118	Q1033	E945	L860	G766	I666	T582	P508	D426	K323
VAL	L1371	V1212	V1212	Q1128	Y1035	V946	G861	Q767	P683	P583	L509	L426	K324
TYR	D1373	E1214	E1214	E1129	R1036	E951	Q865	R774	I670	H587	S513	V432	R326
MET	Y1287	R1215	R1215	K1132	T1038	E952	F866	A776	A671	D672	P514	F433	E433
PRO	K1290	I1216	I1216	L1134	K1039	N953	R867	F777	G673	E593	Q515	R434	R327
GLU	TL377	K1217	K1217	R1135	F1042	W954	Y868	G778	P674	G594	N517	R436	R328
GLN	L1381	Q1218	Q1218	S1136	D1043	L956	G869	F779	T675	T595	K318	L436	K332
ILE	T1382	T1219	T1219	A1137	W1044	P957	E870	W780	M676	T596	P519	M439	K336
THR	S1383	K1221	K1221	I1138	V1045	I960	G872	D781	R677	L597	C520	V442	R337
GLU	V1384	L1224	L1224	E1139	L1046	R961	R873	R782	E678	K601	G522	V443	N339
ILE	TL385	F1225	F1225	H1140	N1047	R962	D874	T783	I679	M605	T523	L443	L340
GLY	H1387	V1226	V1226	L1143	S1048	I963	A875	P785	I683	L606	D526	R446	G341
GLN	M1390	I1227	I1227	L1148	E1050	I973	H877	H786	A684	I607	T527	D447	G342
ASP	V1397	S1229	S1229	T1149	A1051	D974	L878	K789	K687	I608	L528	P448	K343
GLY	M1398	K1235	K1235	A1149	R1055	H975	E879	D790	K688	Q611	C529	H451	R344
VAL	R1399	L1236	L1236	E1150	V1056	L981	K880	P794	L691	I612	T531	K452	R350
THR	E1400	I1237	I1237	E1151	S1057	L986	Q881	W795	K695	I613	R532	M455	T351
PRO	S1401	T1238	T1238	E1165	V1058	I986	S882	S796	K696	F614	K533	M456	V352
TYR	F1402	R1239	R1239	D1166	G1061	V990	T895	K797	A697	V617	L534	A457	I353
SER	E1403	C1240	C1240	E1167	Q1070	L993	D890	G799	Q698	E818	T535	A458	S354
ASN	E1404	R1241	R1241	I1169	S1071	Q994	R898	W800	Q698	K619	L536	R459	G355
GLU	TL405	V1242	V1242	L1170	E1065	L995	V899	R801	A704	K620	D538	I463	D356
GLY	E1407	I1243	I1243	L1171	A1069	E995	R899	N802	L710	T621	T539	I463	E360
LEU	I1408	ARG	ARG	L1172	Q1070	N996	D900	S803	R711	G623	F540	P464	L361
VAL	A1416	PRO	PRO	L1176	S1071	L997	L901	Y804	L718	S624	V546	Y465	D362
ASN	E1417	LYS	LYS	L1176	E1074	L1000	L902	R806	V718	S625	N548	S466	Q363
ALA	L1418	LEU	LEU	ASP	E1074	L1000	N903	R806	L722	N626	N549	R469	V364
LEU	L1418	ASP	ASP	GLU	T1077	N1004	H906	E812	L722	N626	N549	L470	G365
VAL	R1422	ALA	ALA	GLU	T1077	E1005	T907	F813	L722	N626	N549	L470	K368
LYS	I1333	THR	THR	ALA	L1081	I1006	L908	F814	D727	T634	L550	L471	S369
ASP	D1334	GLU	GLU	ALA	ASN	I1007	P909	F815	K728	R635	V551	L472	I370
ASP	I1335	GLU	GLU	GLN	THR	A1010	L912	M818	A729	C642	N556	V473	T375
GLU	M1336	ALA	ALA	GLN	THR	A1010	L912	M818	G730	C642	N556	V473	T375
LEU	E1337	GLU	GLU	PHE	THR	A1010	L912	M818	G730	C642	N556	V473	T375
MET	V1428	GLU	GLU	PHE	THR	A1010	L912	M818	G730	C642	N556	V473	T375
PHE	I1429	GLU	GLU	ASP	THR	A1010	L912	M818	G730	C642	N556	V473	T375
SER	L1430	D1257	D1257	GLN	ALA	A1014	S915	G820	L732	L645	V559	Y478	Y376
SER	G1431	K1262	K1262	Q1198	GLY	V1015	G916	L824	N736	F646	P663	N479	E378
LEU	E1342	I1263	I1263	L1192	VAL	V1015	G916	L824	N736	F646	P663	N479	E378
VAL	R1345	E1264	E1264	L1192	ALA	F1018	I919	T834	L740	N648	I565	A480	V380
VAL	A1434	E1264	E1264	L1192	ALA	F1018	I919	T834	L740	N648	I565	A480	V380
ASP	P1435	E1264	E1264	L1192	ALA	F1018	I919	T834	L740	N648	I565	A480	V380
ASP	A1347	E1264	E1264	L1192	ALA	F1018	I919	T834	L740	N648	I565	A480	V380
SER	L1348	L1268	L1268	R1194	SER	C1019	N741	Q835	N742	K651	I566	D481	F379
GLY	G1437	L1268	L1268	L1195	K1092	C1020	N741	Q835	N742	K651	I566	D481	F379
SER	TL438	I1271	I1271	L1195	K1092	C1020	N741	Q835	N742	K651	I566	D481	F379
SER	E1350	T1272	T1272	L1197	P1099	L1021	E932	R839	Q745	W656	P570	M487	L391
ASN	I1351	L1273	L1273	L1197	P1099	L1021	E932	R839	Q745	W656	P570	M487	L391
ASP	V1352	L1273	L1273	D1198	E1103	S1024	Y933	R840	M746	L657	N572	H490	V392



• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

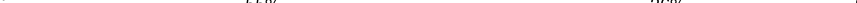


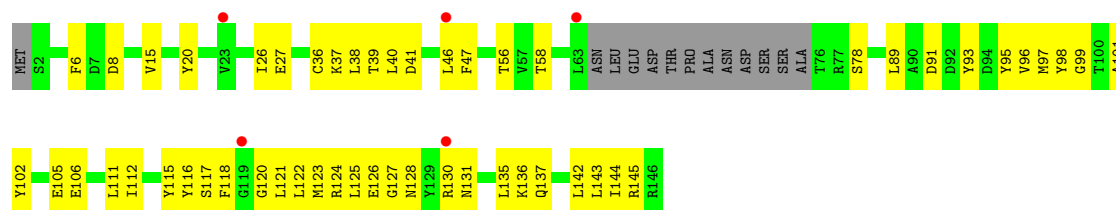
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

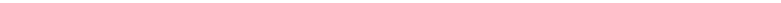


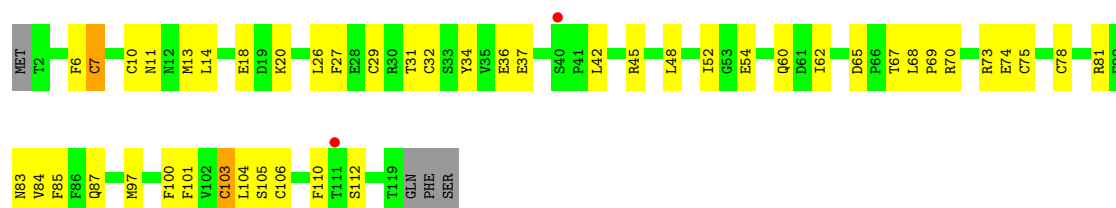
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

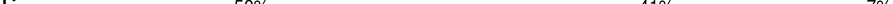


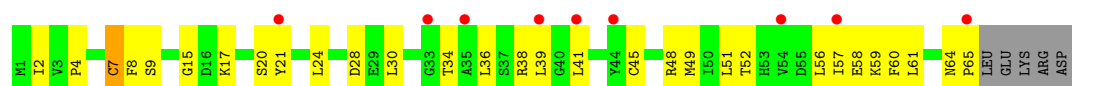
- Chain H: 

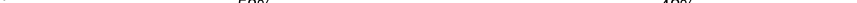


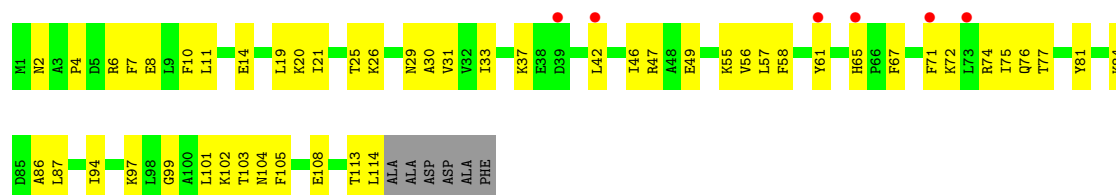
- Chain I:  2% 59% 36% ..



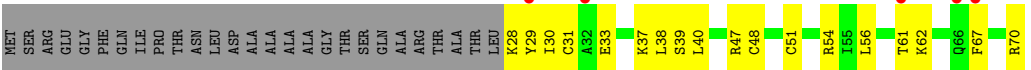
- Chain J: 



- Chain K: 



- 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.54Å 223.49Å 191.47Å 90.00° 98.38° 90.00°	Depositor
Resolution (Å)	48.44 – 3.50 48.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.44-3.50) 99.3 (48.44-3.50)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.268 , 0.302 0.268 , 0.303	Depositor DCC
R_{free} test set	2000 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	94.4	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28981	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: MG, ZN, WVQ

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	0.14	0/218	0.36	0/339
2	T	0.22	0/507	0.50	0/775
3	N	0.20	0/311	0.39	0/479
4	A	0.17	0/11020	0.42	2/14907 (0.0%)
5	B	0.16	0/9046	0.39	0/12210
6	C	0.15	0/2139	0.37	0/2899
7	E	0.16	0/1767	0.39	0/2378
8	F	0.14	0/696	0.36	0/943
9	H	0.20	0/1082	0.50	0/1466
10	I	0.14	0/970	0.41	0/1308
11	J	0.18	0/541	0.44	0/727
12	K	0.17	0/937	0.44	0/1265
13	L	0.16	0/339	0.42	0/450
All	All	0.17	0/29573	0.41	2/40146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	56	PRO	CA-C-N	5.53	132.10	121.54
4	A	56	PRO	C-N-CA	5.53	132.10	121.54

There are no chirality outliers.

There are no planarity outliers.

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	194	0	98	6	0
2	T	481	0	262	18	0
3	N	275	0	144	11	0
4	A	10828	0	10876	484	0
5	B	8874	0	8823	365	0
6	C	2101	0	2056	91	0
7	E	1731	0	1758	66	0
8	F	684	0	692	19	0
9	H	1064	0	1029	58	0
10	I	952	0	897	45	0
11	J	532	0	542	31	0
12	K	919	0	929	48	0
13	L	337	0	352	14	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	28981	0	28458	1100	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 19.

All (1100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:30:ALA:HA	12:K:75:ILE:O	1.74	0.88
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.57	0.85
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.60	0.84
4:A:109:HIS:CE1	4:A:110:CYS:SG	2.71	0.83
4:A:672:ASP:H	4:A:736:ASN:HD21	1.27	0.81
4:A:111:GLY:HA3	4:A:214:ILE:HA	1.62	0.80
9:H:101:ALA:HA	9:H:116:TYR:HA	1.61	0.80
4:A:446:ARG:HG3	4:A:448:PRO:HD2	1.62	0.80
4:A:110:CYS:SG	4:A:112:LYS:NZ	2.54	0.79
5:B:68:THR:HA	5:B:90:ILE:O	1.80	0.79
4:A:179:LEU:HD22	4:A:297:GLN:HG2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:621:GLU:HB3	5:B:623:GLU:HB2	1.65	0.77
5:B:828:ALA:O	5:B:834:ASN:ND2	2.17	0.77
4:A:67:CYS:SG	4:A:70:CYS:HB2	2.24	0.77
4:A:1136:SER:HB3	4:A:1206:ASP:HB2	1.66	0.76
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.68	0.75
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.70	0.74
5:B:392:ARG:HH12	10:I:52:ILE:HG22	1.53	0.73
5:B:1165:ILE:HB	5:B:1185:CYS:HB3	1.69	0.73
4:A:246:VAL:HA	5:B:1202:LEU:HD11	1.70	0.73
4:A:370:ILE:HD13	5:B:1105:ALA:HB2	1.71	0.73
5:B:310:MET:HE3	5:B:386:LEU:HD12	1.69	0.72
9:H:96:VAL:HA	9:H:142:LEU:O	1.89	0.72
4:A:23:SER:HB3	4:A:26:GLU:HG2	1.70	0.72
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.71	0.72
4:A:1136:SER:O	4:A:1274:ARG:NH1	2.23	0.72
3:N:7:DA:H2'	3:N:8:DG:C8	2.24	0.72
4:A:69:THR:HA	5:B:1174:LYS:HE2	1.71	0.71
4:A:960:ILE:HG21	4:A:1025:ARG:HB3	1.72	0.71
4:A:575:LYS:HE2	9:H:120:GLY:HA3	1.71	0.71
4:A:1219:THR:HG21	4:A:1271:ILE:HD12	1.71	0.71
4:A:1352:VAL:HG12	4:A:1368:MET:HE2	1.72	0.71
5:B:465:ASN:HB3	5:B:474:SER:HB3	1.70	0.71
4:A:1004:ASN:HD22	4:A:1007:ILE:HG12	1.56	0.71
4:A:37:PHE:H	4:A:52:GLY:HA3	1.55	0.70
4:A:42:ASP:HB2	4:A:49:LYS:H	1.56	0.70
12:K:30:ALA:HB2	12:K:76:GLN:HG2	1.74	0.70
7:E:52:ARG:HE	7:E:53:PRO:HD2	1.57	0.69
12:K:42:LEU:HG	12:K:46:ILE:HD11	1.74	0.69
8:F:81:THR:HB	8:F:136:ARG:HH11	1.56	0.69
5:B:778:MET:HE2	5:B:1094:ARG:HB3	1.74	0.69
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.74	0.69
5:B:910:VAL:HG11	5:B:938:SER:HB3	1.74	0.69
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	1.75	0.69
5:B:25:ILE:HG12	5:B:651:LEU:HD22	1.74	0.69
5:B:1210:MET:O	5:B:1211:ASN:ND2	2.26	0.69
6:C:99:LEU:HD12	6:C:118:LEU:HB3	1.74	0.69
7:E:97:VAL:HG13	7:E:127:ILE:HD11	1.75	0.69
4:A:42:ASP:HB3	4:A:46:THR:HB	1.75	0.68
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.75	0.68
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.75	0.68
4:A:302:THR:HG22	4:A:308:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:463:ILE:HD13	4:A:469:ARG:HG2	1.75	0.68
5:B:896:ASP:OD2	13:L:29:TYR:OH	2.08	0.68
4:A:861:GLY:HA3	7:E:174:GLN:HE21	1.59	0.67
5:B:915:THR:HB	5:B:934:LYS:HB3	1.76	0.67
7:E:5:ASN:HB3	7:E:52:ARG:HH12	1.60	0.67
4:A:202:LEU:HB3	4:A:207:ILE:HD11	1.77	0.67
5:B:426:LYS:O	5:B:430:ARG:HG2	1.95	0.67
4:A:53:LEU:HD21	4:A:266:LEU:HD11	1.75	0.67
4:A:540:PHE:HB3	4:A:571:LEU:HD12	1.75	0.67
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.75	0.67
4:A:1192:LEU:HD21	4:A:1239:ARG:HG2	1.78	0.66
9:H:128:ASN:O	9:H:131:ASN:ND2	2.29	0.66
5:B:904:ARG:HG2	5:B:948:ILE:HG12	1.75	0.66
5:B:997:GLU:HB2	6:C:35:ARG:HG2	1.77	0.66
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.76	0.66
5:B:519:TRP:HD1	5:B:635:ARG:HH12	1.43	0.66
5:B:570:VAL:HG23	5:B:573:GLN:HB2	1.77	0.66
5:B:1167:GLY:H	5:B:1215:ARG:HG2	1.61	0.66
4:A:1268:LEU:HD22	10:I:48:LEU:HD11	1.77	0.66
4:A:1227:ILE:HD11	4:A:1239:ARG:HE	1.60	0.66
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.78	0.65
7:E:47:CYS:HB3	7:E:51:GLY:HA2	1.78	0.65
5:B:234:ILE:HG21	5:B:257:LYS:HB3	1.78	0.65
4:A:665:GLY:HA2	5:B:1086:PHE:CD2	2.31	0.65
11:J:28:ASP:HB2	11:J:30:LEU:HG	1.79	0.65
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.29	0.65
5:B:950:ASP:HB3	5:B:967:ARG:HG2	1.79	0.65
5:B:643:ASP:HB3	5:B:646:LEU:HA	1.79	0.65
5:B:883:LEU:HB2	5:B:932:HIS:HB3	1.79	0.65
6:C:25:VAL:HG23	6:C:228:PHE:CE1	2.32	0.65
4:A:565:ILE:HG21	9:H:46:LEU:HD13	1.78	0.65
5:B:957:ASN:ND2	5:B:961:LEU:O	2.30	0.65
4:A:856:THR:HB	4:A:865:GLN:HB2	1.79	0.65
6:C:31:ASN:OD1	6:C:34:ARG:NH1	2.29	0.65
10:I:68:LEU:HD13	10:I:84:VAL:HG11	1.79	0.65
4:A:662:PHE:HE2	4:A:746:MET:HE2	1.61	0.64
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	1.79	0.64
6:C:10:ILE:H	12:K:108:GLU:HG2	1.62	0.64
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.80	0.64
5:B:1060:ARG:NH2	6:C:199:LYS:O	2.30	0.64
9:H:125:LEU:HG	9:H:130:ARG:HH22	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:7:SER:OG	5:B:1159:ARG:NH1	2.31	0.64
4:A:635:ARG:HE	4:A:877:HIS:HA	1.62	0.64
4:A:1197:LEU:HB2	4:A:1209:MET:HE1	1.80	0.64
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.80	0.64
4:A:569:LYS:HD3	6:C:221:TYR:HB2	1.79	0.64
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.80	0.64
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.80	0.64
4:A:666:ILE:HD11	5:B:1067:ARG:HA	1.80	0.63
4:A:1386:ARG:HA	4:A:1390:ASN:HB2	1.80	0.63
4:A:1188:GLN:HA	4:A:1243:VAL:HA	1.79	0.63
10:I:78:CYS:CB	10:I:103:CYS:SG	2.85	0.63
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.30	0.63
4:A:22:PHE:HD2	5:B:1211:ASN:HA	1.64	0.63
7:E:72:PHE:HE1	7:E:157:SER:HA	1.63	0.63
4:A:88:LYS:NZ	4:A:203:SER:OG	2.32	0.63
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.81	0.63
4:A:858:ASN:HD21	4:A:860:LEU:HB2	1.63	0.63
9:H:56:THR:HB	9:H:145:ARG:HB3	1.81	0.63
5:B:1220:ARG:HH11	5:B:1221:SER:H	1.46	0.63
5:B:780:VAL:HG22	5:B:795:ILE:HG23	1.80	0.62
5:B:842:ASN:ND2	5:B:845:SER:OG	2.32	0.62
4:A:1325:THR:HA	7:E:147:HIS:HA	1.81	0.62
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.81	0.62
6:C:163:ILE:HD12	6:C:165:LYS:HB3	1.79	0.62
10:I:65:ASP:OD2	10:I:67:THR:OG1	2.13	0.62
6:C:262:LEU:HD11	12:K:87:LEU:HD23	1.81	0.62
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.82	0.62
11:J:36:LEU:HD22	11:J:41:LEU:HD11	1.80	0.62
7:E:119:SER:O	7:E:123:LEU:HG	1.99	0.62
5:B:664:THR:HG21	5:B:679:TYR:H	1.64	0.62
11:J:20:SER:O	11:J:24:LEU:HG	2.00	0.62
13:L:47:ARG:HB2	13:L:54:ARG:HA	1.82	0.61
4:A:474:VAL:HG23	4:A:521:MET:HE2	1.82	0.61
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.81	0.61
4:A:267:ALA:O	4:A:271:LYS:HG3	2.01	0.61
5:B:620:ARG:NH2	10:I:68:LEU:HD21	2.15	0.61
5:B:1166:CYS:HB3	5:B:1185:CYS:SG	2.40	0.61
9:H:38:LEU:HB2	9:H:125:LEU:HD13	1.82	0.61
4:A:344:ARG:O	5:B:1155:SER:OG	2.13	0.61
5:B:620:ARG:HH22	10:I:68:LEU:HD21	1.65	0.61
4:A:169:ASN:O	4:A:171:GLN:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:704:ALA:HA	4:A:710:LEU:HD11	1.81	0.61
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.81	0.61
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.83	0.61
4:A:467:THR:HG21	5:B:977:GLY:HA3	1.83	0.61
4:A:1444:MET:HE1	8:F:135:ARG:HD2	1.82	0.61
2:T:12:DT:H2'	2:T:13:DC:C6	2.36	0.60
4:A:208:LEU:HD13	4:A:235:ILE:HD11	1.84	0.60
4:A:23:SER:HB2	4:A:233:TRP:CE2	2.35	0.60
6:C:123:ASN:ND2	6:C:125:MET:SD	2.74	0.60
12:K:57:LEU:N	12:K:76:GLN:O	2.35	0.60
5:B:892:LYS:HD2	5:B:909:ASP:HB3	1.82	0.60
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.84	0.60
4:A:550:LEU:HD12	4:A:577:ILE:HD13	1.83	0.60
7:E:87:SER:HA	7:E:115:ASN:HB2	1.83	0.60
4:A:818:MET:HG2	5:B:514:LEU:HD23	1.84	0.60
5:B:977:GLY:HA2	5:B:989:THR:HB	1.83	0.60
6:C:249:ASP:OD1	12:K:102:LYS:NZ	2.35	0.60
4:A:566:ILE:HD11	9:H:98:TYR:HB2	1.83	0.60
4:A:813:PHE:HE2	5:B:749:LEU:HD21	1.67	0.59
9:H:125:LEU:HG	9:H:130:ARG:HH12	1.67	0.59
5:B:693:ILE:HG21	5:B:701:ILE:HD13	1.83	0.59
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.67	0.59
7:E:114:ASN:OD1	7:E:115:ASN:ND2	2.35	0.59
2:T:6:DT:H2''	2:T:7:DC:C4	2.38	0.59
4:A:106:VAL:HG13	4:A:111:GLY:HA2	1.85	0.59
4:A:559:VAL:HG13	9:H:78:SER:HA	1.85	0.59
4:A:666:ILE:O	4:A:669:THR:OG1	2.20	0.59
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.83	0.59
5:B:848:ARG:NH1	11:J:8:PHE:O	2.36	0.59
13:L:28:LYS:HG3	13:L:39:SER:HA	1.83	0.59
4:A:1282:VAL:HG22	4:A:1308:THR:HG22	1.84	0.59
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.85	0.58
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.85	0.58
7:E:32:GLN:O	7:E:36:GLU:OE1	2.20	0.58
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.85	0.58
4:A:517:ASN:O	4:A:626:ASN:ND2	2.27	0.58
5:B:354:ASP:HB3	5:B:358:LYS:HE3	1.85	0.58
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.38	0.58
1:R:2:U:H2'	1:R:3:C:C6	2.39	0.58
4:A:512:VAL:HA	4:A:519:PRO:HA	1.84	0.58
6:C:146:LYS:NZ	11:J:58:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:73:ARG:HH12	10:I:112:SER:HA	1.68	0.58
5:B:243:ALA:HB1	5:B:249:ARG:HG3	1.83	0.58
5:B:1060:ARG:NH1	6:C:200:GLU:O	2.36	0.58
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.67	0.58
4:A:1371:LEU:HG	4:A:1375:MET:HE2	1.84	0.58
5:B:862:GLN:O	5:B:914:LYS:NZ	2.37	0.58
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.68	0.58
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.86	0.58
4:A:446:ARG:HH21	4:A:480:ALA:HA	1.69	0.58
4:A:265:LYS:O	4:A:269:ILE:HD12	2.04	0.58
4:A:782:ARG:HH21	4:A:785:PRO:HA	1.69	0.58
5:B:841:MET:HB3	5:B:846:ILE:HD11	1.84	0.58
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.86	0.58
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.37	0.57
12:K:61:TYR:HB3	12:K:71:PHE:HE1	1.67	0.57
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.85	0.57
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.86	0.57
4:A:325:ILE:HD12	5:B:1210:MET:HE2	1.86	0.57
4:A:880:LYS:HD3	4:A:953:ASN:HB3	1.86	0.57
4:A:1165:GLU:OE1	4:A:1235:LYS:NZ	2.36	0.57
9:H:91:ASP:HB2	9:H:93:TYR:HD1	1.70	0.57
4:A:974:ASP:HB3	9:H:136:LYS:HE3	1.86	0.57
5:B:884:ARG:HH21	5:B:935:ARG:HB3	1.69	0.57
7:E:11:ARG:HD2	7:E:141:VAL:HG21	1.85	0.57
13:L:39:SER:N	13:L:40:LEU:HD12	2.20	0.57
2:T:27:DA:H2'	2:T:28:DT:C6	2.38	0.57
4:A:102:VAL:O	4:A:106:VAL:HG23	2.05	0.57
4:A:1290:LYS:HA	4:A:1300:LYS:HA	1.87	0.57
5:B:1065:GLN:HE21	6:C:200:GLU:HG2	1.70	0.57
7:E:173:SER:HA	7:E:177:ARG:HH12	1.69	0.57
2:T:22:DT:OP1	4:A:344:ARG:NH1	2.38	0.57
4:A:58:LEU:HB3	4:A:244:PRO:HD2	1.85	0.57
4:A:18:GLN:NE2	4:A:19:PHE:O	2.35	0.57
4:A:181:LEU:HB2	4:A:202:LEU:HD22	1.87	0.57
4:A:569:LYS:HG2	4:A:570:PRO:HD2	1.87	0.57
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.69	0.57
4:A:1192:LEU:HD11	4:A:1239:ARG:HB3	1.85	0.57
5:B:276:ILE:HG12	5:B:334:ILE:HG23	1.86	0.57
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.40	0.57
5:B:408:LEU:HD21	5:B:545:ILE:HG13	1.86	0.57
4:A:484:GLY:H	5:B:989:THR:HG23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:134:ILE:HG12	6:C:141:GLY:HA2	1.86	0.56
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.40	0.56
12:K:58:PHE:HB3	12:K:76:GLN:HB2	1.87	0.56
4:A:579:SER:HB3	4:A:611:GLN:HA	1.86	0.56
5:B:424:LEU:HD11	5:B:448:ILE:HG13	1.86	0.56
5:B:825:VAL:HG22	5:B:1010:LEU:HB3	1.87	0.56
4:A:14:VAL:HA	5:B:1218:THR:HA	1.87	0.56
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.20	0.56
5:B:346:GLU:HA	5:B:349:ILE:HD12	1.88	0.56
10:I:78:CYS:HB3	10:I:103:CYS:SG	2.45	0.56
13:L:33:GLU:HB3	13:L:51:CYS:HB2	1.87	0.56
4:A:859:SER:HB2	4:A:1422:ARG:HB3	1.87	0.56
8:F:90:ARG:HH11	8:F:90:ARG:HB3	1.70	0.56
11:J:9:SER:OG	11:J:48:ARG:NH2	2.37	0.56
4:A:1341:ILE:HD11	7:E:179:GLN:HG2	1.88	0.56
4:A:117:GLU:HG3	4:A:126:LEU:HD11	1.87	0.56
5:B:859:TYR:HE2	5:B:942:ARG:HD3	1.70	0.56
5:B:1207:LEU:HD12	5:B:1214:PRO:HG3	1.86	0.56
4:A:578:LEU:O	4:A:582:ILE:HG13	2.06	0.56
4:A:779:PHE:HB2	4:A:782:ARG:HG3	1.87	0.56
4:A:1329:THR:HG22	4:A:1331:SER:H	1.71	0.56
5:B:50:SER:HB3	5:B:408:LEU:HD12	1.87	0.56
9:H:6:PHE:CE1	9:H:8:ASP:HB2	2.41	0.56
4:A:268:ASP:HA	4:A:271:LYS:HE2	1.87	0.56
4:A:874:ASP:HB2	4:A:1058:VAL:HA	1.88	0.56
6:C:177:GLU:HB3	6:C:231:ASN:HB3	1.88	0.56
4:A:472:LEU:HD21	5:B:835:GLN:CD	2.31	0.55
4:A:752:LYS:HG2	5:B:1015:HIS:O	2.06	0.55
5:B:882:THR:HG22	5:B:934:LYS:HB2	1.87	0.55
4:A:12:ARG:HB2	5:B:1218:THR:HB	1.88	0.55
4:A:961:ARG:HE	4:A:1025:ARG:HH22	1.54	0.55
5:B:886:LYS:NZ	5:B:936:ASP:O	2.38	0.55
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.41	0.55
5:B:262:GLU:HA	5:B:267:ARG:HH21	1.70	0.55
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.87	0.55
4:A:1199:ARG:HE	4:A:1236:LEU:HD11	1.72	0.55
7:E:91:LYS:HE2	7:E:94:LYS:HD2	1.87	0.55
4:A:951:GLU:O	4:A:954:TRP:NE1	2.39	0.55
5:B:293:PRO:HB3	10:I:11:ASN:HB3	1.87	0.55
5:B:842:ASN:HD21	5:B:844:SER:HB2	1.72	0.55
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:361:LEU:HD21	5:B:377:PHE:HB3	1.89	0.55
4:A:132:LYS:NZ	4:A:1417:GLU:OE2	2.40	0.55
5:B:104:GLU:HG2	5:B:110:HIS:CE1	2.42	0.55
4:A:575:LYS:O	4:A:579:SER:OG	2.24	0.55
6:C:34:ARG:HA	6:C:37:MET:HE2	1.87	0.55
4:A:538:ASP:CG	9:H:20:TYR:HB3	2.32	0.55
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	1.88	0.55
9:H:36:CYS:HA	9:H:126:GLU:O	2.07	0.55
4:A:115:LEU:HB3	4:A:122:MET:HE3	1.88	0.55
4:A:563:PRO:HG2	4:A:566:ILE:HG12	1.89	0.55
4:A:1004:ASN:HD21	4:A:1006:ILE:HB	1.70	0.55
4:A:1168:GLU:O	4:A:1171:GLN:HG3	2.07	0.55
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.89	0.54
4:A:323:LYS:HD3	4:A:328:ARG:HG2	1.88	0.54
7:E:166:LYS:HE3	7:E:167:ARG:HG2	1.88	0.54
4:A:88:LYS:HE3	4:A:204:THR:HB	1.89	0.54
4:A:782:ARG:NH2	5:B:701:ILE:O	2.41	0.54
4:A:1194:ARG:HE	4:A:1237:ILE:HG13	1.73	0.54
5:B:977:GLY:H	5:B:990:ILE:HB	1.71	0.54
6:C:256:ALA:HA	6:C:259:LEU:HD12	1.90	0.54
4:A:304:MET:O	4:A:324:SER:OG	2.24	0.54
4:A:244:PRO:HA	4:A:247:ARG:HG2	1.87	0.54
4:A:1051:ALA:O	4:A:1055:ARG:HG2	2.07	0.54
11:J:4:PRO:HG2	11:J:49:MET:HG3	1.88	0.54
4:A:380:VAL:HG12	4:A:388:LEU:HD12	1.90	0.54
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.90	0.54
4:A:1262:LYS:HE3	4:A:1263:ILE:HG12	1.90	0.54
3:N:8:DG:H2"	3:N:9:DA:C8	2.42	0.54
5:B:845:SER:HB3	11:J:8:PHE:HB3	1.88	0.54
7:E:79:TRP:O	7:E:109:ILE:N	2.41	0.54
9:H:58:THR:HB	9:H:143:LEU:HB2	1.88	0.54
4:A:34:LYS:HB2	4:A:36:ARG:HD3	1.90	0.54
4:A:711:ARG:HE	10:I:97:MET:HG2	1.73	0.54
4:A:1336:MET:HE2	4:A:1381:LEU:HB2	1.90	0.54
5:B:520:GLY:HA2	5:B:748:ILE:HG22	1.90	0.54
7:E:78:LEU:HD21	7:E:109:ILE:HD12	1.90	0.54
5:B:186:GLU:HG3	5:B:196:PRO:HB3	1.89	0.54
5:B:512:ARG:HH21	5:B:532:ALA:HA	1.73	0.53
6:C:167:HIS:CG	13:L:70:ARG:HG2	2.43	0.53
5:B:349:ILE:HG22	5:B:353:LYS:HE3	1.90	0.53
5:B:800:GLN:HB3	11:J:52:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:863:GLU:HG2	5:B:872:GLU:HB3	1.89	0.53
4:A:592:ASP:N	4:A:595:THR:OG1	2.40	0.53
4:A:1425:SER:HA	5:B:1135:ARG:HH12	1.73	0.53
5:B:896:ASP:OD1	5:B:896:ASP:N	2.40	0.53
5:B:956:THR:OG1	5:B:960:GLY:O	2.26	0.53
12:K:7:PHE:HA	12:K:10:PHE:CE1	2.44	0.53
4:A:336:ILE:HA	4:A:340:LEU:HD12	1.90	0.53
13:L:38:LEU:HD21	13:L:48:CYS:HB3	1.89	0.53
4:A:777:PHE:HA	4:A:783:THR:HA	1.91	0.53
4:A:1011:GLN:O	4:A:1015:VAL:HG22	2.09	0.53
4:A:1274:ARG:HG2	4:A:1274:ARG:HH11	1.74	0.53
5:B:1104:HIS:HB2	5:B:1122:ARG:HG2	1.89	0.53
6:C:33:LEU:HA	6:C:36:VAL:HG12	1.91	0.53
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.42	0.53
6:C:97:VAL:HG21	6:C:129:ILE:HG22	1.90	0.53
10:I:87:GLN:HE22	10:I:97:MET:HE3	1.74	0.53
4:A:42:ASP:N	4:A:46:THR:O	2.42	0.53
4:A:99:ILE:HA	4:A:102:VAL:HG12	1.91	0.53
4:A:116:ASP:OD1	4:A:164:ARG:NE	2.42	0.53
4:A:662:PHE:O	5:B:828:ALA:HA	2.09	0.53
4:A:761:MET:HE2	5:B:1021:MET:HA	1.91	0.53
5:B:882:THR:OG1	5:B:885:MET:SD	2.63	0.53
4:A:339:ASN:O	4:A:343:LYS:HG2	2.09	0.53
4:A:388:LEU:HD13	4:A:432:VAL:HB	1.91	0.53
4:A:1282:VAL:HA	4:A:1307:GLU:O	2.09	0.53
6:C:7:GLN:HB3	6:C:9:LYS:HZ3	1.73	0.53
4:A:122:MET:HE1	4:A:138:ILE:HG12	1.91	0.53
5:B:1060:ARG:HH12	6:C:200:GLU:C	2.17	0.53
6:C:8:VAL:HG22	6:C:22:LEU:HD12	1.91	0.53
4:A:1000:LEU:HD22	4:A:1007:ILE:HD12	1.90	0.52
5:B:771:SER:O	5:B:775:LYS:HG2	2.09	0.52
5:B:1004:GLU:HB2	5:B:1006:ILE:HG12	1.90	0.52
9:H:96:VAL:HG22	9:H:143:LEU:HG	1.91	0.52
4:A:276:LEU:HD11	4:A:293:GLU:HG3	1.91	0.52
4:A:1027:ALA:O	4:A:1031:VAL:N	2.30	0.52
6:C:6:PRO:HB2	12:K:101:LEU:HB2	1.89	0.52
6:C:76:ASP:HB2	6:C:129:ILE:HG12	1.92	0.52
8:F:85:MET:HE1	8:F:148:VAL:HG13	1.90	0.52
9:H:135:LEU:HB3	9:H:137:GLN:HG2	1.90	0.52
4:A:882:SER:H	4:A:961:ARG:NH2	2.06	0.52
5:B:390:LEU:HD13	5:B:392:ARG:HH21	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:484:GLY:HA3	5:B:979:LYS:HE2	1.91	0.52
5:B:519:TRP:O	5:B:635:ARG:NH1	2.42	0.52
4:A:579:SER:OG	4:A:612:ILE:HG22	2.10	0.52
4:A:1229:SER:HB3	4:A:1237:ILE:H	1.75	0.52
4:A:490:HIS:HB3	5:B:1150:ARG:CZ	2.40	0.52
5:B:311:LEU:O	5:B:315:LYS:HG3	2.10	0.52
5:B:796:LEU:HD23	5:B:799:PRO:HA	1.90	0.52
5:B:806:THR:HG23	5:B:1045:SER:HA	1.90	0.52
5:B:1116:ARG:HG3	5:B:1198:TYR:CD1	2.45	0.52
4:A:387:ARG:O	4:A:391:LEU:HG	2.10	0.52
4:A:527:THR:O	4:A:653:VAL:HG11	2.09	0.52
4:A:1166:ASP:CG	4:A:1239:ARG:HD2	2.35	0.52
4:A:75:ASN:OD1	5:B:1116:ARG:NH1	2.43	0.52
4:A:308:ILE:HB	4:A:312:PRO:HD2	1.91	0.52
4:A:802:ASN:OD1	5:B:729:ILE:N	2.41	0.52
4:A:1436:ILE:HB	5:B:1144:ALA:HB2	1.91	0.52
5:B:997:GLU:O	6:C:34:ARG:NH2	2.43	0.52
9:H:99:GLY:HA3	9:H:118:PHE:HA	1.91	0.52
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.92	0.52
5:B:1135:ARG:O	5:B:1139:ILE:HG12	2.10	0.51
6:C:177:GLU:O	6:C:230:MET:HA	2.10	0.51
4:A:633:VAL:HG21	4:A:645:LEU:HD22	1.92	0.51
4:A:1004:ASN:ND2	4:A:1007:ILE:HG12	2.25	0.51
5:B:414:ALA:O	5:B:418:LYS:HG3	2.10	0.51
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.92	0.51
5:B:1187:ASN:HB2	5:B:1190:ASP:HB3	1.92	0.51
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.93	0.51
5:B:519:TRP:HD1	5:B:635:ARG:NH1	2.07	0.51
6:C:55:THR:OG1	6:C:152:GLU:N	2.43	0.51
7:E:12:LEU:HD21	7:E:55:ARG:NH2	2.25	0.51
4:A:1194:ARG:HG3	4:A:1237:ILE:HG23	1.92	0.51
5:B:803:LEU:HD13	5:B:1032:SER:HB3	1.93	0.51
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.75	0.51
4:A:890:ASP:HA	4:A:940:ARG:HH12	1.76	0.51
9:H:15:VAL:HG12	9:H:26:ILE:HG23	1.92	0.51
4:A:306:ASN:H	4:A:324:SER:HB2	1.75	0.51
4:A:507:VAL:HG13	4:A:521:MET:HE1	1.93	0.51
4:A:1099:PRO:O	4:A:1103:GLU:HG3	2.11	0.51
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.93	0.51
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.93	0.51
2:T:12:DT:H2''	2:T:13:DC:H5'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:627:PHE:O	5:B:632:ARG:NH2	2.43	0.51
4:A:800:VAL:HG22	4:A:812:GLU:HG2	1.91	0.51
4:A:898:ARG:NH1	4:A:899:VAL:O	2.43	0.51
4:A:1342:GLU:OE1	7:E:200:ARG:NH2	2.44	0.51
4:A:1345:ARG:HE	7:E:200:ARG:NH2	2.08	0.51
5:B:121:ASN:HD22	5:B:860:MET:HE3	1.76	0.51
6:C:183:TRP:CG	6:C:213:PRO:HD3	2.46	0.51
3:N:7:DA:H2''	3:N:8:DG:H5'	1.91	0.51
4:A:206:GLU:O	4:A:210:ILE:HG12	2.11	0.51
6:C:108:GLU:HA	6:C:149:LYS:HB2	1.91	0.51
7:E:190:LEU:HD21	7:E:196:VAL:HB	1.91	0.51
9:H:47:PHE:HB3	9:H:95:TYR:CD2	2.46	0.51
12:K:21:ILE:HD13	12:K:84:LYS:HE2	1.92	0.51
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.92	0.51
4:A:873:MET:HE3	4:A:1056:SER:HB3	1.92	0.51
5:B:40:GLU:CD	5:B:681:TRP:HB3	2.36	0.51
8:F:97:ARG:O	8:F:100:GLN:HG2	2.11	0.51
4:A:81:PHE:CD2	4:A:240:PRO:HB2	2.46	0.50
4:A:523:ILE:HG23	4:A:527:THR:HB	1.92	0.50
4:A:901:LEU:HD13	4:A:919:ILE:HG23	1.92	0.50
5:B:228:LYS:HG3	5:B:234:ILE:HG13	1.92	0.50
5:B:763:GLN:HG3	5:B:765:PRO:HD2	1.93	0.50
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.45	0.50
12:K:113:THR:O	12:K:114:LEU:HD22	2.11	0.50
4:A:350:ARG:HD2	5:B:1128:LEU:HD11	1.92	0.50
6:C:234:SER:HB2	6:C:240:VAL:HG12	1.93	0.50
7:E:42:PHE:O	7:E:46:TYR:HB2	2.11	0.50
10:I:54:GLU:HB2	10:I:100:PHE:CE2	2.46	0.50
4:A:50:ILE:HG23	4:A:52:GLY:H	1.76	0.50
4:A:368:LYS:NZ	4:A:399:HIS:H	2.09	0.50
4:A:551:TYR:HB2	12:K:58:PHE:HZ	1.77	0.50
4:A:1134:ILE:O	4:A:1138:ILE:HG22	2.11	0.50
5:B:1147:LEU:O	5:B:1151:LEU:HB3	2.11	0.50
9:H:125:LEU:HG	9:H:130:ARG:NH2	2.26	0.50
2:T:9:DC:H2''	2:T:10:DT:H2'	1.94	0.50
4:A:782:ARG:NH2	4:A:785:PRO:O	2.44	0.50
5:B:364:ILE:HG12	5:B:585:VAL:HG22	1.94	0.50
2:T:20:DC:H2''	2:T:21:DC:H6	1.77	0.50
5:B:660:LYS:O	5:B:664:THR:HG23	2.11	0.50
5:B:809:MET:HA	5:B:812:LEU:HB2	1.93	0.50
5:B:859:TYR:OH	5:B:945:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:259:LEU:O	6:C:263:THR:HG23	2.12	0.50
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.94	0.50
4:A:180:LYS:HD2	4:A:201:VAL:HG13	1.93	0.50
4:A:336:ILE:HD12	5:B:1203:LEU:HD22	1.93	0.50
4:A:565:ILE:HG13	9:H:97:MET:HG2	1.93	0.50
4:A:742:ASN:HA	4:A:745:GLN:HG3	1.92	0.50
5:B:1054:GLY:HA2	5:B:1057:LYS:HD2	1.92	0.50
12:K:10:PHE:CD2	12:K:11:LEU:HD13	2.46	0.50
12:K:29:ASN:OD1	12:K:77:THR:OG1	2.21	0.50
4:A:218:ASP:O	4:A:222:LEU:HG	2.12	0.50
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.76	0.50
7:E:52:ARG:NE	7:E:53:PRO:HD2	2.26	0.50
9:H:38:LEU:HA	9:H:124:ARG:O	2.12	0.50
4:A:761:MET:HA	4:A:804:TYR:HB2	1.93	0.50
4:A:1115:SER:HA	4:A:1308:THR:O	2.12	0.50
5:B:350:GLN:HA	5:B:353:LYS:HD2	1.94	0.50
5:B:648:HIS:NE2	5:B:710:LEU:O	2.43	0.50
10:I:69:PRO:HB2	10:I:85:PHE:CE1	2.47	0.50
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.93	0.50
6:C:25:VAL:HG23	6:C:228:PHE:HE1	1.73	0.50
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.46	0.50
4:A:684:ALA:O	4:A:688:LYS:HD3	2.12	0.49
6:C:245:VAL:HA	6:C:248:ILE:HD12	1.93	0.49
12:K:47:ARG:HD3	12:K:61:TYR:CD1	2.47	0.49
4:A:340:LEU:HD22	4:A:1429:ILE:HA	1.93	0.49
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.93	0.49
4:A:1421:CYS:O	4:A:1427:ASN:ND2	2.44	0.49
11:J:45:CYS:HA	11:J:48:ARG:HE	1.77	0.49
4:A:332:LYS:HE2	4:A:337:ARG:NH2	2.27	0.49
4:A:614:PHE:HB2	9:H:122:LEU:HD11	1.94	0.49
4:A:687:LYS:NZ	4:A:795:GLU:OE1	2.42	0.49
4:A:1199:ARG:NE	4:A:1236:LEU:HD11	2.27	0.49
4:A:1346:ALA:O	4:A:1350:LYS:HG3	2.12	0.49
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.78	0.49
5:B:211:VAL:HG21	5:B:483:LEU:HD13	1.94	0.49
5:B:221:ASN:HB3	5:B:584:GLY:HA3	1.93	0.49
5:B:883:LEU:HG	5:B:884:ARG:HG3	1.94	0.49
9:H:39:THR:O	9:H:123:MET:HA	2.13	0.49
9:H:106:GLU:HB2	9:H:112:ILE:HD12	1.93	0.49
12:K:21:ILE:HG23	12:K:31:VAL:HG21	1.94	0.49
4:A:464:PRO:O	12:K:2:ASN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:261:ARG:HB2	5:B:264:SER:HB3	1.93	0.49
5:B:641:GLU:HG3	5:B:652:LYS:HD2	1.94	0.49
4:A:443:LEU:HD12	4:A:501:LEU:HD11	1.94	0.49
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.95	0.49
5:B:99:LYS:NZ	5:B:183:GLU:OE1	2.46	0.49
6:C:148:ARG:HG3	6:C:149:LYS:N	2.28	0.49
4:A:248:PRO:HD3	5:B:1114:LEU:HD22	1.95	0.49
4:A:786:HIS:NE2	5:B:742:GLU:HG3	2.27	0.49
4:A:990:VAL:O	4:A:994:GLN:HG3	2.12	0.49
4:A:1129:GLU:CD	4:A:1129:GLU:H	2.21	0.49
5:B:850:LEU:HB2	11:J:8:PHE:CG	2.47	0.49
4:A:225:ASN:HB3	4:A:228:PHE:HB2	1.94	0.49
4:A:434:ARG:HH12	4:A:436:ILE:HA	1.77	0.49
4:A:568:PRO:HB2	9:H:46:LEU:HD22	1.95	0.49
4:A:729:ALA:HA	4:A:732:LEU:HD12	1.95	0.49
5:B:70:ILE:HA	5:B:88:TYR:O	2.13	0.49
5:B:551:PRO:O	5:B:555:ILE:HG12	2.13	0.49
5:B:616:ILE:HG12	5:B:697:GLU:HA	1.95	0.49
5:B:807:ARG:O	5:B:810:GLU:HG2	2.13	0.49
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.45	0.49
6:C:22:LEU:HD11	12:K:101:LEU:HD11	1.93	0.49
4:A:392:VAL:HG11	4:A:424:ILE:HD11	1.95	0.49
4:A:1397:LEU:HB3	4:A:1429:ILE:HD13	1.94	0.49
1:R:4:G:H2'	1:R:5:A:C8	2.48	0.49
4:A:909:ASP:HB3	4:A:912:LEU:HD13	1.94	0.49
6:C:7:GLN:HB3	6:C:9:LYS:NZ	2.28	0.49
10:I:75:CYS:HB3	10:I:110:PHE:CD1	2.48	0.49
4:A:210:ILE:O	4:A:214:ILE:HG13	2.13	0.49
4:A:534:LEU:HA	4:A:539:THR:HG21	1.94	0.49
4:A:781:ASP:O	4:A:790:ASP:N	2.43	0.49
7:E:91:LYS:O	7:E:95:THR:HG23	2.13	0.49
9:H:105:GLU:HG2	9:H:115:TYR:HE1	1.77	0.49
4:A:942:PHE:O	4:A:946:VAL:HG23	2.12	0.48
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.44	0.48
8:F:74:ILE:HG21	8:F:144:GLU:OE2	2.13	0.48
4:A:211:PHE:HA	4:A:214:ILE:HD12	1.96	0.48
5:B:51:PHE:O	5:B:55:VAL:HG23	2.13	0.48
5:B:114:PRO:O	5:B:118:ARG:HG3	2.12	0.48
5:B:120:ARG:NE	5:B:956:THR:O	2.46	0.48
5:B:544:CYS:HB2	5:B:634:TYR:CE2	2.47	0.48
5:B:618:ASP:HB3	5:B:621:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:701:ILE:HB	5:B:739:THR:OG1	2.12	0.48
6:C:46:ILE:HA	6:C:159:ALA:HA	1.95	0.48
4:A:100:LYS:HD3	4:A:100:LYS:C	2.38	0.48
4:A:167:CYS:SG	4:A:168:GLY:N	2.87	0.48
4:A:727:ASP:O	4:A:731:ARG:HG2	2.13	0.48
4:A:794:PRO:HB2	4:A:799:PHE:HB3	1.94	0.48
5:B:282:ILE:HA	5:B:285:ILE:HD12	1.93	0.48
4:A:973:ILE:HG22	4:A:975:HIS:H	1.78	0.48
4:A:1209:MET:HE3	4:A:1236:LEU:HD22	1.94	0.48
5:B:757:PRO:HG2	5:B:984:HIS:CE1	2.48	0.48
7:E:118:PRO:HA	7:E:121:MET:HG2	1.94	0.48
11:J:8:PHE:H	11:J:49:MET:HE3	1.78	0.48
4:A:96:ILE:HA	4:A:99:ILE:HB	1.95	0.48
4:A:356:ASP:CG	12:K:65:HIS:HE2	2.22	0.48
4:A:954:TRP:HB3	7:E:203:GLU:OE2	2.13	0.48
4:A:1221:LYS:HD2	4:A:1221:LYS:O	2.13	0.48
5:B:612:GLU:O	5:B:632:ARG:NH1	2.43	0.48
5:B:635:ARG:HE	5:B:637:LEU:HD11	1.78	0.48
5:B:780:VAL:HB	5:B:817:LEU:HD11	1.96	0.48
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.95	0.48
4:A:148:CYS:O	4:A:168:GLY:HA2	2.13	0.48
4:A:180:LYS:NZ	4:A:202:LEU:O	2.32	0.48
5:B:598:GLU:OE2	5:B:601:ARG:NH2	2.47	0.48
5:B:620:ARG:HG2	10:I:62:ILE:HD11	1.95	0.48
5:B:992:ILE:HG13	12:K:67:PHE:HE1	1.79	0.48
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.60	0.48
8:F:125:LEU:HD11	8:F:153:VAL:HG21	1.94	0.48
4:A:248:PRO:HD2	4:A:260:ASP:OD2	2.14	0.48
4:A:442:VAL:O	4:A:457:ALA:HA	2.13	0.48
4:A:594:GLY:H	4:A:601:LYS:HZ3	1.60	0.48
5:B:212:LEU:HD21	5:B:466:TRP:CH2	2.49	0.48
6:C:36:VAL:HG23	6:C:40:GLU:HG3	1.94	0.48
6:C:239:PRO:O	6:C:243:VAL:HG23	2.13	0.48
9:H:26:ILE:O	9:H:39:THR:HA	2.14	0.48
9:H:125:LEU:HB3	9:H:130:ARG:HH12	1.79	0.48
11:J:58:GLU:HA	11:J:61:LEU:HD12	1.96	0.48
1:R:3:C:H2'	1:R:4:G:C8	2.49	0.48
4:A:269:ILE:HG13	4:A:299:HIS:HB3	1.96	0.48
4:A:767:GLN:HA	4:A:799:PHE:HA	1.95	0.48
5:B:857:ARG:HG2	5:B:859:TYR:CZ	2.49	0.48
5:B:1033:LYS:O	5:B:1037:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1072:MET:HG3	5:B:1085:ILE:HB	1.95	0.48
4:A:913:LEU:HG	4:A:1032:LEU:HD13	1.95	0.48
5:B:1163:CYS:HB2	5:B:1187:ASN:HD21	1.78	0.48
7:E:88:VAL:HG11	7:E:112:TYR:CD2	2.49	0.48
4:A:244:PRO:HD3	4:A:247:ARG:HH21	1.79	0.48
4:A:836:TYR:O	4:A:840:ARG:HG3	2.14	0.48
5:B:400:HIS:O	5:B:404:LYS:HG2	2.13	0.48
5:B:710:LEU:HD21	5:B:738:PHE:HB2	1.95	0.48
7:E:31:THR:HB	7:E:34:GLU:H	1.79	0.48
4:A:277:GLU:O	4:A:280:GLU:HG3	2.13	0.47
4:A:513:SER:OG	4:A:515:GLN:O	2.19	0.47
4:A:665:GLY:HA2	5:B:1086:PHE:HD2	1.78	0.47
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.96	0.47
4:A:975:HIS:HA	4:A:1036:ARG:HB2	1.96	0.47
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.95	0.47
6:C:17:ASN:HA	6:C:232:VAL:O	2.14	0.47
6:C:62:PHE:CE1	6:C:66:ARG:HD2	2.49	0.47
8:F:90:ARG:HB3	8:F:90:ARG:NH1	2.29	0.47
2:T:5:DC:H5"	2:T:5:DC:H6	1.79	0.47
4:A:76:GLU:CD	5:B:1159:ARG:HH21	2.22	0.47
4:A:1143:LEU:HG	4:A:1268:LEU:HD23	1.95	0.47
4:A:1333:ILE:O	4:A:1337:GLU:HG2	2.14	0.47
5:B:287:ARG:NH1	5:B:321:GLY:O	2.47	0.47
8:F:109:VAL:HG21	8:F:123:LYS:HG3	1.96	0.47
2:T:6:DT:H2"	2:T:7:DC:C5	2.49	0.47
2:T:12:DT:O2	3:N:8:DG:N2	2.47	0.47
4:A:548:ASN:HD21	12:K:47:ARG:HD2	1.78	0.47
4:A:1037:LEU:HD23	4:A:1042:PHE:HB2	1.96	0.47
5:B:36:ALA:HA	5:B:39:ARG:HD2	1.94	0.47
4:A:18:GLN:HB2	4:A:1418:LEU:HD12	1.97	0.47
4:A:463:ILE:HG21	4:A:469:ARG:HG3	1.96	0.47
4:A:515:GLN:NE2	4:A:1071:SER:OG	2.47	0.47
4:A:674:PRO:HA	4:A:677:ARG:NH1	2.29	0.47
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	1.96	0.47
5:B:542:MET:HE3	5:B:743:ILE:HD12	1.97	0.47
5:B:954:VAL:HA	5:B:964:VAL:HG12	1.96	0.47
5:B:1097:HIS:HB3	5:B:1102:LYS:HE3	1.96	0.47
6:C:255:VAL:HG22	12:K:42:LEU:HD11	1.97	0.47
4:A:662:PHE:HZ	4:A:745:GLN:HB2	1.80	0.47
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.96	0.47
4:A:915:SER:O	4:A:919:ILE:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:586:TRP:NE1	5:B:588:GLY:O	2.47	0.47
5:B:757:PRO:HD3	5:B:983:ARG:HD2	1.96	0.47
5:B:760:ASP:OD1	5:B:760:ASP:N	2.48	0.47
5:B:1063:GLY:O	6:C:202:PRO:HG3	2.15	0.47
7:E:16:PHE:CD2	7:E:20:LYS:HE2	2.49	0.47
7:E:55:ARG:HB3	7:E:82:PHE:HB3	1.96	0.47
4:A:7:SER:OG	5:B:1161:HIS:HE1	1.98	0.47
4:A:434:ARG:HH21	4:A:498:ARG:HH21	1.62	0.47
4:A:517:ASN:HB2	4:A:878:ILE:O	2.14	0.47
4:A:537:ARG:NH1	9:H:41:ASP:OD2	2.47	0.47
4:A:606:LEU:HG	4:A:613:ILE:HD13	1.97	0.47
4:A:1397:LEU:HB2	4:A:1426:GLU:HG2	1.97	0.47
5:B:483:LEU:HD12	5:B:484:ASN:H	1.80	0.47
5:B:566:LEU:HG	5:B:587:HIS:HA	1.96	0.47
5:B:876:LYS:HB2	5:B:894:ASP:O	2.14	0.47
6:C:104:PHE:HD1	6:C:152:GLU:HB3	1.80	0.47
6:C:258:ILE:HD12	12:K:19:LEU:HD21	1.96	0.47
4:A:592:ASP:N	4:A:592:ASP:OD1	2.47	0.47
4:A:783:THR:O	5:B:516:ASN:ND2	2.44	0.47
4:A:916:GLY:HA2	4:A:919:ILE:HB	1.95	0.47
5:B:101:MET:HA	5:B:112:LEU:H	1.78	0.47
5:B:121:ASN:ND2	5:B:860:MET:HE3	2.29	0.47
5:B:293:PRO:HB2	5:B:296:GLU:HB2	1.97	0.47
5:B:728:ARG:NE	5:B:1049:ASP:OD1	2.45	0.47
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.96	0.47
7:E:64:PRO:HG3	7:E:76:GLY:HA2	1.97	0.47
8:F:100:GLN:HA	8:F:103:MET:HE2	1.96	0.47
11:J:64:ASN:N	11:J:65:PRO:HD2	2.29	0.47
13:L:30:ILE:HG13	13:L:37:LYS:HA	1.97	0.47
4:A:30:ILE:O	5:B:1183:LYS:HD3	2.14	0.47
4:A:106:VAL:HG12	4:A:107:CYS:O	2.14	0.47
10:I:10:CYS:SG	10:I:31:THR:HB	2.55	0.47
4:A:14:VAL:HG11	5:B:1216:LEU:HB3	1.97	0.47
4:A:57:ARG:CB	4:A:68:GLN:HB3	2.44	0.47
4:A:181:LEU:O	4:A:202:LEU:HB2	2.15	0.47
4:A:994:GLN:OE1	4:A:1023:ARG:NE	2.47	0.47
5:B:223:VAL:HG21	5:B:381:MET:HG2	1.97	0.47
6:C:60:ASP:HB2	13:L:67:PHE:HE2	1.80	0.47
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.49	0.47
4:A:86:LEU:HD13	4:A:296:LEU:HD11	1.97	0.47
4:A:115:LEU:HD11	4:A:119:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:691:LEU:O	4:A:695:LYS:HG3	2.15	0.47
4:A:900:ASP:H	4:A:906:HIS:HB3	1.80	0.47
5:B:1099:VAL:O	5:B:1103:ILE:HG13	2.15	0.47
6:C:11:ARG:N	6:C:19:ASP:O	2.48	0.47
4:A:353:ILE:HG21	4:A:487:MET:HB2	1.96	0.46
4:A:567:LYS:HE3	9:H:89:LEU:HD12	1.98	0.46
4:A:1207:LEU:HD11	4:A:1273:LEU:HB2	1.96	0.46
4:A:1376:THR:HG22	7:E:212:ARG:NH2	2.30	0.46
5:B:100:PRO:O	5:B:180:TYR:OH	2.28	0.46
9:H:125:LEU:HG	9:H:130:ARG:NH1	2.30	0.46
12:K:81:TYR:CE2	12:K:86:ALA:HB2	2.50	0.46
4:A:342:GLY:O	5:B:1129:ARG:NH1	2.47	0.46
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.15	0.46
5:B:680:THR:HG1	5:B:683:SER:H	1.63	0.46
6:C:26:ASP:OD1	6:C:26:ASP:N	2.45	0.46
6:C:108:GLU:HG2	6:C:149:LYS:HD2	1.96	0.46
4:A:981:LEU:HD22	4:A:986:ILE:HG13	1.96	0.46
4:A:1074:GLU:O	4:A:1077:THR:OG1	2.28	0.46
11:J:34:THR:O	11:J:38:ARG:HG2	2.16	0.46
4:A:551:TYR:OH	12:K:72:LYS:HG2	2.14	0.46
6:C:148:ARG:HH12	11:J:64:ASN:HA	1.80	0.46
4:A:994:GLN:HE22	4:A:1023:ARG:HH21	1.63	0.46
4:A:1111:MET:HB3	4:A:1114:PRO:HG3	1.97	0.46
10:I:78:CYS:HB2	10:I:105:SER:OG	2.15	0.46
4:A:478:TYR:CD2	4:A:487:MET:HE1	2.50	0.46
6:C:148:ARG:HD3	11:J:61:LEU:O	2.16	0.46
4:A:781:ASP:HB2	4:A:789:LYS:HG2	1.98	0.46
4:A:815:PHE:HD1	4:A:818:MET:HE3	1.81	0.46
4:A:1148:ILE:N	4:A:1196:GLU:O	2.47	0.46
4:A:1215:ARG:O	4:A:1219:THR:HG23	2.16	0.46
4:A:1377:THR:HA	7:E:212:ARG:HH12	1.81	0.46
5:B:464:GLY:HA2	5:B:480:SER:HB3	1.97	0.46
5:B:579:ARG:HH11	5:B:623:GLU:HG3	1.80	0.46
6:C:37:MET:HA	6:C:41:ILE:HD11	1.96	0.46
8:F:82:THR:HG22	8:F:84:TYR:H	1.80	0.46
4:A:851:HIS:ND1	8:F:139:PRO:HG3	2.31	0.46
5:B:258:LEU:HD13	5:B:269:ILE:HG12	1.98	0.46
5:B:954:VAL:O	13:L:56:LEU:N	2.47	0.46
2:T:26:DG:H4'	5:B:482:VAL:HG21	1.98	0.46
4:A:378:GLU:OE1	4:A:434:ARG:HD3	2.16	0.46
5:B:1168:LEU:HB2	5:B:1170:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1:A:H2'	1:R:2:U:C6	2.52	0.45
3:N:3:DA:H4'	3:N:4:DG:H5'	1.98	0.45
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.16	0.45
5:B:90:ILE:HA	5:B:133:LYS:O	2.16	0.45
5:B:262:GLU:HA	5:B:267:ARG:NH2	2.31	0.45
5:B:563:MET:HG3	5:B:588:GLY:HA3	1.97	0.45
6:C:147:LEU:HD23	6:C:147:LEU:HA	1.68	0.45
9:H:47:PHE:HB3	9:H:95:TYR:HD2	1.78	0.45
4:A:107:CYS:HB3	4:A:110:CYS:O	2.15	0.45
4:A:325:ILE:HD12	5:B:1210:MET:HG3	1.99	0.45
4:A:1135:ARG:HH21	4:A:1284:MET:HG3	1.80	0.45
5:B:181:LEU:HD11	5:B:194:GLU:HG3	1.98	0.45
5:B:255:GLN:O	5:B:257:LYS:NZ	2.50	0.45
5:B:899:ILE:HD12	5:B:899:ILE:HA	1.87	0.45
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	1.98	0.45
4:A:528:LEU:O	4:A:531:ILE:HG22	2.16	0.45
4:A:722:LEU:HD13	4:A:799:PHE:HB2	1.97	0.45
4:A:806:ARG:HH12	5:B:729:ILE:HG12	1.80	0.45
10:I:18:GLU:OE1	10:I:20:LYS:NZ	2.32	0.45
4:A:53:LEU:HA	4:A:53:LEU:HD23	1.68	0.45
5:B:292:ILE:HD11	5:B:327:ARG:HB2	1.98	0.45
8:F:116:ASP:HB3	8:F:119:ARG:HG2	1.98	0.45
5:B:333:PHE:O	5:B:334:ILE:HG13	2.16	0.45
10:I:78:CYS:HB3	10:I:106:CYS:HB3	1.98	0.45
3:N:6:DG:C6	3:N:7:DA:C6	3.05	0.45
4:A:360:GLU:OE2	4:A:651:LYS:NZ	2.46	0.45
5:B:461:LEU:HD13	5:B:466:TRP:HH2	1.81	0.45
12:K:37:LYS:HA	12:K:37:LYS:HD3	1.80	0.45
2:T:22:DT:H2'	2:T:23:DC:C6	2.52	0.45
4:A:446:ARG:HE	4:A:480:ALA:HB2	1.81	0.45
5:B:122:LEU:HD23	5:B:122:LEU:HA	1.79	0.45
6:C:205:LYS:O	6:C:208:GLU:HG2	2.17	0.45
4:A:506:ALA:HB3	4:A:509:LEU:HG	1.99	0.45
5:B:378:LEU:HD22	5:B:382:ILE:HD11	1.99	0.45
9:H:27:GLU:HG3	9:H:39:THR:HG23	1.99	0.45
10:I:75:CYS:SG	10:I:78:CYS:N	2.68	0.45
4:A:25:GLU:HA	4:A:28:ARG:HE	1.82	0.45
4:A:326:ARG:HG3	4:A:1406:VAL:HG21	1.98	0.45
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.99	0.45
4:A:666:ILE:HD13	5:B:1030:LEU:HD22	1.98	0.45
4:A:675:THR:O	4:A:679:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1128:GLN:HG2	4:A:1304:TRP:HE1	1.82	0.45
5:B:360:PHE:CE2	5:B:374:LYS:HB3	2.51	0.45
6:C:10:ILE:HA	6:C:20:PHE:HA	1.98	0.45
6:C:10:ILE:HD11	12:K:105:PHE:CE1	2.52	0.45
12:K:55:LYS:HD2	12:K:81:TYR:CG	2.52	0.45
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.98	0.45
1:R:3:C:H2'	1:R:4:G:H8	1.82	0.44
3:N:2:DC:H1'	3:N:3:DA:C8	2.51	0.44
4:A:951:GLU:OE2	4:A:953:ASN:ND2	2.50	0.44
5:B:213:ILE:HG23	5:B:497:ARG:HG2	1.99	0.44
5:B:373:ARG:H	5:B:373:ARG:HG3	1.58	0.44
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.98	0.44
5:B:858:SER:HA	5:B:966:VAL:O	2.17	0.44
6:C:166:GLU:HB2	12:K:10:PHE:CE1	2.52	0.44
7:E:128:PRO:HG2	7:E:129:PRO:HD3	1.99	0.44
4:A:340:LEU:HD21	5:B:1200:ALA:HB2	1.99	0.44
4:A:420:ARG:NH2	4:A:423:ASP:OD2	2.50	0.44
4:A:993:LEU:HD11	4:A:1050:GLU:HB2	1.99	0.44
4:A:1135:ARG:NH2	4:A:1284:MET:HG3	2.32	0.44
4:A:1438:THR:HA	8:F:88:TYR:HB3	1.99	0.44
5:B:281:PRO:HD2	5:B:284:ILE:HD12	2.00	0.44
5:B:470:LYS:HB2	5:B:473:MET:H	1.83	0.44
5:B:487:THR:OG1	5:B:777:ALA:O	2.35	0.44
5:B:706:GLN:HG2	5:B:708:GLU:H	1.81	0.44
9:H:142:LEU:HD22	9:H:144:ILE:HD11	1.99	0.44
4:A:125:ALA:HB1	4:A:138:ILE:HG13	1.99	0.44
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.98	0.44
4:A:756:ILE:O	4:A:760:GLN:HG3	2.17	0.44
4:A:820:GLY:O	4:A:824:LEU:HG	2.18	0.44
5:B:527:THR:OG1	5:B:534:GLY:N	2.50	0.44
6:C:62:PHE:O	6:C:66:ARG:HG3	2.18	0.44
7:E:175:LEU:HD23	7:E:213:ILE:HB	2.00	0.44
8:F:71:GLU:O	8:F:71:GLU:HG2	2.17	0.44
9:H:118:PHE:O	9:H:121:LEU:HB2	2.17	0.44
4:A:230:ARG:HB3	4:A:233:TRP:CG	2.52	0.44
4:A:675:THR:HG21	4:A:736:ASN:HB2	1.99	0.44
5:B:384:ARG:HA	5:B:387:LEU:HD12	2.00	0.44
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.17	0.44
5:B:1008:PRO:HD3	5:B:1087:PHE:HE1	1.82	0.44
9:H:116:TYR:HB3	9:H:118:PHE:HE1	1.82	0.44
4:A:452:LYS:HB2	5:B:1141:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:932:GLU:O	4:A:936:LEU:HG	2.17	0.44
4:A:1035:TYR:CE1	4:A:1037:LEU:HD22	2.52	0.44
5:B:488:TYR:O	5:B:492:LEU:HG	2.18	0.44
5:B:1162:ILE:O	5:B:1192:TYR:HB2	2.18	0.44
10:I:13:MET:HE3	10:I:13:MET:HB2	1.90	0.44
4:A:98:LYS:HD2	4:A:224:PHE:HZ	1.82	0.44
5:B:25:ILE:HG12	5:B:651:LEU:CD2	2.46	0.44
5:B:563:MET:HE2	5:B:580:VAL:HG21	1.99	0.44
5:B:801:LYS:HG2	11:J:52:THR:HA	1.99	0.44
5:B:1138:MET:HG2	5:B:1147:LEU:HG	2.00	0.44
7:E:55:ARG:HG3	7:E:83:CYS:O	2.17	0.44
4:A:351:THR:HB	4:A:468:PHE:CD2	2.53	0.44
4:A:362:ASP:OD1	4:A:362:ASP:N	2.50	0.44
4:A:781:ASP:HB3	4:A:790:ASP:H	1.83	0.44
5:B:1098:MET:HE3	5:B:1098:MET:HB2	1.83	0.44
6:C:36:VAL:HA	6:C:40:GLU:HG2	2.00	0.44
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.53	0.44
4:A:202:LEU:HD23	4:A:207:ILE:HD11	1.99	0.44
4:A:1036:ARG:HA	4:A:1036:ARG:HD3	1.81	0.44
4:A:1398:MET:H	4:A:1398:MET:HG2	1.64	0.44
5:B:197:PHE:O	5:B:488:TYR:OH	2.27	0.44
12:K:7:PHE:HA	12:K:10:PHE:CZ	2.53	0.44
4:A:91:PHE:HZ	4:A:207:ILE:HD13	1.82	0.44
4:A:242:PRO:O	4:A:247:ARG:NE	2.48	0.44
4:A:420:ARG:O	4:A:424:ILE:HG23	2.18	0.44
5:B:63:ILE:O	5:B:67:SER:HB3	2.18	0.44
5:B:1174:LYS:HB2	5:B:1177:HIS:HB2	1.99	0.44
6:C:186:LEU:HB3	6:C:188:HIS:ND1	2.33	0.44
4:A:18:GLN:HE22	4:A:1416:ALA:C	2.26	0.43
4:A:679:ILE:O	4:A:683:ILE:HG12	2.18	0.43
5:B:379:GLY:HA2	5:B:382:ILE:HD12	2.00	0.43
5:B:426:LYS:HE3	5:B:426:LYS:HB3	1.78	0.43
5:B:581:PHE:CG	5:B:586:TRP:HB2	2.53	0.43
5:B:914:LYS:HB3	5:B:937:ALA:HB3	2.00	0.43
6:C:3:GLU:HB2	12:K:104:ASN:HD21	1.82	0.43
6:C:105:GLY:O	6:C:149:LYS:HA	2.18	0.43
10:I:6:PHE:HD1	10:I:13:MET:HA	1.83	0.43
3:N:8:DG:OP2	3:N:8:DG:H8	2.01	0.43
4:A:114:LEU:HB2	4:A:142:CYS:SG	2.58	0.43
4:A:340:LEU:HD13	4:A:1429:ILE:HG12	2.00	0.43
5:B:555:ILE:HD12	5:B:587:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:60:ASP:HB2	13:L:67:PHE:CE2	2.53	0.43
9:H:125:LEU:CG	9:H:130:ARG:HH12	2.32	0.43
10:I:78:CYS:HB3	10:I:106:CYS:SG	2.57	0.43
4:A:67:CYS:SG	4:A:70:CYS:CB	2.96	0.43
4:A:125:ALA:O	4:A:134:ARG:HB2	2.17	0.43
4:A:698:GLN:HA	10:I:97:MET:O	2.18	0.43
5:B:802:PRO:HG2	5:B:805:THR:HG22	1.99	0.43
5:B:1114:LEU:HD12	5:B:1114:LEU:HA	1.82	0.43
10:I:7:CYS:HB2	10:I:34:TYR:HD2	1.82	0.43
11:J:7:CYS:HA	11:J:49:MET:HE3	2.00	0.43
4:A:25:GLU:CD	4:A:25:GLU:H	2.27	0.43
4:A:82:GLY:O	4:A:241:VAL:HB	2.18	0.43
4:A:130:ASP:HB3	4:A:133:LYS:HG3	1.99	0.43
4:A:399:HIS:HD2	4:A:435:HIS:HB3	1.84	0.43
4:A:1105:LEU:HB3	4:A:1384:VAL:CG2	2.48	0.43
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.19	0.43
4:A:1341:ILE:HG13	7:E:182:ASP:OD1	2.18	0.43
5:B:244:LEU:O	5:B:249:ARG:HB2	2.18	0.43
5:B:975:GLN:O	5:B:990:ILE:HD12	2.17	0.43
7:E:94:LYS:O	7:E:98:ILE:HG12	2.19	0.43
10:I:42:LEU:HD21	10:I:45:ARG:HB3	2.01	0.43
10:I:68:LEU:HD23	10:I:68:LEU:HA	1.82	0.43
3:N:7:DA:C6	3:N:8:DG:C6	3.07	0.43
4:A:439:ASN:HA	4:A:459:ARG:HD2	2.00	0.43
4:A:774:ARG:HD2	4:A:797:LYS:HB3	2.00	0.43
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	2.01	0.43
4:A:1129:GLU:HA	4:A:1132:LYS:HD2	2.01	0.43
4:A:1192:LEU:HB2	4:A:1241:ARG:HG3	2.01	0.43
6:C:222:LYS:HB3	6:C:222:LYS:HE3	1.92	0.43
7:E:94:LYS:HG2	7:E:123:LEU:HD13	2.01	0.43
9:H:40:LEU:HD13	9:H:123:MET:HB3	1.99	0.43
4:A:587:HIS:HB3	4:A:608:ILE:HD13	2.00	0.43
5:B:640:VAL:HB	5:B:738:PHE:O	2.19	0.43
5:B:642:ASP:HA	5:B:649:LYS:HG2	2.00	0.43
5:B:903:VAL:HG12	5:B:905:VAL:HG13	2.00	0.43
7:E:156:LEU:HD22	7:E:160:GLU:HB3	2.01	0.43
4:A:147:VAL:HG23	4:A:169:ASN:C	2.43	0.43
4:A:1215:ARG:HG3	4:A:1273:LEU:HD23	2.01	0.43
4:A:1341:ILE:HG22	4:A:1376:THR:HG23	1.99	0.43
5:B:272:THR:HA	5:B:279:ASP:HA	2.01	0.43
5:B:1082:MET:HE2	6:C:190:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1149:GLU:HA	5:B:1153:GLU:CD	2.44	0.43
9:H:38:LEU:HD13	9:H:125:LEU:HB2	2.00	0.43
4:A:31:SER:O	5:B:1183:LYS:NZ	2.40	0.43
4:A:426:LEU:HD23	4:A:426:LEU:HA	1.87	0.43
4:A:1217:LYS:HD3	4:A:1226:VAL:HG23	2.01	0.43
5:B:579:ARG:NH1	5:B:623:GLU:HG3	2.33	0.43
6:C:143:LEU:HD21	11:J:2:ILE:HD11	2.01	0.43
10:I:97:MET:HE2	10:I:97:MET:HB3	1.84	0.43
10:I:104:LEU:HD12	10:I:104:LEU:HA	1.84	0.43
4:A:465:TYR:CD2	5:B:976:ILE:HD12	2.54	0.43
4:A:667:GLY:O	4:A:670:ILE:HG22	2.19	0.43
4:A:901:LEU:HA	4:A:907:THR:HG23	2.01	0.43
4:A:1404:GLU:O	4:A:1408:ILE:HD12	2.18	0.43
4:A:1427:ASN:HA	4:A:1430:LEU:HD12	2.01	0.43
5:B:40:GLU:OE2	5:B:681:TRP:N	2.51	0.43
5:B:805:THR:OG1	5:B:1041:GLU:OE2	2.24	0.43
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	2.01	0.43
5:B:1054:GLY:O	5:B:1058:LEU:HG	2.18	0.43
6:C:77:ILE:N	6:C:129:ILE:HD11	2.34	0.43
6:C:251:LEU:O	6:C:255:VAL:HG23	2.19	0.43
9:H:106:GLU:HA	9:H:112:ILE:HA	2.01	0.43
9:H:125:LEU:CB	9:H:130:ARG:HH12	2.32	0.43
3:N:6:DG:H2''	3:N:7:DA:H5''	2.01	0.43
4:A:867:ILE:HD11	4:A:1010:ALA:HB1	2.00	0.43
4:A:1286:LYS:HG2	4:A:1302:PRO:HB3	2.00	0.43
5:B:30:SER:O	5:B:34:ILE:HG13	2.19	0.43
5:B:602:THR:HA	5:B:605:ARG:HH11	1.84	0.43
5:B:639:ILE:HD12	5:B:688:GLY:O	2.19	0.43
7:E:15:ALA:O	7:E:19:VAL:HG23	2.19	0.43
7:E:52:ARG:HE	7:E:52:ARG:HA	1.83	0.43
8:F:111:LEU:HD23	8:F:111:LEU:H	1.84	0.43
10:I:34:TYR:OH	10:I:36:GLU:OE1	2.37	0.43
4:A:137:ALA:O	4:A:141:LEU:HG	2.19	0.42
4:A:353:ILE:CG2	4:A:487:MET:HB2	2.49	0.42
5:B:546:SER:OG	5:B:631:GLY:N	2.52	0.42
5:B:749:LEU:HD22	5:B:753:ALA:HB1	2.00	0.42
6:C:246:ARG:O	6:C:250:THR:OG1	2.29	0.42
2:T:25:DC:H2'	2:T:26:DG:C8	2.54	0.42
4:A:23:SER:HB2	4:A:233:TRP:CZ2	2.54	0.42
4:A:1193:LEU:HD22	4:A:1264:GLU:HB2	2.01	0.42
5:B:816:GLU:OE1	5:B:816:GLU:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:848:ARG:HG2	6:C:69:LEU:HD11	2.01	0.42
5:B:904:ARG:HE	5:B:948:ILE:HD11	1.84	0.42
7:E:52:ARG:O	7:E:54:GLN:NE2	2.50	0.42
7:E:113:GLN:O	7:E:136:ASN:ND2	2.52	0.42
2:T:15:DC:OP2	2:T:15:DC:H2'	2.19	0.42
4:A:304:MET:C	4:A:324:SER:HG	2.23	0.42
4:A:620:LYS:HE2	4:A:620:LYS:HB2	1.62	0.42
4:A:986:ILE:HD12	4:A:1028:THR:HG23	2.01	0.42
5:B:29:ASP:HB3	5:B:658:ILE:HG21	2.01	0.42
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.85	0.42
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.54	0.42
7:E:124:VAL:HB	7:E:125:PRO:HD3	2.02	0.42
9:H:37:LYS:O	9:H:125:LEU:HA	2.19	0.42
1:R:4:G:H2'	1:R:5:A:H8	1.83	0.42
4:A:28:ARG:HG2	4:A:83:HIS:CE1	2.55	0.42
4:A:880:LYS:HA	4:A:955:PRO:HA	2.00	0.42
4:A:1317:MET:HG3	4:A:1318:THR:HG23	2.01	0.42
5:B:486:TYR:CE2	5:B:1096:ARG:HB3	2.53	0.42
5:B:856:PHE:CD2	5:B:969:ARG:HB2	2.55	0.42
5:B:872:GLU:HG3	5:B:916:THR:HA	1.99	0.42
6:C:58:LEU:HB2	6:C:63:ILE:HD11	2.01	0.42
7:E:60:PHE:CZ	7:E:80:VAL:HG11	2.55	0.42
4:A:83:HIS:ND1	4:A:85:ASP:OD1	2.52	0.42
4:A:114:LEU:HD21	4:A:171:GLN:HG3	2.01	0.42
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.42
4:A:760:GLN:HG2	4:A:765:VAL:HA	2.01	0.42
4:A:775:ILE:HG21	4:A:815:PHE:CE1	2.54	0.42
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	2.02	0.42
5:B:23:ALA:O	5:B:654:ARG:HG3	2.18	0.42
5:B:33:VAL:HG11	5:B:638:PHE:HE1	1.84	0.42
5:B:195:CYS:SG	5:B:782:LEU:HB3	2.59	0.42
10:I:81:ARG:HE	10:I:81:ARG:HB3	1.70	0.42
12:K:25:THR:HG22	12:K:26:LYS:HG3	2.01	0.42
4:A:98:LYS:HD2	4:A:224:PHE:CZ	2.55	0.42
4:A:316:GLN:N	4:A:320:ARG:O	2.52	0.42
4:A:648:ASN:O	4:A:652:VAL:HG23	2.19	0.42
4:A:839:ARG:NH2	4:A:1402:PHE:O	2.46	0.42
4:A:981:LEU:HG	4:A:1039:LYS:HD3	2.01	0.42
4:A:1030:ARG:O	4:A:1034:GLU:HG2	2.19	0.42
4:A:1044:TRP:O	4:A:1048:ASN:ND2	2.52	0.42
4:A:1215:ARG:NH2	4:A:1272:THR:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1383:SER:OG	4:A:1387:HIS:O	2.34	0.42
5:B:221:ASN:N	5:B:241:ARG:O	2.41	0.42
5:B:268:THR:OG1	5:B:270:LYS:NZ	2.53	0.42
5:B:485:ARG:CZ	5:B:782:LEU:HD11	2.49	0.42
5:B:851:PHE:CG	5:B:980:PHE:HE2	2.37	0.42
5:B:898:LEU:HD11	5:B:954:VAL:HG22	2.02	0.42
5:B:1060:ARG:HD2	5:B:1060:ARG:HA	1.68	0.42
11:J:48:ARG:O	11:J:52:THR:OG1	2.20	0.42
11:J:56:LEU:HB3	11:J:60:PHE:CZ	2.55	0.42
12:K:99:GLY:O	12:K:103:THR:HG23	2.19	0.42
4:A:231:PRO:HA	4:A:234:MET:SD	2.60	0.42
4:A:363:GLN:NE2	4:A:459:ARG:HH21	2.17	0.42
4:A:526:ASP:HB3	4:A:657:LEU:HD23	2.02	0.42
4:A:573:SER:OG	4:A:575:LYS:HG3	2.19	0.42
4:A:183:GLY:O	4:A:199:LEU:N	2.53	0.42
4:A:944:ARG:HH21	4:A:1292:PRO:HB3	1.85	0.42
5:B:310:MET:HE2	5:B:310:MET:HB3	1.83	0.42
5:B:579:ARG:NH1	5:B:621:GLU:O	2.37	0.42
7:E:31:THR:HB	7:E:34:GLU:HB3	2.01	0.42
7:E:112:TYR:O	7:E:136:ASN:HA	2.20	0.42
10:I:68:LEU:O	10:I:70:ARG:NH1	2.52	0.42
11:J:36:LEU:HD11	11:J:51:LEU:HD13	2.00	0.42
12:K:49:GLU:OE2	12:K:97:LYS:NZ	2.35	0.42
4:A:74:MET:HE2	4:A:74:MET:HB3	1.67	0.42
4:A:515:GLN:OE1	4:A:1071:SER:HA	2.20	0.42
4:A:740:LEU:HD13	6:C:192:TRP:CD1	2.55	0.42
4:A:1135:ARG:O	4:A:1139:GLU:HG3	2.20	0.42
5:B:372:SER:OG	5:B:567:GLU:HG3	2.18	0.42
5:B:519:TRP:NE1	5:B:742:GLU:OE2	2.53	0.42
6:C:56:THR:HG22	6:C:147:LEU:HD21	2.01	0.42
6:C:75:MET:HB2	6:C:75:MET:HE2	1.81	0.42
2:T:23:DC:H2'	2:T:24:DT:C6	2.55	0.42
4:A:519:PRO:O	4:A:624:SER:HB2	2.20	0.42
4:A:775:ILE:HG21	4:A:815:PHE:CD1	2.55	0.42
5:B:982:SER:HB3	5:B:1092:TYR:CZ	2.55	0.42
6:C:84:ARG:HD2	12:K:11:LEU:HD21	2.01	0.42
6:C:251:LEU:HD12	6:C:251:LEU:HA	1.86	0.42
4:A:22:PHE:HB2	5:B:1211:ASN:HB2	2.02	0.41
4:A:1289:ARG:HG2	4:A:1290:LYS:N	2.34	0.41
5:B:40:GLU:OE2	5:B:680:THR:HB	2.20	0.41
5:B:199:MET:SD	5:B:199:MET:N	2.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:886:LYS:H	5:B:886:LYS:HD2	1.85	0.41
5:B:1059:LEU:HD12	5:B:1059:LEU:HA	1.88	0.41
6:C:62:PHE:HE1	6:C:66:ARG:HD2	1.84	0.41
7:E:56:LYS:HE3	7:E:56:LYS:HB3	1.92	0.41
4:A:500:GLU:OE1	5:B:1146:PHE:N	2.53	0.41
4:A:546:VAL:O	4:A:550:LEU:HD13	2.20	0.41
9:H:97:MET:HE2	9:H:118:PHE:HB3	2.02	0.41
12:K:10:PHE:HD2	12:K:11:LEU:HD13	1.85	0.41
2:T:22:DT:H2'	2:T:23:DC:H6	1.85	0.41
4:A:529:CYS:O	4:A:533:LYS:HG3	2.20	0.41
4:A:597:LEU:HD22	9:H:102:TYR:HD2	1.86	0.41
4:A:939:ASP:O	4:A:943:LEU:HG	2.19	0.41
4:A:1287:TYR:CE2	4:A:1305:VAL:HG11	2.55	0.41
5:B:128:LEU:HB2	5:B:168:GLY:O	2.20	0.41
5:B:267:ARG:HH11	5:B:313:MET:HE1	1.85	0.41
5:B:407:ASP:N	5:B:407:ASP:OD1	2.52	0.41
5:B:639:ILE:HB	5:B:652:LYS:HD3	2.02	0.41
9:H:37:LYS:HB2	9:H:126:GLU:OE2	2.20	0.41
10:I:78:CYS:HB3	10:I:106:CYS:CB	2.51	0.41
4:A:203:SER:O	4:A:206:GLU:N	2.53	0.41
7:E:171:LYS:HA	7:E:171:LYS:HD2	1.94	0.41
10:I:34:TYR:CE1	10:I:36:GLU:HB3	2.56	0.41
10:I:69:PRO:HB2	10:I:85:PHE:CZ	2.55	0.41
10:I:74:GLU:OE1	10:I:81:ARG:HD2	2.20	0.41
4:A:11:LEU:HD22	5:B:1195:HIS:NE2	2.35	0.41
4:A:65:LEU:HD22	4:A:73:GLY:HA2	2.03	0.41
4:A:903:ASN:HD22	4:A:906:HIS:CG	2.38	0.41
4:A:1441:PHE:CE1	8:F:92:ARG:HD3	2.56	0.41
5:B:36:ALA:O	5:B:40:GLU:HG3	2.21	0.41
5:B:298:LEU:HG	5:B:314:LEU:HD13	2.01	0.41
5:B:654:ARG:O	5:B:658:ILE:HG12	2.20	0.41
5:B:755:ILE:HD13	5:B:755:ILE:HA	1.89	0.41
5:B:952:VAL:HG13	5:B:966:VAL:HG22	2.03	0.41
10:I:84:VAL:O	10:I:101:PHE:HA	2.20	0.41
4:A:27:VAL:HG11	4:A:240:PRO:HD3	2.03	0.41
4:A:840:ARG:HE	4:A:1384:VAL:HG23	1.84	0.41
4:A:1140:HIS:HD1	4:A:1277:GLU:HA	1.85	0.41
4:A:1169:ILE:HA	4:A:1172:LEU:HD12	2.01	0.41
4:A:1390:ASN:ND2	4:A:1399:ARG:O	2.53	0.41
5:B:283:VAL:HG21	5:B:317:CYS:O	2.21	0.41
5:B:1060:ARG:HH12	6:C:200:GLU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:70:ARG:NH1	10:I:84:VAL:HG22	2.36	0.41
12:K:20:LYS:HD3	12:K:21:ILE:N	2.36	0.41
2:T:17:DG:H4'	4:A:1403:GLU:HG2	2.03	0.41
4:A:311:GLN:N	4:A:312:PRO:HD3	2.35	0.41
4:A:424:ILE:HD12	4:A:424:ILE:O	2.21	0.41
4:A:683:ILE:O	4:A:687:LYS:HG3	2.21	0.41
4:A:1220:PHE:O	4:A:1221:LYS:HG3	2.21	0.41
5:B:112:LEU:HD11	5:B:117:ALA:HB2	2.03	0.41
5:B:127:GLY:HA2	5:B:166:PHE:HE1	1.86	0.41
5:B:622:LYS:HA	5:B:622:LYS:HD2	1.89	0.41
5:B:660:LYS:HE2	5:B:679:TYR:CD2	2.56	0.41
7:E:143:ASN:HB3	7:E:146:HIS:CG	2.56	0.41
4:A:140:THR:HA	4:A:143:LYS:HD3	2.01	0.41
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.85	0.41
4:A:376:TYR:CZ	4:A:498:ARG:HD2	2.55	0.41
4:A:913:LEU:HD23	4:A:913:LEU:HA	1.84	0.41
5:B:37:PHE:HD2	5:B:681:TRP:CE2	2.39	0.41
5:B:118:ARG:HA	5:B:207:GLY:HA2	2.02	0.41
5:B:706:GLN:HG2	5:B:708:GLU:HB2	2.02	0.41
11:J:17:LYS:HB3	11:J:39:LEU:HD13	2.03	0.41
4:A:33:ALA:C	4:A:34:LYS:HD3	2.45	0.41
4:A:58:LEU:HD23	4:A:247:ARG:HH21	1.86	0.41
4:A:92:HIS:HB3	4:A:95:PHE:CD2	2.56	0.41
4:A:230:ARG:NE	4:A:232:GLU:HB3	2.35	0.41
4:A:534:LEU:HG	4:A:574:GLY:HA3	2.03	0.41
4:A:718:VAL:O	4:A:722:LEU:HG	2.21	0.41
4:A:765:VAL:HG22	4:A:800:VAL:HB	2.02	0.41
4:A:870:GLU:OE1	7:E:202:SER:HB2	2.21	0.41
4:A:873:MET:HE2	4:A:873:MET:HB3	1.76	0.41
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.55	0.41
4:A:1151:GLU:O	4:A:1193:LEU:HD12	2.21	0.41
5:B:101:MET:HB2	5:B:110:HIS:O	2.21	0.41
5:B:396:ASP:OD1	5:B:396:ASP:N	2.54	0.41
5:B:497:ARG:HH21	5:B:538:ASN:HD21	1.69	0.41
5:B:878:GLN:HB2	5:B:881:ASN:HB3	2.03	0.41
5:B:952:VAL:HG22	5:B:966:VAL:HG22	2.03	0.41
6:C:167:HIS:CD2	13:L:70:ARG:HG2	2.56	0.41
7:E:12:LEU:HD22	7:E:137:GLU:OE2	2.21	0.41
10:I:73:ARG:O	10:I:83:ASN:ND2	2.54	0.41
12:K:31:VAL:O	12:K:74:ARG:HA	2.21	0.41
4:A:472:LEU:HD21	5:B:835:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:619:LYS:O	4:A:623:GLY:N	2.54	0.41
4:A:1037:LEU:HD12	4:A:1037:LEU:HA	1.95	0.41
5:B:604:ARG:NH2	5:B:614:SER:HA	2.36	0.41
5:B:953:LEU:O	5:B:964:VAL:HA	2.21	0.41
5:B:1082:MET:HA	6:C:189:THR:HA	2.03	0.41
5:B:1213:THR:O	5:B:1213:THR:OG1	2.38	0.41
9:H:112:ILE:HG22	9:H:127:GLY:O	2.21	0.41
11:J:59:LYS:H	11:J:59:LYS:HG2	1.58	0.41
4:A:605:MET:HE2	4:A:605:MET:HB2	1.82	0.40
5:B:186:GLU:HA	5:B:189:LEU:HD12	2.03	0.40
5:B:286:PHE:HB3	5:B:297:ILE:HG12	2.03	0.40
5:B:313:MET:HE2	5:B:313:MET:HB3	1.89	0.40
5:B:579:ARG:HB3	5:B:586:TRP:NE1	2.35	0.40
5:B:658:ILE:HG12	5:B:658:ILE:H	1.69	0.40
5:B:874:PHE:CZ	5:B:914:LYS:HD3	2.56	0.40
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.21	0.40
7:E:178:ILE:HG23	7:E:214:CYS:HA	2.02	0.40
8:F:132:LEU:O	8:F:148:VAL:HG23	2.21	0.40
9:H:106:GLU:HG3	9:H:111:LEU:O	2.22	0.40
3:N:5:DC:H2"	3:N:6:DG:OP2	2.21	0.40
4:A:135:PHE:HD1	4:A:222:LEU:HA	1.87	0.40
4:A:451:HIS:NE2	4:A:515:GLN:OE1	2.54	0.40
4:A:688:LYS:O	4:A:691:LEU:HG	2.22	0.40
4:A:867:ILE:HG22	4:A:872:GLY:N	2.36	0.40
4:A:1295:THR:HB	4:A:1297:GLU:HG2	2.02	0.40
5:B:199:MET:HE2	5:B:492:LEU:HD23	2.03	0.40
5:B:406:LEU:HD23	5:B:406:LEU:HA	1.95	0.40
5:B:736:THR:HG22	5:B:737:THR:HG23	2.03	0.40
6:C:9:LYS:HA	6:C:9:LYS:HD3	1.85	0.40
7:E:116:ILE:H	7:E:116:ILE:HG13	1.71	0.40
7:E:180:ARG:HH12	7:E:192:ARG:HB3	1.86	0.40
12:K:8:GLU:O	12:K:37:LYS:HD2	2.21	0.40
12:K:14:GLU:OE1	12:K:14:GLU:HA	2.21	0.40
13:L:62:LYS:HD3	13:L:62:LYS:HA	1.83	0.40
4:A:332:LYS:HE2	4:A:337:ARG:HH21	1.86	0.40
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.56	0.40
4:A:665:GLY:HA3	5:B:1069:PHE:CZ	2.56	0.40
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.44	0.40
4:A:1014:ALA:HA	7:E:205:SER:HB3	2.02	0.40
4:A:1034:GLU:HB2	4:A:1035:TYR:CD2	2.57	0.40
4:A:1055:ARG:NE	8:F:154:ASP:OD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:224:GLN:HE21	5:B:224:GLN:HB2	1.75	0.40
5:B:1069:PHE:HB2	6:C:201:TRP:HH2	1.87	0.40
6:C:258:ILE:HG23	12:K:19:LEU:HD21	2.02	0.40
7:E:13:TRP:NE1	7:E:37:LEU:O	2.51	0.40
10:I:14:LEU:HB3	10:I:27:PHE:HB3	2.04	0.40
2:T:9:DC:H2''	2:T:10:DT:H5'	2.03	0.40
4:A:375:THR:HB	4:A:433:GLU:HB3	2.04	0.40
4:A:613:ILE:HG23	9:H:117:SER:CB	2.51	0.40
4:A:845:LEU:HD21	4:A:1371:LEU:HA	2.03	0.40
4:A:862:ASN:HA	7:E:174:GLN:HA	2.03	0.40
4:A:1434:ALA:HB3	4:A:1436:ILE:HG12	2.02	0.40
5:B:661:LEU:HG	5:B:679:TYR:CD2	2.56	0.40
5:B:998:ASP:HB3	5:B:1076:HIS:HE1	1.85	0.40
6:C:44:LEU:HD21	6:C:97:VAL:HB	2.03	0.40
9:H:97:MET:HE1	9:H:121:LEU:HD12	2.02	0.40
10:I:60:GLN:HA	10:I:104:LEU:HD11	2.03	0.40
4:A:28:ARG:HA	4:A:83:HIS:CD2	2.57	0.40
4:A:91:PHE:CE1	4:A:204:THR:HG23	2.57	0.40
4:A:597:LEU:HD23	4:A:597:LEU:HA	1.83	0.40
5:B:267:ARG:NH1	5:B:313:MET:HE1	2.37	0.40
5:B:822:ASN:O	11:J:48:ARG:NH1	2.54	0.40
5:B:975:GLN:HE22	5:B:1100:ASP:CG	2.30	0.40
11:J:2:ILE:HD12	11:J:57:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1370/1733 (79%)	1341 (98%)	29 (2%)	0	100	100
5	B	1108/1224 (90%)	1088 (98%)	20 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	265/318 (83%)	263 (99%)	2 (1%)	0	100	100
7	E	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
10	I	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	3498/4173 (84%)	3429 (98%)	69 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1194/1520 (79%)	1190 (100%)	4 (0%)	86	83
5	B	955/1061 (90%)	952 (100%)	3 (0%)	86	83
6	C	235/274 (86%)	234 (100%)	1 (0%)	84	81
7	E	193/197 (98%)	193 (100%)	0	100	100
8	F	73/137 (53%)	72 (99%)	1 (1%)	59	71
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	106 (96%)	4 (4%)	31	57
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	70
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	36 (97%)	1 (3%)	39	62
All	All	3072/3657 (84%)	3057 (100%)	15 (0%)	81	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	67	CYS
4	A	70	CYS
4	A	77	CYS
4	A	109	HIS
5	B	1163	CYS
5	B	1182	CYS
5	B	1185	CYS
6	C	86	CYS
8	F	124	GLU
10	I	7	CYS
10	I	29	CYS
10	I	32	CYS
10	I	103	CYS
11	J	7	CYS
13	L	31	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	71	GLN
4	A	281	HIS
4	A	282	ASN
4	A	358	ASN
4	A	493	GLN
4	A	515	GLN
4	A	517	ASN
4	A	548	ASN
4	A	611	GLN
4	A	654	ASN
4	A	736	ASN
4	A	742	ASN
4	A	768	GLN
4	A	906	HIS
4	A	935	GLN
4	A	965	GLN
4	A	1009	ASN
4	A	1390	ASN
4	A	1432	GLN
5	B	103	ASN
5	B	115	GLN
5	B	481	GLN
5	B	776	GLN

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Mol	Chain	Res	Type
5	B	842	ASN
5	B	862	GLN
5	B	1097	HIS
5	B	1161	HIS
5	B	1179	GLN
5	B	1187	ASN
6	C	135	GLN
6	C	252	GLN
7	E	115	ASN
9	H	128	ASN
9	H	131	ASN
10	I	60	GLN
11	J	23	ASN
12	K	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	7/9 (77%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
2	WVQ	T	19	2	19,24,25	3.62	7 (36%)	18,33,36	1.57	4 (22%)

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
2	WVQ	T	19	2	-	4/6/40/41	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	WVQ	C5-N7	12.72	1.46	1.28
2	T	19	WVQ	C4-N9	4.83	1.45	1.35
2	T	19	WVQ	C2-N2	4.17	1.45	1.34
2	T	19	WVQ	C6-C5	-3.93	1.36	1.47
2	T	19	WVQ	C6-N1	-3.21	1.32	1.38
2	T	19	WVQ	O6-C6	-2.66	1.18	1.23
2	T	19	WVQ	C5-C4	-2.23	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.25	119.71	126.44
2	T	19	WVQ	C2'-C3'-C4'	2.48	107.83	102.80
2	T	19	WVQ	N2-C2-N3	2.18	120.04	116.57
2	T	19	WVQ	N2-C2-N1	2.04	120.25	117.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	WVQ	O4'-C4'-C5'-O5'
2	T	19	WVQ	C3'-C4'-C5'-O5'
2	T	19	WVQ	C4'-C5'-O5'-P
2	T	19	WVQ	O4'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	R	9/9 (100%)	0.51	0	100	100	104, 120, 189, 222	0
2	T	23/29 (79%)	0.67	0	100	100	107, 185, 252, 281	0
3	N	13/18 (72%)	0.46	0	100	100	203, 228, 274, 280	0
4	A	1384/1733 (79%)	0.44	66 (4%)	35	19	77, 117, 187, 248	0
5	B	1126/1224 (91%)	0.51	59 (5%)	33	19	47, 108, 163, 210	0
6	C	267/318 (83%)	0.46	13 (4%)	35	19	46, 100, 155, 201	0
7	E	212/215 (98%)	0.44	11 (5%)	33	19	88, 137, 215, 274	0
8	F	86/155 (55%)	0.27	3 (3%)	47	26	80, 108, 157, 183	0
9	H	133/146 (91%)	0.37	5 (3%)	44	24	90, 137, 196, 280	0
10	I	118/122 (96%)	0.32	2 (1%)	69	43	93, 133, 178, 231	0
11	J	65/70 (92%)	0.70	9 (13%)	6	5	47, 100, 133, 150	0
12	K	114/120 (95%)	0.33	6 (5%)	32	18	64, 108, 144, 179	0
13	L	43/70 (61%)	0.95	5 (11%)	9	6	94, 170, 235, 272	0
All	All	3593/4229 (84%)	0.46	179 (4%)	34	19	46, 115, 186, 281	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	775	LYS	6.5
5	B	543	SER	6.5
7	E	93	MET	5.8
5	B	779	GLY	5.2
7	E	112	TYR	5.1
5	B	386	LEU	5.0
5	B	819	ALA	4.5
5	B	823	ALA	4.3
9	H	23	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
12	K	42	LEU	4.1
4	A	1149	ALA	4.1
4	A	62	ASP	4.1
6	C	178	PHE	3.8
6	C	29	MET	3.8
5	B	525	ALA	3.8
4	A	1328	TYR	3.7
5	B	681	TRP	3.7
4	A	355	GLY	3.6
12	K	65	HIS	3.6
9	H	119	GLY	3.5
13	L	32	ALA	3.5
12	K	71	PHE	3.4
4	A	775	ILE	3.4
4	A	1390	ASN	3.4
5	B	740	HIS	3.4
6	C	97	VAL	3.4
5	B	533	CYS	3.4
4	A	1020	CYS	3.3
4	A	1434	ALA	3.3
9	H	63	LEU	3.3
5	B	489	SER	3.3
9	H	130	ARG	3.2
4	A	722	LEU	3.2
13	L	67	PHE	3.2
11	J	54	VAL	3.2
4	A	646	PHE	3.2
4	A	664	THR	3.1
4	A	815	PHE	3.1
5	B	869	SER	3.1
4	A	642	CYS	3.1
5	B	488	TYR	3.1
12	K	61	TYR	3.0
12	K	39	ASP	3.0
5	B	814	PHE	3.0
11	J	39	LEU	3.0
4	A	784	LEU	3.0
13	L	66	GLN	3.0
5	B	753	ALA	3.0
11	J	44	TYR	2.9
5	B	1214	PRO	2.9
4	A	873	MET	2.9

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Mol	Chain	Res	Type	RSRZ
10	I	111	THR	2.9
5	B	381	MET	2.9
5	B	780	VAL	2.9
12	K	73	LEU	2.9
4	A	1429	ILE	2.8
7	E	111	VAL	2.8
4	A	872	GLY	2.8
11	J	35	ALA	2.8
4	A	91	PHE	2.8
5	B	787	VAL	2.8
5	B	1047	PHE	2.8
7	E	110	PHE	2.8
5	B	51	PHE	2.8
4	A	48	ALA	2.8
4	A	834	THR	2.8
5	B	493	SER	2.7
5	B	1009	ASP	2.7
6	C	159	ALA	2.7
4	A	885	THR	2.7
7	E	109	ILE	2.7
11	J	33	GLY	2.7
4	A	86	LEU	2.7
5	B	811	TYR	2.7
6	C	38	ILE	2.6
4	A	622	VAL	2.6
5	B	1072	MET	2.6
4	A	957	PRO	2.6
4	A	466	SER	2.6
5	B	407	ASP	2.6
6	C	57	VAL	2.6
5	B	310	MET	2.5
8	F	85	MET	2.5
4	A	1061	GLY	2.5
4	A	776	ALA	2.5
6	C	30	ALA	2.5
5	B	751	VAL	2.5
4	A	135	PHE	2.5
5	B	27	ALA	2.5
8	F	93	ILE	2.5
5	B	113	TYR	2.5
5	B	698	GLU	2.5
4	A	1193	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
5	B	830	TYR	2.4
5	B	818	PRO	2.4
4	A	963	ILE	2.4
4	A	365	GLY	2.4
6	C	36	VAL	2.4
5	B	446	LEU	2.4
4	A	92	HIS	2.4
4	A	341	MET	2.4
4	A	1197	LEU	2.4
5	B	495	LEU	2.4
4	A	687	LYS	2.4
6	C	146	LYS	2.4
6	C	96	SER	2.4
4	A	696	GLU	2.4
5	B	75	ALA	2.4
4	A	199	LEU	2.3
4	A	1371	LEU	2.3
5	B	771	SER	2.3
6	C	23	SER	2.3
5	B	25	ILE	2.3
5	B	114	PRO	2.3
5	B	1211	ASN	2.3
6	C	129	ILE	2.3
5	B	802	PRO	2.3
13	L	61	THR	2.3
11	J	57	ILE	2.3
4	A	617	VAL	2.3
4	A	1397	LEU	2.3
5	B	778	MET	2.3
4	A	1400	CYS	2.2
5	B	620	ARG	2.2
4	A	668	ASP	2.2
4	A	577	ILE	2.2
5	B	37	PHE	2.2
8	F	84	TYR	2.2
4	A	798	GLY	2.2
4	A	932	GLU	2.2
5	B	939	THR	2.2
5	B	1212	ILE	2.2
4	A	540	PHE	2.2
4	A	659	HIS	2.2
5	B	999	MET	2.2

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Mol	Chain	Res	Type	RSRZ
5	B	877	PRO	2.2
11	J	65	PRO	2.2
4	A	1018	PHE	2.2
7	E	94	LYS	2.2
4	A	862	ASN	2.2
5	B	954	VAL	2.2
5	B	773	MET	2.2
4	A	137	ALA	2.1
4	A	612	ILE	2.1
7	E	127	ILE	2.1
6	C	251	LEU	2.1
7	E	123	LEU	2.1
11	J	41	LEU	2.1
4	A	473	SER	2.1
4	A	939	ASP	2.1
7	E	97	VAL	2.1
5	B	611	PRO	2.1
4	A	237	THR	2.1
5	B	390	LEU	2.1
7	E	90	VAL	2.1
5	B	524	PRO	2.1
4	A	1382	THR	2.1
4	A	214	ILE	2.1
4	A	1150	SER	2.1
13	L	29	TYR	2.1
5	B	1077	THR	2.1
5	B	824	ILE	2.1
4	A	482	PHE	2.1
5	B	1093	GLN	2.1
4	A	236	LEU	2.1
9	H	46	LEU	2.1
5	B	733	HIS	2.1
5	B	379	GLY	2.1
4	A	370	ILE	2.1
4	A	162	VAL	2.1
4	A	1081	LEU	2.1
11	J	21	TYR	2.0
7	E	120	ALA	2.0
10	I	40	SER	2.0
4	A	997	LEU	2.0
4	A	996	ASN	2.0
4	A	868	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	136	ALA	2.0
5	B	48	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WVQ	T	19	23/24	0.83	0.14	140,145,169,176	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	I	202	1/1	0.80	0.10	273,273,273,273	0
14	ZN	L	101	1/1	0.81	0.14	363,363,363,363	0
14	ZN	A	1801	1/1	0.91	0.08	301,301,301,301	0
14	ZN	C	401	1/1	0.96	0.07	120,120,120,120	0
15	MG	A	1803	1/1	0.97	0.05	129,129,129,129	0
14	ZN	B	1301	1/1	0.98	0.04	204,204,204,204	0
14	ZN	J	101	1/1	0.98	0.10	133,133,133,133	0
14	ZN	A	1802	1/1	0.98	0.03	167,167,167,167	0
14	ZN	I	201	1/1	0.98	0.04	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.