



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 01:58 PM EDT

PDB ID : 8UKU / pdb_00008uku
Title : RNA polymerase II elongation complex with Fapy-dG lesion with CMP added
Authors : Hou, P.; Oh, J.; Wang, D.
Deposited on : 2023-10-15
Resolution : 3.60 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

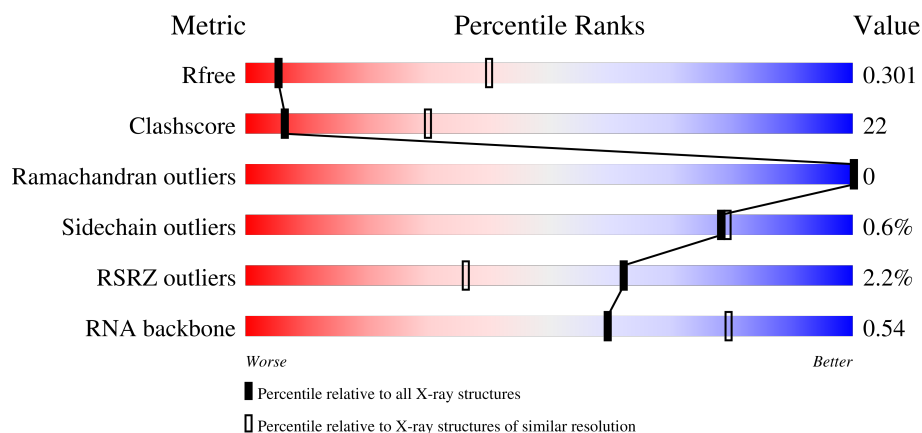
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

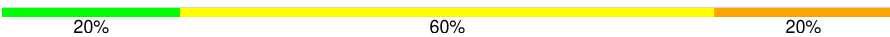
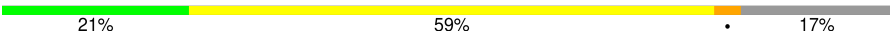
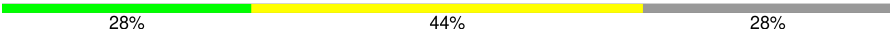
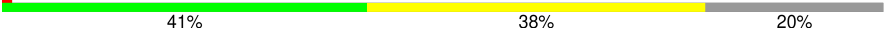
The reported resolution of this entry is 3.60 Å.

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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	R	10	
2	T	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 [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28991 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	10	Total	C	N	O	P	0	0	0
			215	97	43	66	9			

- Molecule 2 is a DNA chain called tsDNA with Fapy-dG.

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	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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
			332	205	64	59	4			

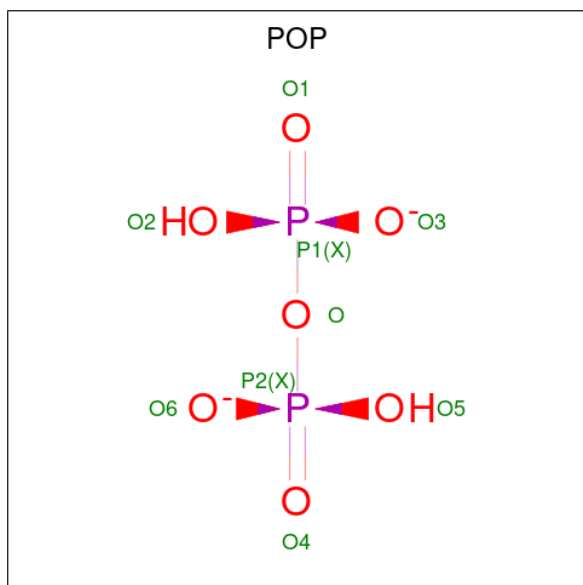
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 16 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total 9	O 7	P 2	0	0

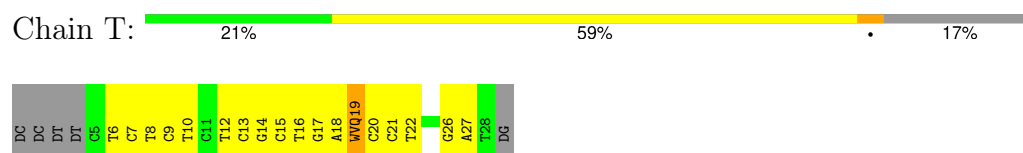
3 Residue-property plots [i](#)

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

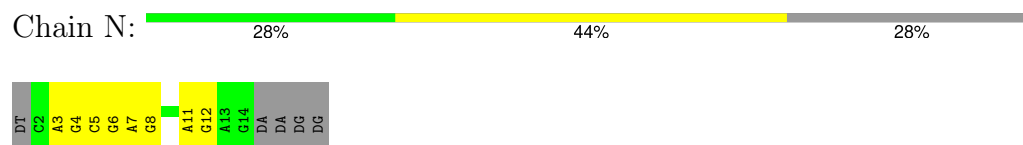
- Molecule 1: RNA



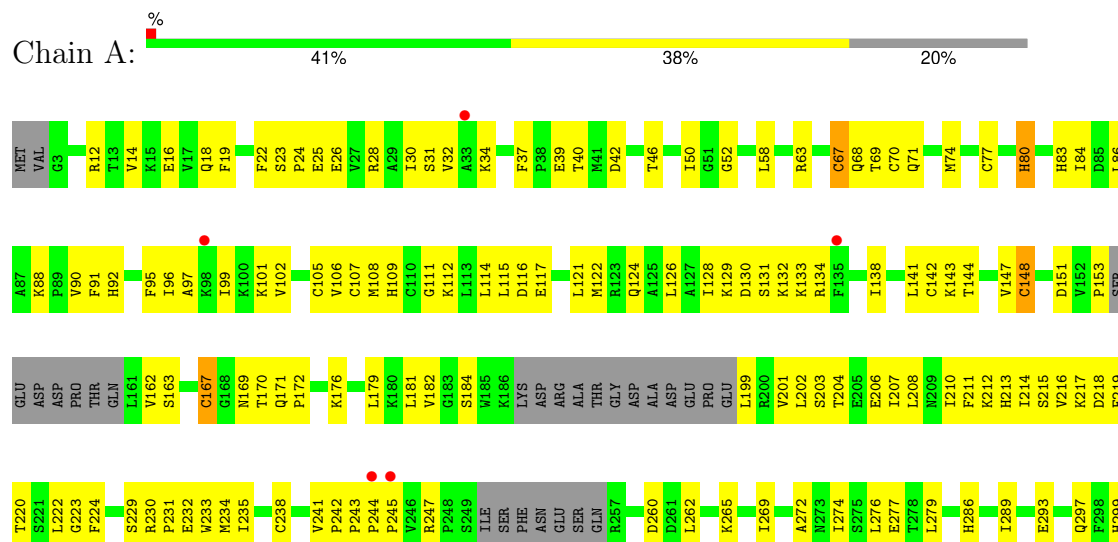
- Molecule 2: tsDNA with Fapy-dG



- Molecule 3: ntsDNA

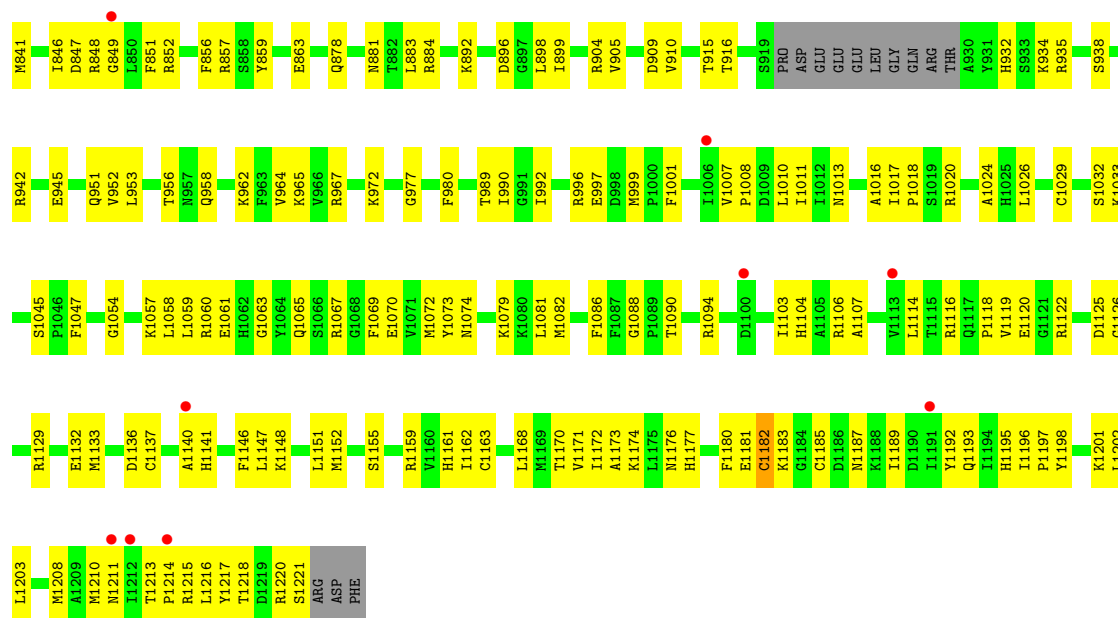


- Molecule 4: DNA-directed RNA polymerase II subunit RPB1

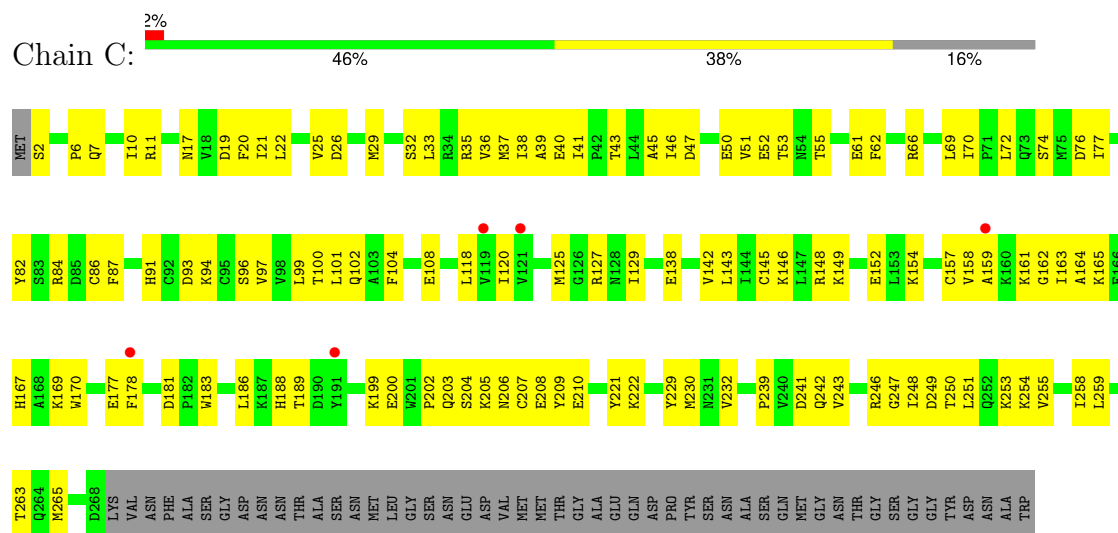


V1372	S1383	K1217	S1136	V1084	L981	A891	E812	R711	P639	I560	L489	L388	T302
D1373	T1289	Q1218	A1137	G1065	T982	A892	E812	E712	C642	P561	P492	L391	Y303
V1374	K1290	T1219	E1138	A1069	T983	K895	F815	K728	L645	I565	Q493	V392	M304
M1375	V1291	F1220	H1140	S1071	T986	K896	M818	L732	F646	K567	S494	H399	D305
S1383	P1292	L1224	T1141	P1076	L986	K898	G819	E734	G647	K568	E495	A402	N306
V1384	K1300	F1225	T1142	A1076	L989	V899	G820	W735	Q650	P570	L501	K403	Q311
T1385	V1226	V1227	K1144	T1077	Q994	D900	E822	N736	L646	K569	E496	R407	P312
R1386	L1306	V1228	T1147	Q1078	L997	L901	E823	L737	Q651	K571	L502	K403	Q311
H1387	E1307	S1229	T1147	M1079	L998	L902	G823	K738	V652	K575	S502	R407	S324
R1391	T1308	E1230	S1150	T1080	V999	N903	L804	D739	N653	Q576	Q503	D411	I325
G1395	V1311	D1231	E1151	L1081	L1000	H906	T826	L740	N654	K577	L504	D411	I326
A1396	M1312	L1236	I1152	ASN	R1001	T907	T827	N741	F655	I577	Q505	L415	R327
L1397	L1313	T1237	D1155	THR	L1004	L908	D826	N742	W656	S579	A506	L415	R328
M1398	I1238	I1239	I1163	PHE	M1004	D909	T831	V743	W657	P508	P508	S418	L329
R1399	V1316	C1240	T1163	HIS	I1007	L912	E833	K744	H659	L509	Q510	K419	K330
C1400	M1317	C1240	F1164	ALA	Q1008	L913	E833	W746	G661	P583	I511	R420	R335
S1401	T1318	V1243	E1165	ALA	Q1009	E914	Y836	V747	F662	I586	V512	I424	I336
F1402	D1323	ARG	D1166	GLY	Q1010	S915	T837	M748	G665	H587	S513	E433	R337
E1403	P1324	PRO	D1166	VAL	Q1011	G916	R839	A749	I666	F591	P514	R434	G338
E1404	T1325	LYS	I1169	ALA	R1012	R843	R840	W758	G667	O515	O515	H435	N339
V1405	R1326	SER	I1170	SER	D1013	E918	R840	Q760	D668	I523	I523	P447	L340
V1406	T1327	LEU	I1170	K1092	A1014	T919	R840	Q760	D672	P600	G222	P448	F347
E1407	I1328	ASP	L1176	K1093	V1015	L920	R841	Q760	T675	K601	D526	S449	S348
I1408	T1328	ALA	L1176	V1094	F1018	L923	E842	W756	M676	M605	C520	V442	R340
L1409	T1329	GLU	L1176	T1095	L1021	L925	Y842	I757	E677	L527	L528	R446	V345
G1413	T1333	THR	L1176	G1096	L1022	Q926	R843	I758	I679	L606	L607	D447	D346
A1416	D1334	GLU	L1176	P1098	L1023	R927	R844	W758	T680	I607	I607	P448	F347
E1417	T1335	ALA	L1176	F1099	L1024	L928	E844	Q760	I679	I607	I607	P448	S348
E1418	H1336	GLU	L1176	P1099	S1024	L928	E844	Q760	E685	I608	I608	S449	R349
L1418	E1337	GLU	L1176	K1102	R1025	L929	E844	Q760	E685	I608	I608	L450	R350
G1423	V1339	GLU	L1176	E1103	L1026	L933	E844	Q760	E685	I608	I608	V456	V351
V1424	H1258	ASP	L1176	I1104	A1027	Y933	E844	Q760	E685	I608	I608	A457	T351
S1425	M1259	PHE	L1176	L1105	T1028	Y933	E844	Q760	E685	I608	I608	V456	I353
E1426	L1261	GLN	L1176	L1106	T1028	Y933	E844	Q760	E685	I608	I608	A457	G355
N1427	K1262	GLN	L1176	V1107	R1029	L936	E844	Q760	E685	I608	I608	A457	D356
V1428	I1263	GLU	L1176	K1108	R1030	L936	E844	Q760	E685	I608	I608	A457	P357
E1429	E1264	GLU	L1176	K1109	R1030	F942	E844	Q760	E685	I608	I608	A457	L361
L1430	E1264	GLU	L1176	K1109	R1030	F942	E844	Q760	E685	I608	I608	A457	G365
G1431	N1265	GLU	L1176	M1110	Q1033	V946	E844	Q760	E685	I608	I608	A457	K368
Q1432	T1266	GLU	L1176	M1111	E1034	F947	E844	Q760	E685	I608	I608	A457	D366
M1433	M1267	GLU	L1176	K1112	Y1035	R1036	E844	Q760	E685	I608	I608	A457	P357
A1434	E1269	GLU	L1176	P1113	R1036	L1037	E844	Q760	E685	I608	I608	A457	L361
P1435	E1270	GLU	L1176	S1115	F1042	F1042	E844	Q760	E685	I608	I608	A457	G365
I1436	N1271	GLU	L1176	L1116	L1046	Q954	E844	Q760	E685	I608	I608	A457	K368
G1437	T1272	GLU	L1176	T1117	L1046	P955	E844	Q760	E685	I608	I608	A457	D366
T1438	L1273	GLU	L1176	V1118	E1050	L956	E844	Q760	E685	I608	I608	A457	P357
F1441	V1276	GLU	L1176	Y1119	A1051	P957	E844	Q760	E685	I608	I608	A457	L361
D1446	V1362	GLU	L1176	L1120	E1051	P957	E844	Q760	E685	I608	I608	A457	G365
GLU	V1363	GLU	L1176	E1121	V958	Q881	E844	Q760	E685	I608	I608	A457	K368
GLU	N1364	GLU	L1176	P1122	R1055	N959	E844	Q760	E685	I608	I608	A457	D366
GLU	V1365	GLU	L1176	D1127	V1058	R961	E844	Q760	E685	I608	I608	A457	P357
GLU	R1366	GLU	L1176	Q1130	H1059	R962	E844	Q760	E685	I608	I608	A457	D366
GLU	H1367	GLU	L1176	Q1130	M1063	H975	E844	Q760	E685	I608	I608	A457	P357
GLU	M1368	GLU	L1176	Q1130	M1063	H975	E844	Q760	E685	I608	I608	A457	P357
VAL	Y1287	VAL	L1216	Q1130	M1063	H975	E844	Q760	E685	I608	I608	A457	P357

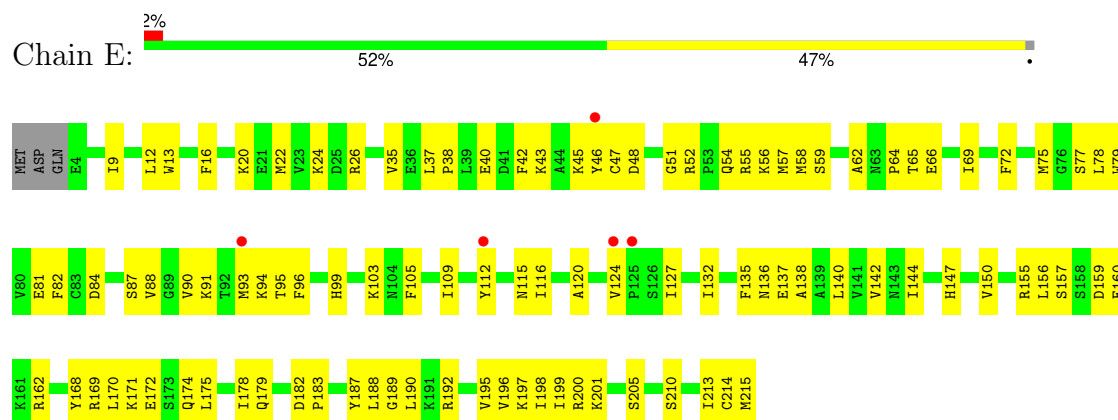




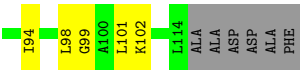
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



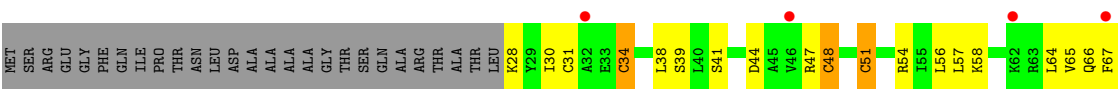
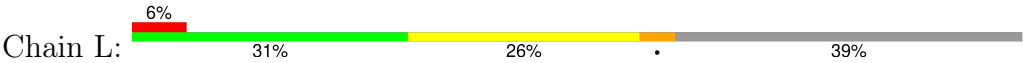
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Chain K:
-
- | State | Category |
|-------|----------|
| W1 | Green |
| N1 | Green |
| A3 | Green |
| P4 | Yellow |
| D5 | Yellow |
| R6 | Yellow |
| F7 | Yellow |
| F10 | Green |
| L11 | Green |
| L12 | Green |
| L19 | Green |
| K20 | Green |
| I21 | Green |
| T25 | Green |
| K26 | Green |
| N29 | Green |
| A30 | Green |
| I33 | Yellow |
| K37 | Green |
| E38 | Green |
| T41 | Yellow |
| L42 | Yellow |
| I46 | Yellow |
| R47 | Yellow |
| A48 | Green |
| E49 | Green |
| L50 | Green |
| L51 | Yellow |
| K55 | Yellow |
| V56 | Yellow |
| L57 | Yellow |
| F58 | Yellow |
| A59 | Yellow |
| A60 | Yellow |
| Y61 | Yellow |
| R65 | Yellow |
| P66 | Yellow |
| F71 | Yellow |
| R74 | Yellow |
| I75 | Yellow |
| Q76 | Yellow |
| T77 | Yellow |
| D82 | Yellow |
| D85 | Yellow |
| Q91 | Yellow |



● Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.10Å 224.01Å 192.54Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	49.24 – 3.60 49.24 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.24-3.60) 98.8 (49.24-3.60)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.258 , 0.301 0.259 , 0.301	Depositor DCC
R_{free} test set	2000 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	112.9	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 130.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28991	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/241	0.40	0/375
2	T	0.28	0/507	0.57	0/775
3	N	0.24	0/311	0.38	0/479
4	A	0.19	0/11020	0.45	0/14907
5	B	0.17	0/9030	0.41	0/12186
6	C	0.20	0/2139	0.44	0/2899
7	E	0.17	0/1767	0.41	0/2378
8	F	0.16	0/696	0.38	0/943
9	H	0.20	0/1082	0.52	0/1466
10	I	0.19	0/970	0.46	0/1308
11	J	0.17	0/541	0.44	0/727
12	K	0.17	0/937	0.43	0/1265
13	L	0.20	0/333	0.48	0/442
All	All	0.18	0/29574	0.44	0/40150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	215	0	111	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	481	0	262	23	0
3	N	275	0	144	11	0
4	A	10828	0	10875	560	1
5	B	8859	0	8816	378	0
6	C	2101	0	2056	107	1
7	E	1731	0	1758	91	0
8	F	684	0	692	26	0
9	H	1064	0	1029	56	0
10	I	952	0	897	48	0
11	J	532	0	542	31	0
12	K	919	0	929	47	0
13	L	332	0	347	19	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
16	B	9	0	0	0	0
All	All	28991	0	28458	1253	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1253) 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)
7:E:168:TYR:HB3	7:E:170:LEU:HD23	1.32	1.08
4:A:981:LEU:HD22	4:A:986:ILE:CG1	1.98	0.94
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.50	0.90
5:B:392:ARG:HD2	10:I:53:GLY:HA3	1.54	0.90
11:J:36:LEU:HD13	11:J:47:ARG:HG2	1.58	0.83
5:B:241:ARG:HB2	5:B:251:ILE:HG12	1.59	0.83
7:E:168:TYR:CB	7:E:170:LEU:HD23	2.09	0.83
5:B:68:THR:HA	5:B:90:ILE:O	1.79	0.82
4:A:981:LEU:HD22	4:A:986:ILE:HG12	1.59	0.82
10:I:78:CYS:HB3	10:I:106:CYS:HB3	1.63	0.81
5:B:102:VAL:HA	5:B:169:ARG:HH12	1.46	0.81
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.63	0.80
4:A:70:CYS:SG	4:A:80:HIS:HE1	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:30:ALA:HA	12:K:75:ILE:O	1.82	0.80
7:E:168:TYR:HB3	7:E:170:LEU:CD2	2.10	0.80
4:A:115:LEU:HD12	4:A:122:MET:HE3	1.64	0.80
4:A:128:ILE:HB	4:A:134:ARG:HB2	1.64	0.79
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.64	0.79
4:A:981:LEU:HD22	4:A:986:ILE:HG13	1.64	0.78
4:A:672:ASP:H	4:A:736:ASN:HD21	1.32	0.78
4:A:351:THR:HG23	5:B:1103:ILE:HG12	1.66	0.78
11:J:28:ASP:HB2	11:J:30:LEU:HG	1.66	0.77
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.65	0.77
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.66	0.77
4:A:1224:LEU:HD21	4:A:1240:CYS:HB3	1.65	0.76
4:A:279:LEU:HD21	4:A:289:ILE:HG12	1.67	0.76
12:K:61:TYR:HB2	12:K:71:PHE:HE1	1.51	0.76
4:A:913:LEU:HD22	4:A:915:SER:H	1.50	0.75
6:C:39:ALA:HB1	6:C:165:LYS:HG2	1.68	0.75
5:B:175:ARG:HG2	5:B:200:GLY:HA3	1.69	0.75
9:H:38:LEU:HA	9:H:124:ARG:O	1.87	0.74
4:A:37:PHE:H	4:A:52:GLY:HA3	1.52	0.74
4:A:1325:THR:HA	7:E:147:HIS:HA	1.68	0.74
5:B:245:GLU:HA	5:B:249:ARG:HH22	1.53	0.74
7:E:93:MET:HE2	7:E:124:VAL:HG22	1.70	0.74
4:A:1152:ILE:HG21	4:A:1261:LYS:HE2	1.69	0.73
4:A:569:LYS:HD2	6:C:221:TYR:HB2	1.70	0.73
5:B:121:ASN:HA	5:B:207:GLY:HA3	1.70	0.73
4:A:1363:VAL:HB	4:A:1368:MET:HE2	1.70	0.73
12:K:47:ARG:HD3	12:K:61:TYR:HD1	1.53	0.72
5:B:736:THR:HG23	5:B:737:THR:HG23	1.71	0.72
5:B:753:ALA:HA	5:B:756:ILE:HD12	1.71	0.72
5:B:1174:LYS:HB2	5:B:1177:HIS:HB2	1.70	0.72
8:F:128:LYS:HD2	8:F:149:GLU:HA	1.69	0.72
4:A:14:VAL:HG11	5:B:1216:LEU:HB3	1.72	0.72
4:A:179:LEU:HD13	4:A:297:GLN:HG2	1.72	0.72
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.70	0.72
5:B:431:TYR:HA	5:B:434:ARG:HE	1.55	0.71
5:B:215:GLN:HE21	5:B:476:ARG:HD3	1.54	0.71
5:B:621:GLU:HG3	5:B:623:GLU:HB2	1.72	0.71
4:A:202:LEU:HB3	4:A:207:ILE:HD11	1.71	0.71
5:B:426:LYS:HG3	5:B:430:ARG:HE	1.55	0.71
4:A:512:VAL:HA	4:A:519:PRO:HA	1.71	0.71
1:R:10:C:N3	2:T:19:WVQ:N1	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:69:THR:HB	5:B:1172:ILE:HD12	1.71	0.70
4:A:983:ILE:HG13	4:A:1028:THR:HG21	1.73	0.70
5:B:910:VAL:HG11	5:B:938:SER:HB3	1.74	0.70
4:A:544:ASP:HB2	12:K:47:ARG:HH22	1.56	0.70
4:A:925:LEU:HA	4:A:928:LEU:HD12	1.73	0.69
7:E:20:LYS:HD2	7:E:35:VAL:HA	1.73	0.69
4:A:14:VAL:HA	5:B:1218:THR:HA	1.73	0.69
4:A:208:LEU:HD13	4:A:235:ILE:HD11	1.75	0.69
10:I:82:GLU:HB3	10:I:104:LEU:HD23	1.73	0.69
5:B:703:ILE:HG22	5:B:740:HIS:HB2	1.73	0.69
6:C:84:ARG:HH21	6:C:163:ILE:HD11	1.57	0.69
4:A:117:GLU:HA	4:A:122:MET:HG3	1.74	0.69
5:B:1182:CYS:SG	5:B:1185:CYS:HB2	2.32	0.69
13:L:38:LEU:HD21	13:L:56:LEU:HD22	1.74	0.69
3:N:4:DG:H2"	3:N:5:DC:C5	2.28	0.68
13:L:38:LEU:HD22	13:L:48:CYS:HB2	1.76	0.68
5:B:261:ARG:HB2	5:B:264:SER:HB2	1.76	0.68
4:A:1102:LYS:HE2	4:A:1106:ASN:HD21	1.59	0.68
9:H:80:ARG:O	9:H:87:ARG:NH2	2.26	0.68
7:E:42:PHE:O	7:E:46:TYR:HB2	1.93	0.68
4:A:881:GLN:HB2	4:A:956:LEU:HD12	1.76	0.68
4:A:31:SER:O	5:B:1183:LYS:NZ	2.26	0.68
5:B:780:VAL:HG22	5:B:795:ILE:HG23	1.74	0.68
7:E:109:ILE:HD12	7:E:135:PHE:HE2	1.57	0.68
4:A:1342:GLU:OE1	7:E:200:ARG:NH1	2.28	0.67
7:E:144:ILE:HD11	7:E:187:TYR:HB2	1.77	0.67
12:K:61:TYR:HB2	12:K:71:PHE:CE1	2.29	0.67
5:B:29:ASP:HB3	5:B:658:ILE:HG21	1.77	0.67
9:H:41:ASP:HB3	9:H:121:LEU:HD22	1.77	0.67
4:A:88:LYS:HG2	4:A:293:GLU:HB2	1.76	0.66
4:A:376:TYR:HD2	4:A:434:ARG:HE	1.42	0.66
4:A:306:ASN:H	4:A:324:SER:HB2	1.60	0.66
4:A:565:ILE:HG13	9:H:97:MET:HE3	1.76	0.66
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.31	0.66
9:H:14:GLU:HG3	9:H:27:GLU:HB2	1.78	0.66
4:A:325:ILE:HB	5:B:1210:MET:HE2	1.78	0.66
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.78	0.66
8:F:81:THR:OG1	8:F:144:GLU:OE1	2.12	0.66
7:E:79:TRP:HB2	7:E:105:PHE:HD2	1.59	0.66
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.77	0.66
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.76	0.65
5:B:186:GLU:HA	5:B:189:LEU:HD12	1.78	0.65
5:B:1060:ARG:NH2	6:C:199:LYS:O	2.29	0.65
8:F:109:VAL:HG21	8:F:127:GLU:HG3	1.78	0.65
4:A:230:ARG:HB2	4:A:233:TRP:CG	2.32	0.65
4:A:540:PHE:HB3	4:A:571:LEU:HD12	1.78	0.65
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.77	0.65
5:B:412:LEU:HD13	5:B:466:TRP:HE1	1.61	0.65
12:K:25:THR:HG22	12:K:26:LYS:HG3	1.78	0.65
4:A:981:LEU:CD2	4:A:986:ILE:HG12	2.26	0.65
12:K:58:PHE:HE1	12:K:74:ARG:HB3	1.62	0.65
7:E:47:CYS:HB3	7:E:51:GLY:HA2	1.79	0.65
7:E:78:LEU:HD11	7:E:109:ILE:HG12	1.78	0.65
5:B:563:MET:HE1	5:B:580:VAL:HB	1.79	0.65
6:C:258:ILE:HD12	12:K:19:LEU:HD21	1.80	0.64
5:B:420:LEU:HB3	5:B:453:ILE:HD13	1.79	0.64
10:I:59:VAL:HG12	10:I:61:ASP:H	1.60	0.64
4:A:18:GLN:HB3	5:B:1217:TYR:HE2	1.62	0.64
4:A:565:ILE:HB	4:A:571:LEU:HB2	1.80	0.64
6:C:46:ILE:HG12	6:C:157:CYS:HB3	1.78	0.64
10:I:111:THR:HG22	10:I:113:ASP:H	1.61	0.64
11:J:21:TYR:HB2	11:J:39:LEU:HD11	1.79	0.64
4:A:513:SER:OG	4:A:515:GLN:O	2.15	0.64
11:J:45:CYS:O	11:J:48:ARG:HG2	1.98	0.64
3:N:6:DG:H2"	3:N:7:DA:H5"	1.78	0.63
4:A:781:ASP:HB3	4:A:790:ASP:H	1.60	0.63
6:C:99:LEU:HD22	6:C:120:ILE:HG23	1.80	0.63
9:H:97:MET:HE1	9:H:121:LEU:HD12	1.79	0.63
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.79	0.63
4:A:286:HIS:HA	4:A:289:ILE:HD12	1.81	0.63
4:A:1193:LEU:HD21	4:A:1264:GLU:HB2	1.80	0.63
7:E:179:GLN:HG3	7:E:182:ASP:HB2	1.81	0.63
5:B:470:LYS:HG3	5:B:473:MET:H	1.64	0.63
5:B:651:LEU:HD12	5:B:653:VAL:O	1.99	0.63
4:A:117:GLU:HB2	4:A:126:LEU:HD11	1.81	0.63
4:A:1115:SER:HA	4:A:1308:THR:O	1.97	0.63
8:F:85:MET:HE1	8:F:148:VAL:HG13	1.81	0.63
4:A:1229:SER:HB3	4:A:1237:ILE:H	1.64	0.63
6:C:47:ASP:OD1	13:L:70:ARG:NH1	2.31	0.63
5:B:883:LEU:HB2	5:B:932:HIS:HB3	1.82	0.62
7:E:52:ARG:NH1	7:E:54:GLN:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:155:ARG:HG3	7:E:188:LEU:HD12	1.79	0.62
4:A:767:GLN:HA	4:A:799:PHE:HA	1.80	0.62
13:L:47:ARG:HB3	13:L:54:ARG:HD3	1.82	0.62
4:A:71:GLN:HE22	5:B:1176:ASN:HB2	1.64	0.62
4:A:830:LYS:HD2	4:A:1098:VAL:HG21	1.81	0.62
4:A:1434:ALA:HB1	4:A:1436:ILE:HD13	1.81	0.62
9:H:91:ASP:HB2	9:H:93:TYR:HD1	1.64	0.62
6:C:76:ASP:HB2	6:C:129:ILE:HG12	1.81	0.62
4:A:50:ILE:HG23	4:A:52:GLY:H	1.63	0.62
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.81	0.62
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.81	0.62
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.31	0.62
4:A:1266:THR:O	4:A:1270:ASN:HB2	1.99	0.62
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.82	0.62
4:A:579:SER:HB3	4:A:611:GLN:HA	1.82	0.62
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	1.81	0.62
6:C:250:THR:HA	6:C:253:LYS:HD2	1.82	0.62
4:A:121:LEU:O	4:A:124:GLN:HG3	2.00	0.61
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.81	0.61
4:A:1070:GLN:HE22	5:B:1137:CYS:HA	1.64	0.61
4:A:747:VAL:HG21	4:A:758:ILE:HD11	1.82	0.61
6:C:36:VAL:HA	6:C:40:GLU:HG2	1.82	0.61
10:I:69:PRO:HB2	10:I:85:PHE:CE1	2.35	0.61
4:A:336:ILE:HD11	5:B:1203:LEU:HD13	1.80	0.61
4:A:960:ILE:HG21	4:A:1025:ARG:HB3	1.82	0.61
3:N:11:DA:H2"	3:N:12:DG:C8	2.36	0.61
4:A:1348:LEU:HD23	4:A:1372:VAL:HG13	1.82	0.61
4:A:1446:ASP:HA	8:F:133:VAL:HG23	1.82	0.61
7:E:12:LEU:HD11	7:E:55:ARG:HE	1.65	0.61
4:A:372:LYS:HA	4:A:435:HIS:CD2	2.36	0.61
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.66	0.61
9:H:101:ALA:HA	9:H:116:TYR:HA	1.81	0.61
4:A:528:LEU:O	4:A:531:ILE:HG22	2.01	0.61
5:B:619:ILE:HD12	10:I:65:ASP:HB2	1.82	0.61
4:A:388:LEU:HD23	4:A:391:LEU:HD12	1.83	0.61
5:B:416:LEU:HD21	5:B:467:GLY:HA2	1.82	0.61
11:J:17:LYS:HB3	11:J:39:LEU:HD22	1.81	0.61
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.82	0.61
4:A:583:PRO:HD3	4:A:645:LEU:HD13	1.83	0.61
4:A:216:VAL:HA	4:A:219:PHE:CD2	2.36	0.60
4:A:1147:THR:HB	10:I:48:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:58:THR:HB	9:H:143:LEU:HB2	1.83	0.60
5:B:1163:CYS:HB2	5:B:1171:VAL:HG13	1.83	0.60
4:A:182:VAL:HG22	4:A:201:VAL:HG12	1.82	0.60
5:B:829:CYS:HA	5:B:834:ASN:HD21	1.65	0.60
7:E:172:GLU:HG2	7:E:213:ILE:HD12	1.82	0.60
9:H:30:SER:HB2	9:H:36:CYS:HB2	1.83	0.60
4:A:913:LEU:HD22	4:A:915:SER:HB3	1.83	0.60
4:A:1387:HIS:O	4:A:1391:ARG:HG2	2.02	0.60
5:B:59:LEU:HB3	5:B:95:ILE:HG21	1.83	0.60
6:C:242:GLN:HB3	6:C:246:ARG:HH12	1.67	0.60
4:A:242:PRO:O	4:A:247:ARG:NH1	2.24	0.60
6:C:94:LYS:HG3	6:C:125:MET:HE1	1.82	0.60
5:B:997:GLU:HB2	6:C:35:ARG:HG2	1.82	0.60
5:B:1082:MET:HA	6:C:189:THR:HA	1.83	0.60
6:C:143:LEU:HD23	11:J:2:ILE:HD11	1.84	0.60
4:A:361:LEU:HB2	4:A:471:ASN:HD22	1.67	0.60
4:A:632:VAL:HG13	4:A:962:ARG:HD3	1.82	0.60
4:A:782:ARG:NH2	5:B:701:ILE:O	2.35	0.60
5:B:122:LEU:HD11	5:B:958:GLN:H	1.67	0.60
2:T:8:DT:O2	3:N:12:DG:N2	2.35	0.60
4:A:1111:MET:HB3	4:A:1114:PRO:HG3	1.84	0.60
5:B:44:VAL:HG11	5:B:495:LEU:HD13	1.84	0.60
4:A:230:ARG:HG3	4:A:233:TRP:CE2	2.36	0.59
10:I:68:LEU:O	10:I:70:ARG:NH1	2.35	0.59
4:A:18:GLN:NE2	4:A:19:PHE:O	2.29	0.59
4:A:884:ASP:HB3	4:A:896:ARG:HH22	1.67	0.59
5:B:841:MET:HB3	5:B:846:ILE:HD11	1.83	0.59
5:B:1029:CYS:HG	5:B:1090:THR:HG1	1.41	0.59
9:H:10:PHE:HZ	9:H:36:CYS:HB3	1.67	0.59
4:A:1059:HIS:CD2	8:F:86:THR:HA	2.37	0.59
12:K:12:LEU:HA	12:K:37:LYS:HD3	1.84	0.59
5:B:210:LYS:HZ1	5:B:462:ALA:HA	1.65	0.59
4:A:1216:ILE:HG22	4:A:1220:PHE:CE2	2.37	0.59
5:B:1106:ARG:NH1	5:B:1118:PRO:HB3	2.18	0.59
13:L:48:CYS:SG	13:L:51:CYS:N	2.75	0.59
5:B:283:VAL:HG13	5:B:297:ILE:HD13	1.83	0.59
5:B:892:LYS:HD2	5:B:909:ASP:HB2	1.84	0.59
5:B:1116:ARG:HG3	5:B:1198:TYR:CG	2.37	0.59
2:T:12:DT:H2'	2:T:13:DC:C6	2.38	0.59
4:A:666:ILE:HD11	5:B:1067:ARG:HA	1.84	0.59
4:A:899:VAL:HG21	4:A:908:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1139:GLU:HG3	4:A:1282:VAL:HG22	1.85	0.59
5:B:562:GLY:O	5:B:590:HIS:ND1	2.35	0.59
5:B:788:ARG:O	5:B:967:ARG:NH1	2.35	0.59
6:C:22:LEU:HB3	6:C:25:VAL:HG21	1.84	0.59
4:A:1106:ASN:HB3	4:A:1385:THR:HG23	1.84	0.59
5:B:31:TRP:HA	5:B:34:ILE:HD12	1.85	0.58
4:A:1220:PHE:CE2	4:A:1224:LEU:HD22	2.38	0.58
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	1.84	0.58
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.85	0.58
6:C:204:SER:HB3	6:C:207:CYS:HB2	1.85	0.58
7:E:45:LYS:NZ	7:E:57:MET:SD	2.65	0.58
4:A:619:LYS:O	4:A:623:GLY:N	2.36	0.58
4:A:1142:THR:HG22	4:A:1144:LYS:H	1.68	0.58
9:H:128:ASN:O	9:H:131:ASN:ND2	2.36	0.58
5:B:617:ARG:NH1	10:I:61:ASP:OD2	2.35	0.58
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.85	0.58
6:C:142:VAL:HG23	11:J:15:GLY:HA3	1.84	0.58
7:E:72:PHE:HE1	7:E:157:SER:HA	1.69	0.58
9:H:96:VAL:HA	9:H:142:LEU:O	2.04	0.58
4:A:1155:ASP:HB2	4:A:1192:LEU:HD23	1.83	0.58
4:A:1100:ARG:HE	4:A:1104:ILE:HD11	1.68	0.58
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.84	0.58
5:B:881:ASN:HB3	5:B:934:LYS:HE2	1.84	0.58
5:B:915:THR:HB	5:B:934:LYS:HB3	1.86	0.58
10:I:55:THR:HG21	10:I:109:ILE:HG21	1.84	0.58
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.67	0.58
12:K:91:CYS:HA	12:K:94:ILE:HD12	1.86	0.58
1:R:10:C:N4	2:T:19:WVQ:O6	2.30	0.58
5:B:904:ARG:HG3	13:L:65:VAL:HG11	1.85	0.58
13:L:41:SER:OG	13:L:44:ASP:OD1	2.12	0.58
5:B:681:TRP:CH2	5:B:690:VAL:HG11	2.38	0.58
4:A:108:MET:HG2	4:A:171:GLN:HE22	1.69	0.57
4:A:675:THR:O	4:A:679:ILE:HG12	2.02	0.57
6:C:33:LEU:O	6:C:37:MET:HG3	2.04	0.57
4:A:42:ASP:HB3	4:A:46:THR:HB	1.86	0.57
4:A:181:LEU:HB2	4:A:202:LEU:HB2	1.86	0.57
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.86	0.57
4:A:1075:PRO:O	4:A:1079:MET:N	2.38	0.57
5:B:21:GLU:O	5:B:654:ARG:HB3	2.04	0.57
5:B:830:TYR:OH	5:B:1074:ASN:ND2	2.36	0.57
4:A:153:PRO:HA	4:A:162:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:230:ARG:NH2	4:A:231:PRO:HD2	2.19	0.57
6:C:99:LEU:HD13	6:C:120:ILE:HG12	1.86	0.57
2:T:26:DG:H3'	2:T:27:DA:H8	1.70	0.57
4:A:374:LEU:HA	5:B:1107:ALA:HB2	1.85	0.57
7:E:192:ARG:HA	7:E:214:CYS:HB3	1.85	0.57
4:A:23:SER:OG	4:A:26:GLU:HG2	2.05	0.57
4:A:1329:THR:H	4:A:1335:ILE:HD11	1.70	0.57
5:B:424:LEU:HD11	5:B:448:ILE:HG13	1.87	0.57
5:B:570:VAL:HG23	5:B:573:GLN:HB2	1.85	0.57
5:B:1033:LYS:HG2	5:B:1059:LEU:HD11	1.87	0.57
13:L:34:CYS:HB3	13:L:51:CYS:HB3	1.85	0.57
4:A:303:TYR:CZ	4:A:325:ILE:HD11	2.39	0.57
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.38	0.57
5:B:43:LEU:HG	5:B:492:LEU:HD22	1.87	0.57
5:B:210:LYS:NZ	5:B:462:ALA:HA	2.20	0.57
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.86	0.57
5:B:1168:LEU:HD23	5:B:1208:MET:HE2	1.87	0.57
6:C:177:GLU:O	6:C:230:MET:HA	2.05	0.57
4:A:450:LEU:HD22	4:A:1077:THR:HG21	1.85	0.57
5:B:308:TRP:H	5:B:308:TRP:CD1	2.22	0.57
6:C:101:LEU:HD13	6:C:118:LEU:HA	1.87	0.57
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.37	0.57
4:A:913:LEU:HD22	4:A:915:SER:CB	2.35	0.57
6:C:46:ILE:HA	6:C:159:ALA:HA	1.87	0.57
7:E:190:LEU:HD22	7:E:214:CYS:SG	2.45	0.57
4:A:71:GLN:OE1	5:B:1177:HIS:ND1	2.39	0.56
4:A:387:ARG:O	4:A:391:LEU:HG	2.05	0.56
4:A:951:GLU:O	4:A:954:TRP:NE1	2.38	0.56
5:B:104:GLU:HG2	5:B:110:HIS:CE1	2.40	0.56
7:E:64:PRO:HD3	7:E:77:SER:H	1.69	0.56
2:T:9:DC:H2'	2:T:10:DT:H71	1.86	0.56
4:A:446:ARG:HG3	4:A:448:PRO:HD2	1.86	0.56
5:B:1016:ALA:O	5:B:1020:ARG:HG2	2.05	0.56
6:C:11:ARG:NH2	6:C:19:ASP:OD1	2.38	0.56
6:C:35:ARG:HA	6:C:38:ILE:HD12	1.86	0.56
4:A:863:VAL:CG2	7:E:170:LEU:HD11	2.34	0.56
4:A:1216:ILE:HG22	4:A:1220:PHE:CZ	2.40	0.56
5:B:30:SER:OG	5:B:743:ILE:O	2.21	0.56
5:B:611:PRO:HG3	5:B:685:LEU:HD21	1.88	0.56
7:E:46:TYR:HE1	7:E:58:MET:HG3	1.70	0.56
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:151:ASP:OD2	4:A:163:SER:OG	2.21	0.56
6:C:52:GLU:HG2	6:C:53:THR:HG23	1.87	0.56
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.40	0.56
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.87	0.56
4:A:613:ILE:HG21	9:H:102:TYR:HB3	1.87	0.56
4:A:665:GLY:HA2	5:B:1086:PHE:CD2	2.41	0.56
5:B:754:SER:HB2	5:B:812:LEU:HD11	1.87	0.56
9:H:91:ASP:HB2	9:H:93:TYR:CD1	2.40	0.56
6:C:17:ASN:HA	6:C:232:VAL:O	2.05	0.56
6:C:203:GLN:OE1	6:C:203:GLN:N	2.39	0.56
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.88	0.56
8:F:83:PRO:HA	8:F:146:TRP:HZ3	1.70	0.56
4:A:18:GLN:HB2	4:A:1418:LEU:HD12	1.87	0.55
4:A:660:ASN:HA	5:B:1082:MET:HB3	1.87	0.55
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.70	0.55
5:B:55:VAL:HA	5:B:59:LEU:HD23	1.88	0.55
4:A:551:TYR:CZ	12:K:74:ARG:HB2	2.42	0.55
4:A:915:SER:O	4:A:918:GLU:HG3	2.06	0.55
5:B:273:LEU:HD13	5:B:355:ILE:HG21	1.89	0.55
5:B:373:ARG:NH2	5:B:587:HIS:HA	2.22	0.55
10:I:22:ASN:HD22	10:I:24:ARG:HD3	1.71	0.55
10:I:89:GLN:O	10:I:91:ARG:NE	2.39	0.55
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.88	0.55
5:B:370:PHE:CE2	5:B:373:ARG:HD3	2.41	0.55
4:A:907:THR:HG21	4:A:920:LEU:HD22	1.88	0.55
5:B:810:GLU:HB3	5:B:815:ARG:NH2	2.22	0.55
11:J:23:ASN:O	11:J:27:GLU:OE1	2.25	0.55
4:A:739:ASP:N	4:A:739:ASP:OD1	2.37	0.55
4:A:131:SER:HB2	4:A:223:GLY:HA3	1.89	0.55
4:A:1212:VAL:O	4:A:1216:ILE:HD12	2.07	0.55
4:A:1290:LYS:HA	4:A:1300:LYS:HA	1.89	0.55
5:B:496:ARG:HH12	5:B:541:LEU:HA	1.70	0.55
6:C:55:THR:OG1	6:C:152:GLU:N	2.39	0.55
3:N:3:DA:H1'	3:N:4:DG:H5'	1.89	0.55
5:B:841:MET:HE3	5:B:990:ILE:HG21	1.87	0.55
5:B:856:PHE:HB3	5:B:967:ARG:HD2	1.88	0.55
7:E:200:ARG:NH2	7:E:210:SER:OG	2.40	0.55
4:A:578:LEU:O	4:A:582:ILE:HG13	2.08	0.55
5:B:99:LYS:HA	5:B:178:ASN:HD21	1.72	0.55
4:A:63:ARG:HA	4:A:74:MET:HE3	1.88	0.54
4:A:1011:GLN:O	4:A:1015:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:702:LEU:HD13	4:A:710:LEU:HG	1.90	0.54
5:B:118:ARG:NH2	5:B:194:GLU:OE2	2.40	0.54
5:B:123:THR:HG23	5:B:205:ILE:HA	1.89	0.54
6:C:206:ASN:HA	6:C:209:TYR:CD2	2.42	0.54
7:E:43:LYS:O	7:E:47:CYS:N	2.34	0.54
5:B:497:ARG:HE	5:B:538:ASN:HD21	1.56	0.54
5:B:835:GLN:O	5:B:838:SER:OG	2.23	0.54
5:B:1106:ARG:HH12	5:B:1118:PRO:HB3	1.73	0.54
4:A:618:GLU:OE1	4:A:620:LYS:N	2.37	0.54
5:B:520:GLY:HA3	5:B:635:ARG:HH21	1.73	0.54
5:B:1152:MET:HE1	5:B:1195:HIS:HB3	1.88	0.54
4:A:122:MET:HE2	4:A:141:LEU:HD12	1.90	0.54
4:A:870:GLU:OE2	4:A:1345:ARG:NH2	2.41	0.54
4:A:1118:VAL:HA	4:A:1327:ILE:HG12	1.88	0.54
5:B:544:CYS:HB2	5:B:634:TYR:CE2	2.43	0.54
4:A:97:ALA:O	4:A:101:LYS:HG2	2.07	0.54
4:A:214:ILE:HB	4:A:219:PHE:CE1	2.43	0.54
4:A:214:ILE:HB	4:A:219:PHE:CZ	2.42	0.54
4:A:350:ARG:HE	4:A:486:GLU:HB3	1.71	0.54
5:B:384:ARG:NH1	5:B:621:GLU:OE2	2.34	0.54
7:E:178:ILE:HG23	7:E:214:CYS:HA	1.90	0.54
4:A:355:GLY:HA3	4:A:482:PHE:CZ	2.43	0.54
4:A:1033:GLN:O	4:A:1036:ARG:NH2	2.41	0.54
4:A:1121:GLU:OE2	4:A:1130:GLN:NE2	2.35	0.54
5:B:801:LYS:N	11:J:52:THR:O	2.36	0.54
5:B:806:THR:HG23	5:B:1045:SER:HA	1.90	0.54
5:B:977:GLY:H	5:B:990:ILE:HG13	1.73	0.54
4:A:22:PHE:HE2	5:B:1208:MET:HA	1.73	0.54
4:A:789:LYS:O	10:I:69:PRO:HG3	2.08	0.54
5:B:806:THR:H	5:B:809:MET:HE3	1.73	0.54
5:B:1057:LYS:O	5:B:1061:GLU:OE1	2.25	0.54
10:I:28:GLU:OE1	10:I:28:GLU:N	2.41	0.54
5:B:116:GLU:O	5:B:120:ARG:HG2	2.08	0.53
4:A:24:PRO:HB3	4:A:238:CYS:HB3	1.90	0.53
4:A:463:ILE:HD13	4:A:469:ARG:HG2	1.89	0.53
4:A:851:HIS:CD2	8:F:139:PRO:HG3	2.42	0.53
4:A:942:PHE:O	4:A:946:VAL:HG23	2.07	0.53
5:B:239:GLU:HB3	5:B:255:GLN:HG2	1.90	0.53
7:E:120:ALA:O	7:E:124:VAL:HG23	2.08	0.53
5:B:243:ALA:HB2	5:B:251:ILE:HD12	1.90	0.53
5:B:635:ARG:HH22	5:B:742:GLU:CD	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:119:ARG:HA	8:F:122:MET:HE2	1.89	0.53
9:H:33:GLN:HB3	9:H:35:GLN:HE22	1.73	0.53
9:H:94:ASP:HB3	9:H:146:ARG:NH1	2.23	0.53
9:H:10:PHE:CZ	9:H:36:CYS:HB3	2.43	0.53
4:A:337:ARG:HG3	5:B:1132:GLU:OE2	2.09	0.53
5:B:21:GLU:HA	5:B:656:GLY:H	1.73	0.53
5:B:857:ARG:HG2	5:B:859:TYR:CZ	2.44	0.53
4:A:229:SER:OG	4:A:1413:GLY:O	2.24	0.53
4:A:335:ARG:HH12	5:B:1202:LEU:HB3	1.74	0.53
4:A:388:LEU:O	4:A:392:VAL:HG23	2.07	0.53
4:A:670:ILE:HG12	4:A:805:LEU:HD11	1.90	0.53
4:A:1140:HIS:ND1	4:A:1277:GLU:O	2.42	0.53
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.44	0.53
10:I:10:CYS:HB3	10:I:32:CYS:SG	2.48	0.53
1:R:2:U:H2'	1:R:3:C:C6	2.44	0.53
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.41	0.53
4:A:800:VAL:HG22	4:A:812:GLU:HG2	1.90	0.53
5:B:129:PHE:HA	5:B:166:PHE:HA	1.90	0.53
5:B:651:LEU:HD13	5:B:653:VAL:HG23	1.89	0.53
5:B:763:GLN:HG3	5:B:765:PRO:HD2	1.91	0.53
4:A:998:LEU:HD13	4:A:1011:GLN:HG3	1.91	0.52
4:A:1001:ARG:HD2	8:F:83:PRO:HD3	1.91	0.52
5:B:31:TRP:CE2	5:B:807:ARG:HD3	2.44	0.52
9:H:37:LYS:H	9:H:126:GLU:HB2	1.74	0.52
11:J:33:GLY:HA2	11:J:36:LEU:HD12	1.90	0.52
4:A:30:ILE:HD12	5:B:1170:THR:HG21	1.91	0.52
4:A:345:VAL:HG23	4:A:348:SER:HB3	1.90	0.52
5:B:282:ILE:HA	5:B:285:ILE:HD12	1.91	0.52
5:B:800:GLN:NE2	11:J:49:MET:SD	2.82	0.52
4:A:550:LEU:HD21	4:A:561:PRO:HD2	1.92	0.52
5:B:332:ASP:OD1	5:B:348:ARG:NH2	2.42	0.52
10:I:74:GLU:HB3	10:I:81:ARG:HA	1.91	0.52
4:A:547:LEU:HD22	12:K:58:PHE:HD2	1.73	0.52
4:A:881:GLN:HA	4:A:961:ARG:HH21	1.74	0.52
4:A:913:LEU:HD22	4:A:915:SER:N	2.20	0.52
4:A:1424:VAL:HG22	4:A:1436:ILE:HG12	1.91	0.52
5:B:496:ARG:NH1	5:B:541:LEU:HA	2.24	0.52
5:B:635:ARG:HG3	5:B:637:LEU:HD13	1.91	0.52
5:B:656:GLY:O	5:B:660:LYS:HG3	2.09	0.52
4:A:535:THR:O	4:A:575:LYS:NZ	2.43	0.52
4:A:913:LEU:CD2	4:A:915:SER:H	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1207:LEU:HD11	4:A:1273:LEU:HB2	1.92	0.52
4:A:1431:GLY:HA3	5:B:1197:PRO:HD3	1.92	0.52
5:B:801:LYS:HG2	11:J:52:THR:HA	1.90	0.52
6:C:241:ASP:OD1	6:C:242:GLN:N	2.42	0.52
9:H:39:THR:O	9:H:123:MET:HA	2.10	0.52
4:A:449:SER:HB3	5:B:1137:CYS:SG	2.49	0.52
4:A:1000:LEU:HD13	4:A:1007:ILE:HD12	1.90	0.52
4:A:1433:MET:HB2	5:B:1148:LYS:HD3	1.91	0.52
5:B:489:SER:HA	5:B:492:LEU:HD12	1.92	0.52
5:B:601:ARG:O	5:B:605:ARG:HD3	2.09	0.52
11:J:7:CYS:HA	11:J:49:MET:HE3	1.92	0.52
4:A:538:ASP:OD1	9:H:20:TYR:HB3	2.10	0.52
4:A:665:GLY:HA3	5:B:1069:PHE:CZ	2.44	0.52
4:A:752:LYS:HE3	5:B:1016:ALA:HA	1.92	0.52
4:A:909:ASP:HB3	4:A:912:LEU:HG	1.92	0.52
5:B:848:ARG:NH1	11:J:8:PHE:O	2.43	0.52
4:A:350:ARG:NE	4:A:486:GLU:HB3	2.24	0.52
4:A:915:SER:OG	4:A:918:GLU:OE2	2.28	0.52
5:B:324:ILE:HD12	5:B:329:THR:HB	1.92	0.52
2:T:6:DT:H4'	2:T:7:DC:H5'	1.92	0.52
2:T:6:DT:H2''	2:T:7:DC:C5	2.45	0.52
4:A:781:ASP:HB3	4:A:790:ASP:N	2.25	0.52
4:A:1009:ASN:HA	4:A:1012:ARG:NE	2.25	0.52
5:B:37:PHE:HB2	5:B:681:TRP:CE3	2.45	0.52
4:A:668:ASP:OD2	4:A:742:ASN:N	2.42	0.52
6:C:177:GLU:N	6:C:177:GLU:OE1	2.43	0.52
4:A:1037:LEU:HD23	4:A:1042:PHE:HB2	1.92	0.51
5:B:167:ILE:HG22	5:B:448:ILE:HD11	1.92	0.51
5:B:693:ILE:HG21	5:B:701:ILE:HD13	1.92	0.51
7:E:103:LYS:HB3	7:E:105:PHE:CG	2.45	0.51
9:H:106:GLU:HG2	9:H:108:SER:O	2.09	0.51
12:K:42:LEU:HG	12:K:46:ILE:HD11	1.93	0.51
4:A:694:THR:O	4:A:698:GLN:HG3	2.09	0.51
4:A:1262:LYS:HA	4:A:1265:ASN:OD1	2.10	0.51
6:C:138:GLU:OE1	6:C:138:GLU:N	2.44	0.51
4:A:684:ALA:O	4:A:688:LYS:HG2	2.10	0.51
5:B:228:LYS:HG3	5:B:234:ILE:HG13	1.91	0.51
7:E:190:LEU:HD11	7:E:196:VAL:HG21	1.91	0.51
10:I:75:CYS:HB2	10:I:110:PHE:CD1	2.44	0.51
4:A:743:VAL:O	4:A:747:VAL:HG23	2.10	0.51
4:A:1105:LEU:HB3	4:A:1384:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.92	0.51
6:C:239:PRO:O	6:C:243:VAL:HG23	2.10	0.51
4:A:272:ALA:O	4:A:276:LEU:HD23	2.11	0.51
4:A:384:ASN:O	4:A:388:LEU:HB2	2.10	0.51
4:A:544:ASP:OD1	4:A:544:ASP:N	2.44	0.51
4:A:863:VAL:HG23	7:E:170:LEU:HD11	1.92	0.51
4:A:900:ASP:HB3	4:A:906:HIS:HB3	1.92	0.51
5:B:199:MET:SD	5:B:199:MET:N	2.82	0.51
5:B:437:GLU:CD	5:B:437:GLU:H	2.19	0.51
10:I:7:CYS:HB2	10:I:34:TYR:HD2	1.75	0.51
4:A:230:ARG:HE	4:A:232:GLU:CD	2.18	0.51
4:A:383:TYR:CD1	8:F:115:THR:HB	2.46	0.51
4:A:679:ILE:O	4:A:683:ILE:HG12	2.09	0.51
4:A:830:LYS:HZ1	4:A:1081:LEU:HB3	1.75	0.51
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.93	0.51
12:K:11:LEU:C	12:K:37:LYS:HG2	2.35	0.51
4:A:492:PRO:HB3	4:A:497:THR:HG22	1.92	0.51
4:A:994:GLN:HE21	4:A:1022:LEU:HD23	1.74	0.51
5:B:881:ASN:HB3	5:B:934:LYS:HG3	1.93	0.51
7:E:12:LEU:HD22	7:E:137:GLU:OE2	2.11	0.51
7:E:79:TRP:HB2	7:E:105:PHE:CD2	2.42	0.51
4:A:339:ASN:O	4:A:343:LYS:HG2	2.10	0.51
4:A:881:GLN:HB3	4:A:1025:ARG:HH22	1.75	0.51
5:B:213:ILE:HG23	5:B:497:ARG:HB3	1.92	0.51
7:E:40:GLU:HA	7:E:43:LYS:HE2	1.93	0.51
4:A:452:LYS:O	5:B:1141:HIS:NE2	2.42	0.51
4:A:523:ILE:HB	4:A:622:VAL:HG22	1.92	0.51
4:A:1427:ASN:OD1	4:A:1432:GLN:HB2	2.10	0.51
5:B:125:SER:OG	5:B:169:ARG:HB3	2.11	0.51
5:B:242:SER:HG	5:B:363:HIS:CE1	2.29	0.51
5:B:350:GLN:HA	5:B:353:LYS:HD3	1.92	0.51
5:B:642:ASP:HA	5:B:649:LYS:HA	1.92	0.51
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.93	0.51
4:A:449:SER:HB2	5:B:1133:MET:HB3	1.93	0.51
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.11	0.51
9:H:17:PRO:HA	9:H:24:CYS:SG	2.51	0.51
5:B:883:LEU:HD12	5:B:884:ARG:H	1.75	0.50
7:E:65:THR:O	7:E:69:ILE:HG23	2.12	0.50
10:I:65:ASP:OD2	10:I:67:THR:OG1	2.20	0.50
4:A:122:MET:O	4:A:126:LEU:HG	2.11	0.50
5:B:384:ARG:HA	5:B:387:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:637:LEU:HD22	5:B:693:ILE:HD12	1.93	0.50
5:B:1114:LEU:HG	5:B:1202:LEU:HD11	1.92	0.50
5:B:1220:ARG:HH11	5:B:1221:SER:H	1.58	0.50
4:A:785:PRO:HG2	5:B:703:ILE:HD11	1.93	0.50
4:A:900:ASP:H	4:A:906:HIS:HB3	1.75	0.50
4:A:1166:ASP:O	4:A:1170:ILE:HG12	2.11	0.50
5:B:527:THR:OG1	5:B:534:GLY:N	2.40	0.50
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.93	0.50
6:C:250:THR:O	6:C:254:LYS:HG3	2.12	0.50
4:A:216:VAL:HA	4:A:219:PHE:HD2	1.77	0.50
4:A:399:HIS:NE2	4:A:462:VAL:HG21	2.27	0.50
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	1.94	0.50
2:T:21:DC:H5'	5:B:1129:ARG:HD3	1.94	0.50
9:H:26:ILE:HB	9:H:40:LEU:HB3	1.94	0.50
4:A:534:LEU:HD23	4:A:578:LEU:HD22	1.93	0.50
4:A:1395:GLY:O	4:A:1399:ARG:NH1	2.44	0.50
13:L:47:ARG:HH21	13:L:54:ARG:HH21	1.58	0.50
4:A:557:ASP:OD1	4:A:559:VAL:N	2.39	0.50
5:B:193:LYS:HD2	5:B:787:VAL:HG11	1.92	0.50
5:B:1054:GLY:O	5:B:1058:LEU:HG	2.11	0.50
7:E:156:LEU:HD12	7:E:160:GLU:HB3	1.93	0.50
4:A:346:ASP:CG	5:B:1106:ARG:HH21	2.19	0.50
6:C:41:ILE:HD11	6:C:247:GLY:HA2	1.93	0.50
8:F:83:PRO:HB2	8:F:152:ILE:HD13	1.93	0.50
11:J:59:LYS:H	11:J:59:LYS:HD2	1.76	0.50
4:A:224:PHE:HB3	4:A:229:SER:HB2	1.92	0.50
5:B:309:GLN:O	5:B:313:MET:HG3	2.11	0.50
5:B:426:LYS:HG3	5:B:430:ARG:NE	2.26	0.50
11:J:8:PHE:H	11:J:49:MET:HE3	1.76	0.50
4:A:482:PHE:O	5:B:989:THR:OG1	2.29	0.49
4:A:1227:ILE:HG13	4:A:1239:ARG:HB2	1.94	0.49
4:A:1327:ILE:O	7:E:147:HIS:NE2	2.36	0.49
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.93	0.49
4:A:335:ARG:HH12	5:B:1202:LEU:HD13	1.77	0.49
4:A:857:ARG:HB3	4:A:861:GLY:HA2	1.94	0.49
5:B:564:GLU:OE2	5:B:591:ARG:NH2	2.44	0.49
5:B:599:THR:O	5:B:603:LEU:HG	2.12	0.49
6:C:97:VAL:HG21	6:C:129:ILE:HG22	1.94	0.49
9:H:128:ASN:OD1	9:H:131:ASN:ND2	2.45	0.49
4:A:368:LYS:N	12:K:2:ASN:HD21	2.11	0.49
4:A:880:LYS:HA	4:A:955:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1138:ILE:HA	4:A:1276:VAL:HG23	1.94	0.49
5:B:915:THR:HG21	5:B:934:LYS:HE3	1.94	0.49
5:B:1103:ILE:C	5:B:1122:ARG:HH12	2.20	0.49
6:C:10:ILE:HA	6:C:20:PHE:HA	1.94	0.49
7:E:37:LEU:HD12	7:E:38:PRO:HD2	1.95	0.49
10:I:37:GLU:OE1	10:I:37:GLU:N	2.43	0.49
4:A:1317:MET:HG3	4:A:1318:THR:HG23	1.94	0.49
4:A:1317:MET:HE3	7:E:142:VAL:HB	1.94	0.49
5:B:21:GLU:HA	5:B:656:GLY:N	2.28	0.49
4:A:482:PHE:CD2	5:B:836:GLU:HB2	2.48	0.49
4:A:1348:LEU:HD21	4:A:1375:MET:SD	2.53	0.49
4:A:1398:MET:HE1	4:A:1423:GLY:HA3	1.94	0.49
5:B:519:TRP:NE1	5:B:742:GLU:OE2	2.35	0.49
4:A:148:CYS:HB2	4:A:167:CYS:HB2	1.93	0.49
4:A:820:GLY:O	4:A:824:LEU:HG	2.13	0.49
4:A:836:TYR:O	4:A:840:ARG:HG3	2.13	0.49
5:B:195:CYS:H	5:B:784:ASN:HD22	1.60	0.49
9:H:5:LEU:HD12	9:H:135:LEU:HD23	1.95	0.49
4:A:25:GLU:HA	4:A:28:ARG:HE	1.78	0.49
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.95	0.49
4:A:591:PHE:HD2	4:A:595:THR:HB	1.78	0.49
5:B:168:GLY:HA2	5:B:450:ALA:HB1	1.93	0.49
6:C:251:LEU:O	6:C:255:VAL:HG23	2.12	0.49
13:L:28:LYS:N	13:L:39:SER:HG	2.11	0.49
4:A:1166:ASP:CG	4:A:1239:ARG:HD2	2.37	0.49
5:B:23:ALA:HB3	5:B:655:LYS:HG3	1.95	0.49
6:C:45:ALA:H	6:C:170:TRP:HE1	1.61	0.49
7:E:171:LYS:HE3	7:E:172:GLU:H	1.78	0.49
11:J:41:LEU:HB3	11:J:46:CYS:HB2	1.95	0.49
4:A:34:LYS:HE3	4:A:83:HIS:CE1	2.48	0.49
4:A:106:VAL:HG11	4:A:214:ILE:HD13	1.93	0.49
4:A:108:MET:SD	4:A:210:ILE:HD13	2.53	0.49
4:A:218:ASP:O	4:A:222:LEU:HG	2.13	0.49
4:A:827:THR:O	4:A:831:THR:HG23	2.13	0.49
4:A:891:ALA:O	4:A:895:LYS:HG3	2.13	0.49
4:A:1035:TYR:HE1	4:A:1037:LEU:HD22	1.78	0.49
5:B:916:THR:OG1	5:B:935:ARG:HB3	2.12	0.49
7:E:55:ARG:H	7:E:84:ASP:CG	2.21	0.49
9:H:113:ALA:HB1	9:H:124:ARG:HH12	1.78	0.49
4:A:777:PHE:HA	4:A:783:THR:HA	1.94	0.49
5:B:1159:ARG:HD3	5:B:1161:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:93:TYR:HA	9:H:145:ARG:HD3	1.95	0.49
13:L:68:GLU:O	13:L:70:ARG:NH1	2.46	0.49
2:T:14:DG:H2''	2:T:15:DC:H5'	1.95	0.48
4:A:728:LYS:O	4:A:732:LEU:HG	2.13	0.48
4:A:782:ARG:HH12	5:B:702:LEU:HD13	1.77	0.48
5:B:454:THR:HG22	5:B:458:LYS:HD3	1.95	0.48
4:A:849:MET:HE1	4:A:1436:ILE:HA	1.96	0.48
4:A:1013:ASP:O	7:E:205:SER:HB2	2.12	0.48
5:B:34:ILE:HD11	5:B:744:HIS:HB2	1.94	0.48
5:B:219:ALA:HB2	5:B:405:ARG:HE	1.78	0.48
9:H:37:LYS:HB2	9:H:126:GLU:HG3	1.95	0.48
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.95	0.48
6:C:108:GLU:HG3	6:C:149:LYS:HD2	1.95	0.48
4:A:779:PHE:CE2	4:A:785:PRO:HD3	2.48	0.48
5:B:847:ASP:O	5:B:852:ARG:NH1	2.44	0.48
5:B:863:GLU:HG3	5:B:962:LYS:HB3	1.94	0.48
4:A:902:LEU:HG	4:A:926:GLN:HG2	1.94	0.48
5:B:194:GLU:OE1	5:B:784:ASN:ND2	2.47	0.48
5:B:282:ILE:HD12	5:B:382:ILE:HD13	1.94	0.48
5:B:834:ASN:HD22	5:B:1013:ASN:HA	1.78	0.48
5:B:1171:VAL:HA	5:B:1181:GLU:O	2.13	0.48
6:C:255:VAL:HG22	12:K:42:LEU:HD11	1.95	0.48
2:T:12:DT:O2	3:N:8:DG:N2	2.46	0.48
4:A:91:PHE:CD1	4:A:96:ILE:HD12	2.49	0.48
4:A:231:PRO:HA	4:A:234:MET:HG3	1.94	0.48
5:B:483:LEU:HD22	5:B:491:THR:HG23	1.96	0.48
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.96	0.48
10:I:108:HIS:HE1	10:I:110:PHE:HB3	1.77	0.48
4:A:109:HIS:CD2	4:A:169:ASN:HB3	2.49	0.48
4:A:550:LEU:HD12	4:A:577:ILE:HD13	1.96	0.48
4:A:1282:VAL:HG12	4:A:1308:THR:HG22	1.95	0.48
4:A:1352:VAL:O	4:A:1356:ILE:HG12	2.14	0.48
5:B:1079:LYS:HE3	6:C:188:HIS:CG	2.49	0.48
7:E:91:LYS:O	7:E:95:THR:HG23	2.13	0.48
8:F:85:MET:HG3	8:F:151:LEU:HD22	1.95	0.48
4:A:709:THR:OG1	4:A:712:GLU:HB2	2.14	0.48
5:B:832:GLY:HA2	5:B:835:GLN:HE21	1.79	0.48
7:E:24:LYS:HE2	7:E:35:VAL:HG21	1.96	0.48
10:I:20:LYS:H	10:I:20:LYS:HD2	1.79	0.48
4:A:203:SER:HB3	4:A:206:GLU:HB3	1.96	0.48
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1193:LEU:HB2	4:A:1260:LEU:HD11	1.96	0.48
5:B:93:GLY:HA3	5:B:131:ASP:HB2	1.96	0.48
5:B:256:VAL:HG12	5:B:385:LEU:HD22	1.96	0.48
7:E:90:VAL:HG23	7:E:120:ALA:HA	1.95	0.48
9:H:138:GLU:OE1	9:H:138:GLU:N	2.47	0.48
4:A:138:ILE:O	4:A:142:CYS:HB2	2.14	0.47
4:A:506:ALA:HB3	4:A:509:LEU:HG	1.95	0.47
4:A:532:ARG:HD3	4:A:749:ALA:HB2	1.96	0.47
5:B:650:GLU:HA	5:B:710:LEU:HD21	1.95	0.47
5:B:992:ILE:HD11	12:K:66:PRO:HB2	1.95	0.47
5:B:1029:CYS:HB3	5:B:1088:GLY:HA3	1.96	0.47
11:J:13:VAL:O	11:J:17:LYS:NZ	2.30	0.47
1:R:7:A:H2'	1:R:8:G:H8	1.79	0.47
4:A:12:ARG:HD2	5:B:1218:THR:HB	1.96	0.47
4:A:22:PHE:CD2	5:B:1213:THR:HG22	2.49	0.47
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.96	0.47
4:A:116:ASP:O	4:A:117:GLU:HG2	2.14	0.47
4:A:357:PRO:HG2	5:B:831:SER:O	2.15	0.47
4:A:1107:VAL:HG22	4:A:1383:SER:HB2	1.95	0.47
5:B:701:ILE:HB	5:B:739:THR:OG1	2.14	0.47
6:C:77:ILE:N	6:C:129:ILE:HD11	2.29	0.47
7:E:87:SER:HA	7:E:115:ASN:O	2.15	0.47
3:N:3:DA:H2''	3:N:4:DG:H2'	1.96	0.47
4:A:901:LEU:HD13	4:A:919:ILE:HG13	1.97	0.47
4:A:924:LYS:O	4:A:927:VAL:HG22	2.14	0.47
4:A:1268:LEU:HD22	10:I:48:LEU:HD11	1.96	0.47
5:B:245:GLU:HA	5:B:249:ARG:NH2	2.26	0.47
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.46	0.47
4:A:1122:PRO:HD3	4:A:1323:ASP:HB2	1.97	0.47
4:A:1127:ASP:HB3	4:A:1130:GLN:HB3	1.95	0.47
6:C:50:GLU:HB2	13:L:66:GLN:HB3	1.95	0.47
11:J:25:LEU:HA	11:J:30:LEU:HB2	1.96	0.47
4:A:565:ILE:HD13	9:H:46:LEU:HD12	1.96	0.47
4:A:786:HIS:CE1	5:B:742:GLU:HG3	2.48	0.47
4:A:1138:ILE:HD11	4:A:1316:VAL:HG22	1.96	0.47
5:B:1208:MET:HE3	5:B:1214:PRO:HG2	1.95	0.47
6:C:104:PHE:HB2	6:C:152:GLU:HG3	1.96	0.47
4:A:86:LEU:HD11	4:A:90:VAL:HG22	1.96	0.47
4:A:244:PRO:HA	4:A:247:ARG:HG2	1.97	0.47
4:A:849:MET:HE3	4:A:1063:MET:SD	2.54	0.47
5:B:345:LYS:HA	5:B:345:LYS:HD3	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:471:LYS:O	5:B:474:SER:OG	2.31	0.47
6:C:6:PRO:HB2	12:K:101:LEU:HD12	1.97	0.47
6:C:11:ARG:NH1	6:C:206:ASN:OD1	2.47	0.47
7:E:22:MET:O	7:E:26:ARG:N	2.38	0.47
7:E:169:ARG:HH12	8:F:138:LEU:HD13	1.80	0.47
10:I:27:PHE:O	10:I:35:VAL:HA	2.15	0.47
11:J:34:THR:O	11:J:38:ARG:HG2	2.14	0.47
4:A:71:GLN:NE2	5:B:1176:ASN:HB2	2.30	0.47
4:A:481:ASP:OD2	5:B:837:ASP:HB2	2.14	0.47
4:A:1215:ARG:O	4:A:1219:THR:HG23	2.14	0.47
5:B:213:ILE:HG12	5:B:479:VAL:O	2.15	0.47
5:B:355:ILE:HA	5:B:359:GLU:HG2	1.96	0.47
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.37	0.47
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	1.97	0.47
6:C:46:ILE:O	6:C:169:LYS:NZ	2.45	0.47
6:C:91:HIS:HB3	6:C:96:SER:OG	2.15	0.47
6:C:205:LYS:HD2	6:C:208:GLU:OE2	2.15	0.47
9:H:100:THR:HA	9:H:138:GLU:O	2.14	0.47
4:A:19:PHE:HB3	4:A:1413:GLY:HA2	1.95	0.47
4:A:92:HIS:HB3	4:A:95:PHE:CD2	2.50	0.47
4:A:1207:LEU:HD22	4:A:1212:VAL:HG22	1.97	0.47
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	1.96	0.47
5:B:298:LEU:HD11	5:B:318:VAL:HG21	1.97	0.47
6:C:26:ASP:OD1	6:C:29:MET:HB3	2.15	0.47
6:C:183:TRP:CD1	6:C:210:GLU:HB2	2.49	0.47
10:I:44:TYR:CE2	10:I:46:HIS:HB2	2.50	0.47
4:A:840:ARG:HG2	4:A:1402:PHE:CZ	2.50	0.47
4:A:1119:TYR:CG	4:A:1326:ARG:HB3	2.50	0.47
5:B:597:MET:O	5:B:601:ARG:HG3	2.14	0.47
5:B:745:PRO:HB2	5:B:1047:PHE:CD2	2.50	0.47
5:B:857:ARG:HD2	5:B:942:ARG:HH21	1.79	0.47
5:B:859:TYR:OH	5:B:945:GLU:OE2	2.29	0.47
6:C:181:ASP:OD2	6:C:186:LEU:HB2	2.15	0.47
7:E:127:ILE:HD11	7:E:132:ILE:HD11	1.97	0.47
2:T:8:DT:H2''	2:T:9:DC:C6	2.50	0.47
4:A:420:ARG:O	4:A:424:ILE:HG23	2.14	0.47
4:A:903:ASN:O	4:A:907:THR:OG1	2.32	0.47
4:A:946:VAL:HA	7:E:201:LYS:HD2	1.96	0.47
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.96	0.47
1:R:4:G:H2'	1:R:5:A:C8	2.50	0.46
4:A:99:ILE:HG23	4:A:211:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:407:ARG:NH2	4:A:411:ASP:HB2	2.30	0.46
4:A:527:THR:O	4:A:653:VAL:HG11	2.15	0.46
7:E:55:ARG:HH11	7:E:84:ASP:HA	1.81	0.46
10:I:54:GLU:HB2	10:I:100:PHE:CE2	2.49	0.46
11:J:10:CYS:SG	11:J:43:ARG:NE	2.88	0.46
4:A:380:VAL:HB	4:A:385:ILE:HD11	1.97	0.46
5:B:551:PRO:O	5:B:555:ILE:HG12	2.14	0.46
5:B:708:GLU:O	5:B:711:GLU:HG3	2.16	0.46
5:B:1159:ARG:HG3	5:B:1193:GLN:HE21	1.80	0.46
6:C:99:LEU:CD1	6:C:120:ILE:HG12	2.45	0.46
13:L:68:GLU:HG2	13:L:70:ARG:H	1.80	0.46
4:A:365:GLY:O	4:A:468:PHE:HD1	1.98	0.46
4:A:1116:LEU:O	4:A:1308:THR:HG23	2.15	0.46
5:B:393:LYS:HA	5:B:393:LYS:HD3	1.69	0.46
5:B:654:ARG:O	5:B:658:ILE:HG12	2.16	0.46
4:A:181:LEU:O	4:A:202:LEU:N	2.41	0.46
4:A:260:ASP:OD2	4:A:262:LEU:HB2	2.14	0.46
4:A:586:ILE:HD11	4:A:637:LYS:HD3	1.96	0.46
4:A:756:ILE:O	4:A:760:GLN:HG3	2.16	0.46
4:A:994:GLN:HE22	4:A:1023:ARG:NE	2.13	0.46
5:B:103:ASN:HA	5:B:109:THR:HA	1.97	0.46
5:B:119:LEU:O	5:B:965:LYS:NZ	2.46	0.46
5:B:453:ILE:O	5:B:457:LEU:HG	2.16	0.46
5:B:520:GLY:HA3	5:B:635:ARG:NH2	2.31	0.46
5:B:951:GLN:OE1	5:B:967:ARG:NH2	2.48	0.46
4:A:91:PHE:HB3	4:A:235:ILE:HG22	1.98	0.46
4:A:262:LEU:HD13	4:A:328:ARG:NH2	2.31	0.46
4:A:368:LYS:H	12:K:2:ASN:HD21	1.64	0.46
5:B:1162:ILE:O	5:B:1192:TYR:HB2	2.15	0.46
6:C:40:GLU:OE2	6:C:165:LYS:HD3	2.16	0.46
9:H:100:THR:HG23	9:H:138:GLU:HB2	1.97	0.46
4:A:16:GLU:OE1	5:B:1220:ARG:HG2	2.15	0.46
4:A:672:ASP:H	4:A:736:ASN:ND2	2.09	0.46
4:A:851:HIS:HD2	8:F:139:PRO:HG3	1.81	0.46
4:A:1209:MET:HB2	4:A:1209:MET:HE2	1.67	0.46
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.97	0.46
5:B:586:TRP:CD1	5:B:588:GLY:H	2.33	0.46
5:B:898:LEU:HD21	5:B:964:VAL:HG11	1.98	0.46
6:C:162:GLY:HA3	6:C:170:TRP:CE2	2.50	0.46
4:A:818:MET:HG2	5:B:514:LEU:HD23	1.98	0.46
4:A:901:LEU:HA	4:A:907:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1187:ASN:HB3	5:B:1189:ILE:HG12	1.97	0.46
6:C:21:ILE:HG12	6:C:229:TYR:CD2	2.50	0.46
7:E:99:HIS:O	7:E:103:LYS:HG2	2.15	0.46
4:A:537:ARG:NH1	9:H:41:ASP:OD2	2.49	0.46
4:A:582:ILE:HD13	4:A:607:ILE:HD13	1.97	0.46
4:A:631:HIS:O	4:A:635:ARG:HG2	2.16	0.46
4:A:975:HIS:HD1	4:A:1036:ARG:HG2	1.81	0.46
4:A:1000:LEU:HD23	4:A:1000:LEU:HA	1.85	0.46
5:B:35:SER:HB2	5:B:39:ARG:HH21	1.80	0.46
5:B:188:ASP:HA	5:B:191:LYS:HD2	1.97	0.46
5:B:218:SER:C	5:B:241:ARG:HH12	2.23	0.46
5:B:291:ILE:HG12	5:B:300:HIS:NE2	2.31	0.46
6:C:11:ARG:N	6:C:19:ASP:O	2.49	0.46
6:C:249:ASP:OD1	12:K:102:LYS:NZ	2.48	0.46
12:K:12:LEU:HD12	12:K:12:LEU:H	1.80	0.46
4:A:356:ASP:CG	12:K:65:HIS:HE2	2.24	0.46
4:A:566:ILE:HD13	9:H:96:VAL:HG12	1.98	0.46
4:A:666:ILE:HG13	4:A:667:GLY:N	2.31	0.46
4:A:1217:LYS:HD3	4:A:1226:VAL:HG22	1.98	0.46
5:B:758:PHE:HB2	5:B:1024:ALA:CB	2.46	0.46
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.51	0.46
4:A:532:ARG:HH12	4:A:745:GLN:HB3	1.80	0.46
4:A:597:LEU:HB3	9:H:102:TYR:HE2	1.81	0.46
4:A:675:THR:HG21	4:A:736:ASN:HB2	1.96	0.46
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.41	0.46
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.96	0.46
6:C:69:LEU:O	11:J:6:ARG:NH2	2.46	0.46
7:E:147:HIS:HB3	7:E:150:VAL:HG23	1.98	0.46
4:A:91:PHE:CE1	4:A:96:ILE:HD12	2.51	0.45
4:A:147:VAL:HB	4:A:170:THR:HA	1.98	0.45
4:A:204:THR:HA	4:A:207:ILE:HD12	1.98	0.45
4:A:606:LEU:O	4:A:613:ILE:N	2.48	0.45
4:A:1287:TYR:CZ	4:A:1305:VAL:HG11	2.51	0.45
5:B:219:ALA:O	5:B:241:ARG:NH1	2.50	0.45
5:B:1173:ALA:HB1	5:B:1180:PHE:HD1	1.80	0.45
7:E:197:LYS:HE2	7:E:199:ILE:HD11	1.99	0.45
9:H:15:VAL:HG11	9:H:49:VAL:HG21	1.98	0.45
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.98	0.45
4:A:32:VAL:HG21	4:A:68:GLN:HG2	1.97	0.45
4:A:1425:SER:O	4:A:1429:ILE:HD12	2.16	0.45
5:B:209:GLU:O	5:B:482:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:649:LYS:HE2	5:B:649:LYS:HB3	1.49	0.45
6:C:61:GLU:HG3	13:L:67:PHE:CE2	2.52	0.45
7:E:96:PHE:HA	7:E:99:HIS:ND1	2.31	0.45
9:H:117:SER:HB2	9:H:122:LEU:HD22	1.98	0.45
4:A:50:ILE:HG23	4:A:52:GLY:N	2.28	0.45
4:A:105:CYS:HA	4:A:142:CYS:HB3	1.97	0.45
4:A:671:ALA:HB3	4:A:676:MET:HE2	1.99	0.45
5:B:800:GLN:HB3	11:J:52:THR:HB	1.99	0.45
5:B:841:MET:HE1	5:B:980:PHE:CZ	2.51	0.45
10:I:17:ARG:NH1	10:I:18:GLU:H	2.14	0.45
4:A:344:ARG:CZ	5:B:1120:GLU:HG3	2.47	0.45
4:A:881:GLN:O	4:A:953:ASN:HA	2.17	0.45
4:A:1142:THR:HG22	4:A:1144:LYS:N	2.32	0.45
4:A:1210:GLY:O	4:A:1214:GLU:HG2	2.16	0.45
6:C:246:ARG:O	6:C:250:THR:OG1	2.29	0.45
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.98	0.45
4:A:537:ARG:NH2	4:A:599:SER:O	2.50	0.45
4:A:1102:LYS:HE2	4:A:1106:ASN:ND2	2.28	0.45
5:B:234:ILE:HG21	5:B:257:LYS:HB3	1.97	0.45
6:C:99:LEU:HB3	6:C:118:LEU:HD22	1.97	0.45
9:H:93:TYR:CD2	9:H:145:ARG:HB2	2.51	0.45
4:A:143:LYS:HG3	4:A:144:THR:HG23	1.97	0.45
4:A:1075:PRO:O	4:A:1079:MET:HG3	2.17	0.45
5:B:418:LYS:HE3	5:B:418:LYS:HB2	1.72	0.45
5:B:728:ARG:H	5:B:728:ARG:HG2	1.55	0.45
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.16	0.45
2:T:21:DC:H3'	2:T:22:DT:H71	1.98	0.45
4:A:338:GLY:O	5:B:1129:ARG:NH1	2.46	0.45
4:A:402:ALA:O	4:A:415:LEU:HD12	2.16	0.45
4:A:446:ARG:HH21	4:A:480:ALA:HA	1.81	0.45
4:A:874:ASP:HB2	4:A:1058:VAL:HA	1.99	0.45
5:B:102:VAL:HG12	5:B:125:SER:HB3	1.98	0.45
5:B:322:PHE:CE1	10:I:13:MET:HG2	2.52	0.45
5:B:582:VAL:HB	5:B:587:HIS:NE2	2.32	0.45
6:C:46:ILE:HG13	6:C:159:ALA:HB2	1.98	0.45
10:I:85:PHE:CD2	10:I:99:LEU:HD13	2.52	0.45
4:A:19:PHE:HZ	4:A:1409:LEU:HD22	1.82	0.45
4:A:37:PHE:CD2	4:A:50:ILE:HG13	2.51	0.45
4:A:1035:TYR:CD1	4:A:1037:LEU:HD13	2.52	0.45
4:A:1282:VAL:HA	4:A:1307:GLU:O	2.16	0.45
5:B:604:ARG:NH2	5:B:614:SER:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:205:LYS:O	6:C:208:GLU:HG2	2.17	0.45
4:A:463:ILE:CD1	4:A:469:ARG:HG2	2.46	0.45
4:A:647:GLY:O	4:A:651:LYS:HG3	2.17	0.45
4:A:1141:THR:HG23	4:A:1205:LYS:HE3	1.99	0.45
4:A:1400:CYS:HB2	4:A:1405:THR:HG23	1.99	0.45
5:B:705:MET:HE3	5:B:705:MET:HB3	1.80	0.45
6:C:86:CYS:SG	6:C:87:PHE:N	2.90	0.45
12:K:51:LEU:HD22	12:K:59:ALA:HB3	1.99	0.45
4:A:58:LEU:O	4:A:80:HIS:HD2	2.00	0.45
4:A:212:LYS:HA	4:A:212:LYS:HD2	1.86	0.45
4:A:469:ARG:HA	4:A:469:ARG:HD2	1.88	0.45
6:C:82:TYR:CD1	6:C:161:LYS:HB3	2.52	0.45
7:E:175:LEU:HD23	7:E:213:ILE:HB	1.99	0.45
13:L:30:ILE:N	13:L:57:LEU:O	2.43	0.45
4:A:1136:SER:HB2	4:A:1206:ASP:HB2	1.98	0.44
4:A:1208:THR:HG23	4:A:1211:GLN:H	1.82	0.44
5:B:1147:LEU:HD23	5:B:1147:LEU:HA	1.74	0.44
6:C:82:TYR:CE2	6:C:161:LYS:HE2	2.52	0.44
6:C:102:GLN:HB3	6:C:154:LYS:HG2	1.99	0.44
7:E:55:ARG:HB3	7:E:82:PHE:O	2.17	0.44
2:T:16:DT:H2"	2:T:17:DG:C8	2.53	0.44
4:A:311:GLN:N	4:A:312:PRO:HD3	2.33	0.44
4:A:375:THR:HB	4:A:433:GLU:HB3	1.98	0.44
4:A:487:MET:HE2	4:A:487:MET:HB3	1.60	0.44
4:A:549:MET:HE1	4:A:656:TRP:CD1	2.51	0.44
4:A:845:LEU:O	4:A:1065:GLY:HA3	2.17	0.44
4:A:1163:ILE:HG21	4:A:1194:ARG:NH1	2.32	0.44
5:B:363:HIS:CE1	5:B:364:ILE:HG12	2.52	0.44
5:B:416:LEU:HD23	5:B:416:LEU:HA	1.74	0.44
5:B:851:PHE:CD1	5:B:1094:ARG:HB2	2.52	0.44
4:A:108:MET:HE2	4:A:171:GLN:OE1	2.17	0.44
4:A:711:ARG:NH1	10:I:95:THR:OG1	2.50	0.44
5:B:839:MET:HB2	5:B:1010:LEU:HD11	1.99	0.44
5:B:878:GLN:HB3	5:B:881:ASN:HB2	1.99	0.44
6:C:36:VAL:HG21	6:C:251:LEU:HD13	2.00	0.44
13:L:38:LEU:HD13	13:L:48:CYS:HA	2.00	0.44
1:R:8:G:H2'	1:R:9:G:C8	2.53	0.44
4:A:86:LEU:HD23	4:A:86:LEU:H	1.82	0.44
4:A:873:MET:HE1	4:A:957:PRO:HB3	2.00	0.44
4:A:1008:GLN:O	4:A:1012:ARG:HG3	2.17	0.44
4:A:1197:LEU:HD12	4:A:1209:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:25:ILE:HA	5:B:655:LYS:HD3	1.99	0.44
11:J:23:ASN:C	11:J:27:GLU:OE1	2.61	0.44
12:K:82:ASP:HB3	12:K:85:ASP:HB2	1.99	0.44
4:A:176:LYS:HG3	4:A:181:LEU:HG	2.00	0.44
4:A:868:TYR:CZ	4:A:1366:ARG:HD3	2.53	0.44
4:A:1116:LEU:HG	4:A:1329:THR:OG1	2.17	0.44
5:B:567:GLU:OE1	5:B:567:GLU:N	2.35	0.44
2:T:8:DT:OP2	2:T:8:DT:H2'	2.18	0.44
4:A:569:LYS:NZ	6:C:222:LYS:HD2	2.33	0.44
4:A:679:ILE:HG21	4:A:763:ALA:HB1	2.00	0.44
4:A:982:THR:O	4:A:986:ILE:HG13	2.17	0.44
4:A:1095:THR:OG1	4:A:1100:ARG:HD2	2.18	0.44
4:A:1258:HIS:CE1	4:A:1259:MET:HG2	2.53	0.44
5:B:189:LEU:O	5:B:193:LYS:N	2.50	0.44
5:B:228:LYS:HA	5:B:228:LYS:HD2	1.80	0.44
5:B:408:LEU:O	5:B:412:LEU:HG	2.18	0.44
5:B:953:LEU:O	5:B:964:VAL:HA	2.17	0.44
4:A:18:GLN:HA	4:A:1418:LEU:HA	1.98	0.44
4:A:26:GLU:O	4:A:30:ILE:HG12	2.18	0.44
4:A:302:THR:HA	4:A:305:ASP:O	2.18	0.44
4:A:700:ASN:HB2	10:I:98:VAL:HG22	2.00	0.44
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.83	0.44
4:A:923:LEU:O	4:A:927:VAL:HG13	2.18	0.44
4:A:1267:MET:O	4:A:1271:ILE:HG12	2.18	0.44
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.99	0.44
5:B:999:MET:SD	5:B:1011:ILE:HD11	2.58	0.44
5:B:1114:LEU:HD12	5:B:1114:LEU:HA	1.84	0.44
7:E:48:ASP:HB3	7:E:54:GLN:NE2	2.33	0.44
7:E:116:ILE:H	7:E:116:ILE:HG13	1.62	0.44
7:E:159:ASP:HA	7:E:162:ARG:HD2	1.98	0.44
8:F:81:THR:HB	8:F:146:TRP:CZ2	2.52	0.44
4:A:452:LYS:N	4:A:1070:GLN:OE1	2.50	0.44
4:A:598:LEU:O	9:H:122:LEU:HD12	2.17	0.44
4:A:737:LEU:HD13	4:A:741:ASN:HD21	1.82	0.44
4:A:775:ILE:HD12	4:A:818:MET:HE3	1.99	0.44
4:A:919:ILE:HD12	4:A:919:ILE:HA	1.89	0.44
5:B:598:GLU:O	5:B:602:THR:HG23	2.18	0.44
5:B:620:ARG:HE	10:I:89:GLN:HE22	1.66	0.44
11:J:24:LEU:HA	11:J:27:GLU:OE2	2.18	0.44
4:A:456:MET:HE2	4:A:478:TYR:CE1	2.53	0.44
4:A:683:ILE:O	4:A:687:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:470:LYS:HE3	5:B:472:ALA:HB3	2.00	0.44
5:B:756:ILE:HG22	5:B:759:PRO:HD3	2.00	0.44
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	2.00	0.44
6:C:26:ASP:OD1	6:C:26:ASP:N	2.48	0.44
4:A:620:LYS:HB2	4:A:620:LYS:HE2	1.81	0.43
4:A:1313:LEU:HB3	4:A:1338:VAL:HG21	1.99	0.43
5:B:329:THR:HA	5:B:332:ASP:HB3	2.00	0.43
5:B:1163:CYS:HB2	5:B:1171:VAL:CG1	2.47	0.43
9:H:37:LYS:O	9:H:125:LEU:HA	2.18	0.43
9:H:87:ARG:HD3	9:H:87:ARG:HA	1.73	0.43
10:I:85:PHE:HD2	10:I:99:LEU:HD13	1.83	0.43
2:T:15:DC:OP2	2:T:15:DC:H2'	2.18	0.43
4:A:325:ILE:O	4:A:329:LEU:HG	2.18	0.43
4:A:826:ASP:O	4:A:830:LYS:HG2	2.18	0.43
4:A:882:SER:H	4:A:961:ARG:NH2	2.16	0.43
4:A:1346:ALA:O	4:A:1350:LYS:HG3	2.18	0.43
5:B:314:LEU:O	5:B:318:VAL:HG23	2.18	0.43
6:C:259:LEU:O	6:C:263:THR:HG23	2.18	0.43
2:T:17:DG:H4'	4:A:1403:GLU:HG2	2.00	0.43
3:N:4:DG:H2''	3:N:5:DC:C6	2.53	0.43
4:A:1063:MET:HE3	4:A:1063:MET:HB3	1.78	0.43
5:B:353:LYS:O	5:B:357:GLN:HG2	2.19	0.43
5:B:849:GLY:HA2	5:B:852:ARG:HD3	2.00	0.43
6:C:51:VAL:O	13:L:64:LEU:HD22	2.19	0.43
7:E:136:ASN:OD1	7:E:138:ALA:N	2.48	0.43
12:K:55:LYS:HB3	12:K:55:LYS:HE2	1.78	0.43
4:A:130:ASP:HB3	4:A:133:LYS:HB2	2.01	0.43
4:A:650:GLN:O	4:A:654:ASN:ND2	2.51	0.43
4:A:1208:THR:HG1	4:A:1231:ASP:CG	2.27	0.43
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.99	0.43
5:B:422:LYS:HA	5:B:422:LYS:HD2	1.84	0.43
9:H:118:PHE:O	9:H:121:LEU:HB2	2.19	0.43
1:R:3:C:H2'	1:R:4:G:H8	1.84	0.43
4:A:84:ILE:HG12	4:A:241:VAL:CG2	2.48	0.43
4:A:353:ILE:HB	4:A:470:LEU:HD22	1.99	0.43
4:A:1030:ARG:HA	4:A:1034:GLU:HG3	2.01	0.43
5:B:1106:ARG:HD2	5:B:1125:ASP:O	2.18	0.43
8:F:147:SER:O	8:F:151:LEU:HD12	2.18	0.43
1:R:4:G:C2	2:T:26:DG:C2	3.06	0.43
2:T:13:DC:C2	2:T:14:DG:N7	2.87	0.43
4:A:1004:ASN:HB3	4:A:1007:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	2.00	0.43
5:B:649:LYS:HZ2	5:B:737:THR:HA	1.82	0.43
5:B:695:ALA:HA	5:B:698:GLU:HB2	2.00	0.43
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.54	0.43
7:E:90:VAL:O	7:E:94:LYS:HG3	2.18	0.43
9:H:93:TYR:CD2	9:H:143:LEU:HB3	2.54	0.43
12:K:57:LEU:N	12:K:76:GLN:O	2.50	0.43
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.51	0.43
4:A:994:GLN:HE22	4:A:1023:ARG:HE	1.65	0.43
5:B:391:ASP:OD2	10:I:92:ARG:HA	2.18	0.43
5:B:803:LEU:HD13	5:B:1032:SER:HB3	2.01	0.43
5:B:1106:ARG:HH11	5:B:1126:GLY:HA2	1.84	0.43
8:F:124:GLU:HB3	8:F:130:ILE:HG13	1.99	0.43
12:K:47:ARG:HD3	12:K:61:TYR:CD1	2.43	0.43
12:K:57:LEU:HD12	12:K:76:GLN:HE21	1.84	0.43
1:R:4:G:H2'	1:R:5:A:H8	1.83	0.43
4:A:265:LYS:HG3	4:A:303:TYR:HB2	2.00	0.43
4:A:587:HIS:HB3	4:A:608:ILE:HD13	2.00	0.43
4:A:883:LEU:O	4:A:886:ILE:HG22	2.18	0.43
4:A:892:ALA:HA	4:A:895:LYS:NZ	2.34	0.43
4:A:900:ASP:HB3	4:A:906:HIS:CB	2.49	0.43
4:A:1100:ARG:O	4:A:1104:ILE:HG13	2.18	0.43
5:B:422:LYS:NZ	5:B:426:LYS:HB2	2.33	0.43
5:B:1213:THR:OG1	5:B:1215:ARG:NH1	2.52	0.43
6:C:52:GLU:HB3	6:C:154:LYS:HB2	2.01	0.43
7:E:66:GLU:O	7:E:69:ILE:HG12	2.18	0.43
7:E:190:LEU:HD22	7:E:214:CYS:CB	2.48	0.43
9:H:56:THR:HB	9:H:145:ARG:HB3	2.01	0.43
4:A:607:ILE:HA	4:A:612:ILE:HA	1.99	0.43
4:A:662:PHE:O	5:B:828:ALA:HA	2.18	0.43
4:A:892:ALA:HA	4:A:895:LYS:HZ3	1.83	0.43
4:A:975:HIS:HA	4:A:1036:ARG:HG3	2.01	0.43
4:A:1147:THR:HA	4:A:1197:LEU:HA	2.01	0.43
4:A:1225:PHE:CZ	4:A:1227:ILE:HG23	2.54	0.43
5:B:99:LYS:HD2	5:B:180:TYR:CE1	2.54	0.43
5:B:312:GLU:HA	5:B:315:LYS:HG3	2.01	0.43
5:B:693:ILE:HG23	5:B:697:GLU:HG2	2.00	0.43
6:C:66:ARG:O	6:C:70:ILE:HG13	2.19	0.43
6:C:248:ILE:HG23	12:K:98:LEU:HB3	2.01	0.43
7:E:16:PHE:CD2	7:E:20:LYS:HE2	2.54	0.43
4:A:95:PHE:C	4:A:99:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:456:MET:HE1	4:A:507:VAL:HG13	2.00	0.43
4:A:711:ARG:HD2	10:I:95:THR:OG1	2.19	0.43
4:A:947:PHE:HB2	4:A:950:GLY:HA2	2.01	0.43
4:A:1263:ILE:HD12	4:A:1263:ILE:HA	1.90	0.43
5:B:796:LEU:HD23	5:B:799:PRO:HA	2.01	0.43
6:C:91:HIS:ND1	6:C:158:VAL:HG11	2.34	0.43
7:E:16:PHE:O	7:E:20:LYS:HG3	2.19	0.43
4:A:129:LYS:NZ	7:E:215:MET:SD	2.92	0.42
4:A:216:VAL:O	4:A:220:THR:HG23	2.19	0.42
4:A:997:LEU:HD21	4:A:1050:GLU:HA	2.01	0.42
4:A:1081:LEU:HD13	4:A:1097:GLY:HA3	2.01	0.42
4:A:1194:ARG:HG3	4:A:1237:ILE:HD12	2.01	0.42
4:A:344:ARG:NH2	5:B:1120:GLU:HG3	2.33	0.42
4:A:605:MET:HE1	4:A:616:VAL:O	2.18	0.42
5:B:259:TYR:CE1	5:B:270:LYS:HB2	2.54	0.42
5:B:301:ILE:O	5:B:383:ASN:HB2	2.18	0.42
5:B:611:PRO:CG	5:B:685:LEU:HD21	2.49	0.42
8:F:128:LYS:HD3	8:F:128:LYS:HA	1.86	0.42
10:I:68:LEU:HB3	10:I:84:VAL:HG13	2.00	0.42
4:A:132:LYS:H	4:A:132:LYS:HG3	1.50	0.42
4:A:269:ILE:HD11	4:A:303:TYR:HB2	2.00	0.42
4:A:274:ILE:HD13	4:A:277:GLU:OE2	2.19	0.42
4:A:388:LEU:HD23	4:A:388:LEU:HA	1.85	0.42
4:A:858:ASN:OD1	4:A:862:ASN:N	2.52	0.42
4:A:933:TYR:HA	4:A:936:LEU:HD12	2.01	0.42
4:A:1438:THR:HA	4:A:1441:PHE:CZ	2.55	0.42
5:B:420:LEU:HD11	5:B:456:GLY:HA3	2.01	0.42
6:C:145:CYS:SG	6:C:146:LYS:N	2.92	0.42
6:C:265:MET:HE3	6:C:265:MET:O	2.19	0.42
11:J:3:VAL:HG21	11:J:18:TRP:HB2	2.01	0.42
12:K:7:PHE:HA	12:K:10:PHE:HB3	2.01	0.42
4:A:494:SER:OG	4:A:496:GLU:OE1	2.30	0.42
4:A:741:ASN:OD1	4:A:744:LYS:HB2	2.20	0.42
4:A:1289:ARG:CZ	4:A:1326:ARG:HH22	2.33	0.42
5:B:37:PHE:HD1	5:B:681:TRP:CE2	2.37	0.42
6:C:199:LYS:HD3	6:C:199:LYS:HA	1.83	0.42
12:K:99:GLY:HA2	12:K:102:LYS:HE3	2.01	0.42
4:A:516:SER:HA	4:A:1362:TYR:CD2	2.54	0.42
4:A:981:LEU:CD2	4:A:986:ILE:CG1	2.83	0.42
4:A:1339:LEU:HB3	7:E:150:VAL:HG22	2.01	0.42
5:B:170:LEU:HD12	5:B:171:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:638:PHE:CD2	5:B:743:ILE:HD13	2.54	0.42
5:B:1176:ASN:OD1	5:B:1176:ASN:N	2.52	0.42
6:C:206:ASN:HA	6:C:209:TYR:HD2	1.83	0.42
7:E:56:LYS:NZ	7:E:84:ASP:HB2	2.34	0.42
7:E:72:PHE:HB2	7:E:75:MET:HG2	2.00	0.42
7:E:190:LEU:HD11	7:E:196:VAL:CG2	2.49	0.42
9:H:44:VAL:HA	9:H:47:PHE:O	2.19	0.42
10:I:59:VAL:HG12	10:I:61:ASP:N	2.28	0.42
4:A:1093:LYS:O	4:A:1113:THR:HG21	2.19	0.42
4:A:1399:ARG:HH21	4:A:1408:ILE:HG23	1.85	0.42
5:B:483:LEU:HD23	5:B:483:LEU:HA	1.93	0.42
5:B:1065:GLN:HE21	6:C:200:GLU:HG3	1.84	0.42
9:H:16:ASP:OD1	9:H:18:GLY:N	2.51	0.42
9:H:59:ILE:HA	9:H:141:TYR:O	2.20	0.42
12:K:20:LYS:O	12:K:33:ILE:HA	2.19	0.42
12:K:29:ASN:HB2	12:K:76:GLN:HE22	1.84	0.42
4:A:18:GLN:HE22	4:A:1416:ALA:C	2.27	0.42
4:A:67:CYS:CB	4:A:70:CYS:HB2	2.44	0.42
4:A:92:HIS:ND1	4:A:304:MET:HE3	2.35	0.42
4:A:822:GLU:HA	4:A:825:ILE:HD12	2.01	0.42
4:A:1202:MET:HE3	4:A:1202:MET:HB3	1.95	0.42
5:B:1063:GLY:O	6:C:202:PRO:HG3	2.19	0.42
5:B:1168:LEU:HD21	5:B:1213:THR:HB	2.02	0.42
6:C:74:SER:HB3	6:C:77:ILE:HB	2.01	0.42
7:E:88:VAL:HG21	7:E:112:TYR:CD2	2.54	0.42
2:T:20:DC:H2'	2:T:21:DC:C6	2.55	0.42
4:A:326:ARG:HB2	4:A:1406:VAL:HG21	2.02	0.42
4:A:587:HIS:HA	4:A:607:ILE:O	2.20	0.42
4:A:598:LEU:HB3	9:H:25:ARG:NH1	2.35	0.42
4:A:1116:LEU:HB2	4:A:1311:VAL:HG22	2.01	0.42
5:B:680:THR:HB	5:B:683:SER:H	1.85	0.42
5:B:698:GLU:O	5:B:701:ILE:HG12	2.20	0.42
10:I:74:GLU:HB3	10:I:81:ARG:HE	1.85	0.42
3:N:7:DA:H2''	3:N:8:DG:C8	2.55	0.42
4:A:37:PHE:N	4:A:52:GLY:HA3	2.28	0.42
4:A:837:ILE:O	4:A:841:LEU:HG	2.20	0.42
4:A:1351:GLU:O	4:A:1355:VAL:HG23	2.20	0.42
5:B:313:MET:HE2	5:B:386:LEU:HD22	2.01	0.42
5:B:459:TYR:CE1	5:B:468:GLU:HA	2.54	0.42
5:B:760:ASP:OD1	5:B:760:ASP:N	2.52	0.42
5:B:780:VAL:O	5:B:817:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1001:PHE:HE2	6:C:178:PHE:HB3	1.84	0.42
6:C:93:ASP:HB3	6:C:125:MET:HE2	2.02	0.42
10:I:77:LYS:HE3	10:I:108:HIS:HB2	2.02	0.42
12:K:59:ALA:HA	12:K:74:ARG:O	2.20	0.42
2:T:21:DC:H2"	4:A:447:GLN:HG3	2.02	0.42
4:A:666:ILE:HG23	5:B:1086:PHE:CE2	2.55	0.42
4:A:734:GLU:O	4:A:744:LYS:NZ	2.39	0.42
5:B:60:GLN:OE1	5:B:94:LYS:HA	2.19	0.42
6:C:43:THR:HG23	6:C:74:SER:OG	2.20	0.42
6:C:100:THR:O	6:C:118:LEU:HD23	2.19	0.42
2:T:8:DT:C2	3:N:12:DG:N2	2.88	0.41
3:N:7:DA:H2"	3:N:8:DG:H8	1.83	0.41
4:A:326:ARG:O	4:A:330:LYS:HB2	2.20	0.41
4:A:336:ILE:HD12	5:B:1203:LEU:HD22	2.01	0.41
4:A:442:VAL:O	4:A:457:ALA:HA	2.20	0.41
4:A:477:PRO:HG3	4:A:521:MET:HE2	2.01	0.41
4:A:1109:LYS:HB2	4:A:1109:LYS:HE2	1.85	0.41
5:B:131:ASP:OD1	5:B:131:ASP:N	2.52	0.41
5:B:802:PRO:HG2	5:B:805:THR:HG22	2.02	0.41
5:B:952:VAL:O	13:L:57:LEU:HA	2.20	0.41
8:F:140:ASP:OD1	8:F:141:GLY:N	2.52	0.41
11:J:21:TYR:HA	11:J:24:LEU:HD12	2.02	0.41
4:A:18:GLN:HB3	5:B:1217:TYR:CE2	2.50	0.41
4:A:24:PRO:HB3	4:A:238:CYS:N	2.35	0.41
4:A:442:VAL:HG11	4:A:489:LEU:HD21	2.03	0.41
4:A:676:MET:O	4:A:680:THR:HG23	2.20	0.41
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	2.02	0.41
5:B:120:ARG:NH2	5:B:956:THR:O	2.54	0.41
5:B:194:GLU:OE1	5:B:195:CYS:N	2.52	0.41
5:B:466:TRP:HA	5:B:466:TRP:CE3	2.55	0.41
6:C:104:PHE:HD1	6:C:152:GLU:HB2	1.85	0.41
4:A:306:ASN:N	4:A:324:SER:HB2	2.33	0.41
4:A:497:THR:HG23	5:B:1146:PHE:HB2	2.02	0.41
4:A:515:GLN:OE1	4:A:1071:SER:HA	2.20	0.41
4:A:958:VAL:HB	4:A:1018:PHE:HZ	1.85	0.41
5:B:89:GLU:O	5:B:134:LYS:HA	2.20	0.41
5:B:601:ARG:HH11	5:B:601:ARG:HG2	1.84	0.41
5:B:1001:PHE:CZ	5:B:1073:TYR:HB2	2.55	0.41
6:C:167:HIS:HA	12:K:6:ARG:HH21	1.86	0.41
6:C:254:LYS:NZ	12:K:38:GLU:OE2	2.37	0.41
7:E:103:LYS:HD2	7:E:105:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:3:C:H2'	1:R:4:G:C8	2.55	0.41
4:A:115:LEU:HG	4:A:142:CYS:SG	2.60	0.41
4:A:773:LYS:HA	4:A:773:LYS:HD2	1.92	0.41
4:A:1033:GLN:HA	4:A:1036:ARG:HH21	1.85	0.41
4:A:1427:ASN:ND2	4:A:1435:PRO:HD3	2.35	0.41
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.55	0.41
5:B:1017:ILE:HB	5:B:1018:PRO:HD3	2.02	0.41
7:E:16:PHE:HB2	7:E:58:MET:HE2	2.01	0.41
2:T:17:DG:H2'	2:T:18:DA:C4	2.55	0.41
4:A:171:GLN:NE2	4:A:172:PRO:HD2	2.35	0.41
4:A:217:LYS:HB2	4:A:217:LYS:HE2	1.86	0.41
4:A:508:PRO:CB	4:A:639:PRO:HB2	2.50	0.41
4:A:595:THR:HG22	4:A:596:THR:O	2.19	0.41
4:A:777:PHE:CD1	4:A:783:THR:HG23	2.56	0.41
4:A:782:ARG:HG3	4:A:789:LYS:HA	2.01	0.41
4:A:916:GLY:O	4:A:919:ILE:HG22	2.20	0.41
4:A:1397:LEU:HD12	4:A:1426:GLU:HA	2.02	0.41
5:B:29:ASP:O	5:B:33:VAL:HG23	2.21	0.41
5:B:257:LYS:HB2	5:B:259:TYR:CE1	2.55	0.41
5:B:899:ILE:O	5:B:952:VAL:HG21	2.20	0.41
7:E:13:TRP:NE1	7:E:37:LEU:O	2.54	0.41
7:E:198:ILE:HB	7:E:210:SER:HB2	2.02	0.41
9:H:26:ILE:O	9:H:39:THR:HA	2.20	0.41
4:A:452:LYS:HD2	5:B:1140:ALA:HB1	2.01	0.41
5:B:470:LYS:HD2	5:B:471:LYS:N	2.36	0.41
5:B:638:PHE:O	5:B:740:HIS:HB3	2.20	0.41
6:C:32:SER:HB3	12:K:41:THR:HG23	2.03	0.41
6:C:148:ARG:CZ	11:J:64:ASN:HA	2.50	0.41
7:E:57:MET:HE2	7:E:57:MET:HB3	1.63	0.41
7:E:135:PHE:CD1	7:E:140:LEU:HD21	2.55	0.41
4:A:108:MET:H	4:A:171:GLN:NE2	2.18	0.41
4:A:567:LYS:HB3	4:A:568:PRO:HD3	2.02	0.41
5:B:23:ALA:O	5:B:655:LYS:HG2	2.21	0.41
5:B:566:LEU:HD21	5:B:586:TRP:CE2	2.56	0.41
5:B:663:ALA:HA	5:B:666:TYR:HD2	1.86	0.41
5:B:1119:VAL:O	5:B:1126:GLY:HA3	2.20	0.41
7:E:79:TRP:NE1	7:E:81:GLU:HB2	2.36	0.41
7:E:171:LYS:HE3	7:E:172:GLU:N	2.36	0.41
8:F:76:LYS:HA	8:F:76:LYS:HD2	1.83	0.41
8:F:76:LYS:HD2	8:F:79:ARG:NE	2.36	0.41
9:H:110:ASP:O	9:H:111:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:39:GLU:OE2	4:A:40:THR:N	2.54	0.41
4:A:102:VAL:O	4:A:106:VAL:HG12	2.21	0.41
4:A:111:GLY:HA2	4:A:213:HIS:O	2.21	0.41
4:A:356:ASP:OD1	12:K:65:HIS:NE2	2.53	0.41
4:A:403:LYS:HB2	4:A:403:LYS:HE2	1.66	0.41
4:A:546:VAL:O	4:A:550:LEU:HD13	2.20	0.41
4:A:1262:LYS:O	4:A:1265:ASN:OD1	2.39	0.41
5:B:352:ALA:O	5:B:356:LEU:HD23	2.21	0.41
5:B:355:ILE:HG23	5:B:359:GLU:HB2	2.03	0.41
5:B:852:ARG:HA	5:B:972:LYS:O	2.21	0.41
5:B:1070:GLU:O	5:B:1072:MET:HG2	2.21	0.41
6:C:62:PHE:O	6:C:66:ARG:HG3	2.21	0.41
12:K:10:PHE:CD2	12:K:11:LEU:HB2	2.56	0.41
4:A:22:PHE:N	5:B:1211:ASN:O	2.46	0.41
4:A:32:VAL:HG21	4:A:68:GLN:CG	2.51	0.41
4:A:71:GLN:O	4:A:71:GLN:HG2	2.20	0.41
4:A:80:HIS:HD1	5:B:1172:ILE:HG21	1.85	0.41
4:A:111:GLY:O	4:A:214:ILE:HA	2.20	0.41
4:A:497:THR:O	4:A:501:LEU:HG	2.20	0.41
4:A:601:LYS:H	4:A:601:LYS:HG2	1.65	0.41
4:A:635:ARG:NH1	4:A:635:ARG:HA	2.36	0.41
4:A:678:GLU:O	4:A:681:GLU:HG3	2.20	0.41
4:A:737:LEU:CB	4:A:744:LYS:HD2	2.51	0.41
4:A:770:VAL:HA	4:A:822:GLU:OE1	2.21	0.41
4:A:839:ARG:O	4:A:843:LYS:HG2	2.20	0.41
4:A:843:LYS:HA	4:A:843:LYS:HD2	1.92	0.41
4:A:1150:SER:OG	10:I:46:HIS:HB3	2.21	0.41
5:B:293:PRO:HB2	5:B:296:GLU:HB2	2.01	0.41
5:B:661:LEU:HD11	5:B:684:LEU:HD11	2.03	0.41
8:F:74:ILE:HD13	8:F:74:ILE:HA	1.91	0.41
9:H:102:TYR:CE2	9:H:115:TYR:HB3	2.55	0.41
4:A:42:ASP:HA	4:A:50:ILE:HD13	2.03	0.41
4:A:131:SER:HB2	4:A:223:GLY:CA	2.51	0.41
4:A:504:LEU:HD22	8:F:87:LYS:HD2	2.03	0.41
4:A:605:MET:SD	4:A:615:GLY:HA3	2.61	0.41
4:A:655:PHE:O	4:A:659:HIS:ND1	2.54	0.41
4:A:682:THR:O	4:A:685:GLU:HG2	2.20	0.41
4:A:707:GLY:HA3	4:A:1281:ARG:CD	2.51	0.41
4:A:862:ASN:HA	7:E:174:GLN:O	2.21	0.41
4:A:1165:GLU:O	4:A:1169:ILE:HG12	2.21	0.41
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:566:LEU:HD23	5:B:566:LEU:HA	1.80	0.41
6:C:2:SER:HB3	6:C:7:GLN:HE22	1.86	0.41
7:E:175:LEU:HD21	7:E:195:VAL:HG13	2.02	0.41
10:I:6:PHE:CD1	10:I:13:MET:HA	2.54	0.41
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.96	0.41
1:R:7:A:H2'	1:R:8:G:C8	2.56	0.40
4:A:1224:LEU:HD21	4:A:1240:CYS:CB	2.44	0.40
4:A:1264:GLU:HA	4:A:1267:MET:HE2	2.02	0.40
4:A:1333:ILE:O	4:A:1337:GLU:HG2	2.21	0.40
5:B:361:LEU:HD21	5:B:377:PHE:HB3	2.02	0.40
6:C:259:LEU:HD21	12:K:91:CYS:HB2	2.03	0.40
9:H:110:ASP:HA	9:H:128:ASN:HD22	1.86	0.40
10:I:22:ASN:HB2	10:I:24:ARG:HG2	2.02	0.40
4:A:112:LYS:NZ	4:A:215:SER:HB2	2.36	0.40
4:A:184:SER:O	4:A:199:LEU:HB2	2.21	0.40
4:A:981:LEU:CD2	4:A:982:THR:O	2.68	0.40
4:A:1012:ARG:HE	4:A:1012:ARG:HB2	1.59	0.40
4:A:1209:MET:HE1	4:A:1236:LEU:HD13	2.04	0.40
5:B:43:LEU:HD13	5:B:496:ARG:HD2	2.02	0.40
5:B:86:ARG:N	5:B:137:TYR:O	2.55	0.40
5:B:613:VAL:HA	5:B:632:ARG:NH2	2.36	0.40
7:E:192:ARG:HD2	7:E:192:ARG:C	2.46	0.40
4:A:519:PRO:O	4:A:624:SER:HB2	2.22	0.40
4:A:526:ASP:HB3	4:A:657:LEU:HD23	2.03	0.40
4:A:1120:LEU:HD12	4:A:1120:LEU:HA	1.87	0.40
5:B:394:ASP:OD2	10:I:91:ARG:NH1	2.54	0.40
5:B:1147:LEU:O	5:B:1151:LEU:HB2	2.21	0.40
7:E:9:ILE:H	7:E:9:ILE:HG13	1.76	0.40
7:E:26:ARG:NH1	7:E:189:GLY:HA3	2.36	0.40
7:E:59:SER:HB2	7:E:81:GLU:HA	2.02	0.40
9:H:107:VAL:HG13	9:H:113:ALA:HB2	2.03	0.40
4:A:350:ARG:HA	4:A:487:MET:O	2.21	0.40
4:A:361:LEU:HA	4:A:471:ASN:HB2	2.03	0.40
4:A:781:ASP:O	4:A:790:ASP:N	2.51	0.40
5:B:892:LYS:HD3	5:B:905:VAL:HG12	2.02	0.40
6:C:52:GLU:N	6:C:154:LYS:O	2.44	0.40
7:E:46:TYR:HE1	7:E:58:MET:CG	2.32	0.40
9:H:42:ILE:HD12	9:H:42:ILE:HA	1.98	0.40
4:A:84:ILE:HD13	4:A:84:ILE:HA	1.87	0.40
4:A:106:VAL:HG21	4:A:214:ILE:HG23	2.03	0.40
4:A:114:LEU:HD23	4:A:148:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:344:ARG:O	5:B:1155:SER:OG	2.21	0.40
4:A:511:ILE:O	4:A:520:CYS:N	2.40	0.40
4:A:744:LYS:O	4:A:748:MET:HG3	2.22	0.40
5:B:167:ILE:H	5:B:167:ILE:HG12	1.73	0.40
5:B:174:LEU:HD22	5:B:202:TYR:CZ	2.56	0.40
5:B:346:GLU:HA	5:B:349:ILE:HD13	2.03	0.40
5:B:613:VAL:HA	5:B:632:ARG:HH22	1.87	0.40
5:B:1072:MET:HE3	5:B:1072:MET:HB3	1.90	0.40
7:E:69:ILE:HA	7:E:72:PHE:O	2.22	0.40
10:I:5:ARG:O	10:I:14:LEU:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:418:SER:OG	6:C:87:PHE:O[2_555]	2.17	0.03

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	1370/1733 (79%)	1342 (98%)	28 (2%)	0	100	100
5	B	1103/1224 (90%)	1082 (98%)	21 (2%)	0	100	100
6	C	265/318 (83%)	263 (99%)	2 (1%)	0	100	100
7	E	210/215 (98%)	208 (99%)	2 (1%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
10	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	41 (100%)	0	0	100	100
All	All	3493/4173 (84%)	3432 (98%)	61 (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%)	1188 (100%)	6 (0%)	81	80
5	B	955/1061 (90%)	953 (100%)	2 (0%)	87	85
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	110/116 (95%)	104 (94%)	6 (6%)	19	47
11	J	60/65 (92%)	59 (98%)	1 (2%)	53	69
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	36/57 (63%)	32 (89%)	4 (11%)	6	27
All	All	3071/3657 (84%)	3052 (99%)	19 (1%)	78	79

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	67	CYS
4	A	77	CYS
4	A	80	HIS
4	A	107	CYS
4	A	148	CYS
4	A	167	CYS

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Mol	Chain	Res	Type
5	B	332	ASP
5	B	1182	CYS
10	I	7	CYS
10	I	29	CYS
10	I	32	CYS
10	I	75	CYS
10	I	78	CYS
10	I	106	CYS
11	J	7	CYS
13	L	31	CYS
13	L	34	CYS
13	L	48	CYS
13	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	64	ASN
4	A	83	HIS
4	A	169	ASN
4	A	171	GLN
4	A	282	ASN
4	A	299	HIS
4	A	306	ASN
4	A	358	ASN
4	A	399	HIS
4	A	584	ASN
4	A	698	GLN
4	A	723	ASN
4	A	851	HIS
4	A	966	ASN
4	A	969	GLN
4	A	1048	ASN
4	A	1078	GLN
4	A	1232	ASN
4	A	1258	HIS
4	A	1265	ASN
5	B	53	GLN
5	B	178	ASN
5	B	215	GLN
5	B	350	GLN
5	B	481	GLN

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Mol	Chain	Res	Type
5	B	494	HIS
5	B	834	ASN
5	B	835	GLN
5	B	932	HIS
5	B	1015	HIS
5	B	1074	ASN
6	C	17	ASN
6	C	31	ASN
6	C	102	GLN
6	C	135	GLN
6	C	224	GLN
6	C	264	GLN
7	E	104	ASN
7	E	146	HIS
9	H	3	ASN
9	H	137	GLN
10	I	12	ASN
11	J	64	ASN
12	K	52	ASN
12	K	76	GLN
13	L	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	9	G

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	3.66	7 (36%)	18,33,36	1.58	3 (16%)

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	-	3/6/40/41	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	12.91	1.47	1.28
2	T	19	WVQ	C4-N9	4.66	1.45	1.35
2	T	19	WVQ	C6-C5	-4.19	1.35	1.47
2	T	19	WVQ	C2-N2	4.19	1.45	1.34
2	T	19	WVQ	C6-N1	-3.13	1.32	1.38
2	T	19	WVQ	O6-C6	-2.70	1.18	1.23
2	T	19	WVQ	C5-C4	-2.23	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	WVQ	N3-C2-N1	-4.52	119.28	126.44
2	T	19	WVQ	N2-C2-N3	2.29	120.20	116.57
2	T	19	WVQ	N2-C2-N1	2.21	120.51	117.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	WVQ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	POP	B	1302	-	6,8,8	0.76	0	12,13,13	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	POP	B	1302	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

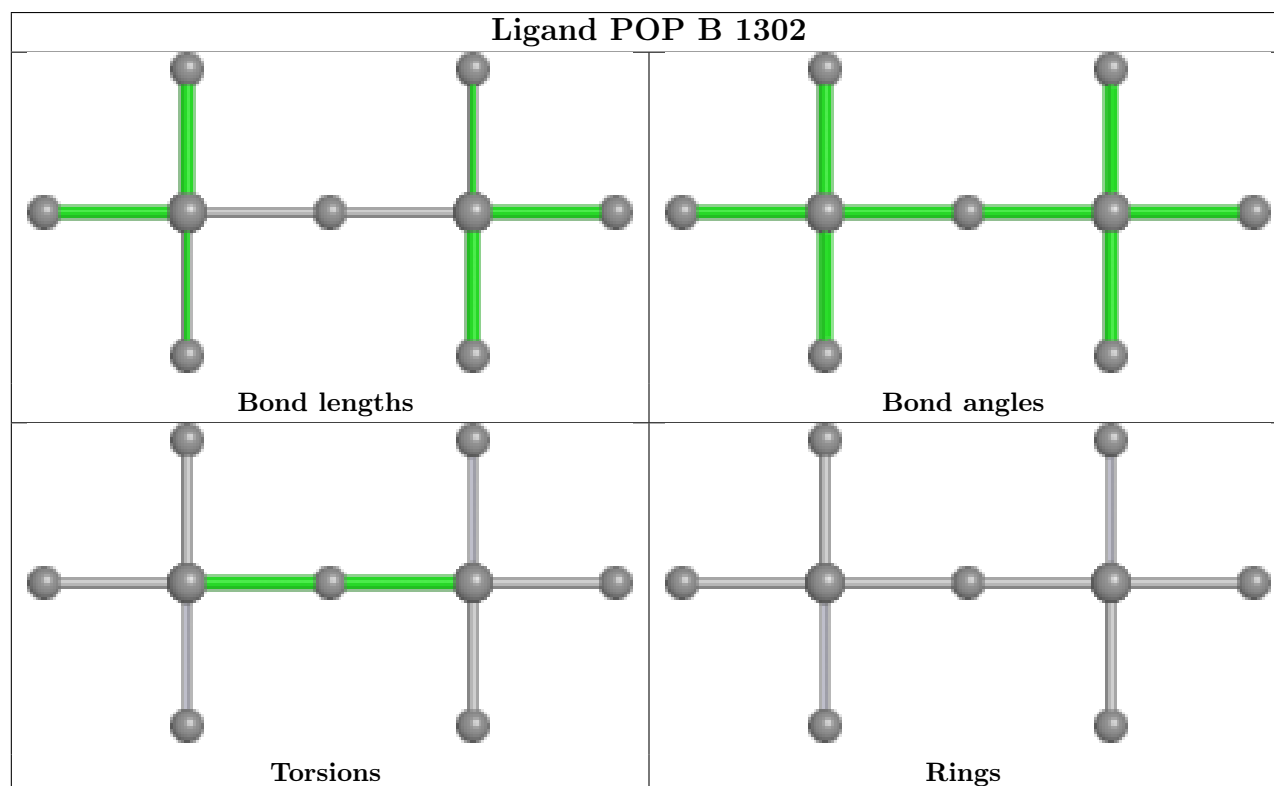
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.23	0  	129, 137, 205, 246	0
2	T	23/29 (79%)	0.17	0  	123, 210, 287, 302	0
3	N	13/18 (72%)	0.11	0  	192, 216, 286, 302	0
4	A	1384/1733 (79%)	0.15	21 (1%)  	96, 144, 221, 331	0
5	B	1123/1224 (91%)	0.21	31 (2%)  	69, 129, 200, 273	0
6	C	267/318 (83%)	0.25	5 (1%)  	65, 130, 196, 235	0
7	E	212/215 (98%)	0.11	5 (2%)  	122, 176, 261, 352	0
8	F	86/155 (55%)	0.03	2 (2%)  	107, 141, 203, 270	0
9	H	133/146 (91%)	0.08	3 (2%)  	116, 164, 252, 364	0
10	I	118/122 (96%)	0.09	0  	102, 148, 215, 251	0
11	J	65/70 (92%)	0.27	6 (9%)  	83, 120, 174, 265	0
12	K	114/120 (95%)	0.12	2 (1%)  	84, 128, 184, 231	0
13	L	43/70 (61%)	0.56	4 (9%)  	129, 240, 312, 407	0
All	All	3591/4230 (84%)	0.17	79 (2%)  	65, 141, 229, 407	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	L	62	LYS	4.2
4	A	642	CYS	4.2
4	A	135	PHE	3.5
5	B	533	CYS	3.4
12	K	42	LEU	3.3
5	B	611	PRO	3.2
11	J	54	VAL	3.2
4	A	448	PRO	3.2
4	A	306	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	646	PHE	3.1
5	B	1100	ASP	3.1
4	A	1328	TYR	3.0
5	B	525	ALA	3.0
5	B	823	ALA	2.9
5	B	1211	ASN	2.9
11	J	44	TYR	2.9
5	B	489	SER	2.9
5	B	811	TYR	2.9
6	C	191	TYR	2.8
4	A	466	SER	2.8
4	A	1329	THR	2.8
5	B	775	LYS	2.8
4	A	503	GLN	2.8
5	B	819	ALA	2.8
5	B	1214	PRO	2.7
4	A	1434	ALA	2.7
5	B	751	VAL	2.7
5	B	753	ALA	2.7
4	A	872	GLY	2.6
5	B	830	TYR	2.6
7	E	93	MET	2.6
5	B	685	LEU	2.6
4	A	244	PRO	2.6
6	C	119	VAL	2.5
4	A	696	GLU	2.5
5	B	386	LEU	2.5
7	E	46	TYR	2.5
6	C	178	PHE	2.4
5	B	829	CYS	2.4
5	B	335	GLY	2.4
7	E	124	VAL	2.3
9	H	23	VAL	2.3
8	F	85	MET	2.3
11	J	61	LEU	2.3
7	E	125	PRO	2.3
5	B	816	GLU	2.3
5	B	779	GLY	2.3
11	J	65	PRO	2.3
5	B	1140	ALA	2.3
4	A	957	PRO	2.3
6	C	121	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	E	112	TYR	2.3
5	B	1212	ILE	2.2
4	A	98	LYS	2.2
12	K	71	PHE	2.2
5	B	681	TRP	2.2
5	B	212	LEU	2.2
5	B	1113	VAL	2.2
8	F	93	ILE	2.2
4	A	33	ALA	2.2
13	L	32	ALA	2.2
5	B	1191	ILE	2.2
4	A	245	PRO	2.1
4	A	776	ALA	2.1
5	B	1006	ILE	2.1
13	L	67	PHE	2.1
5	B	849	GLY	2.1
9	H	63	LEU	2.1
6	C	159	ALA	2.1
4	A	833	GLU	2.1
4	A	620	LYS	2.1
9	H	134	ASN	2.1
13	L	46	VAL	2.1
4	A	815	PHE	2.1
5	B	690	VAL	2.0
11	J	14	VAL	2.0
5	B	692	TYR	2.0
11	J	6	ARG	2.0
5	B	477	ALA	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	0.88	0.15	133,170,190,209	0

6.3 Carbohydrates [i](#)

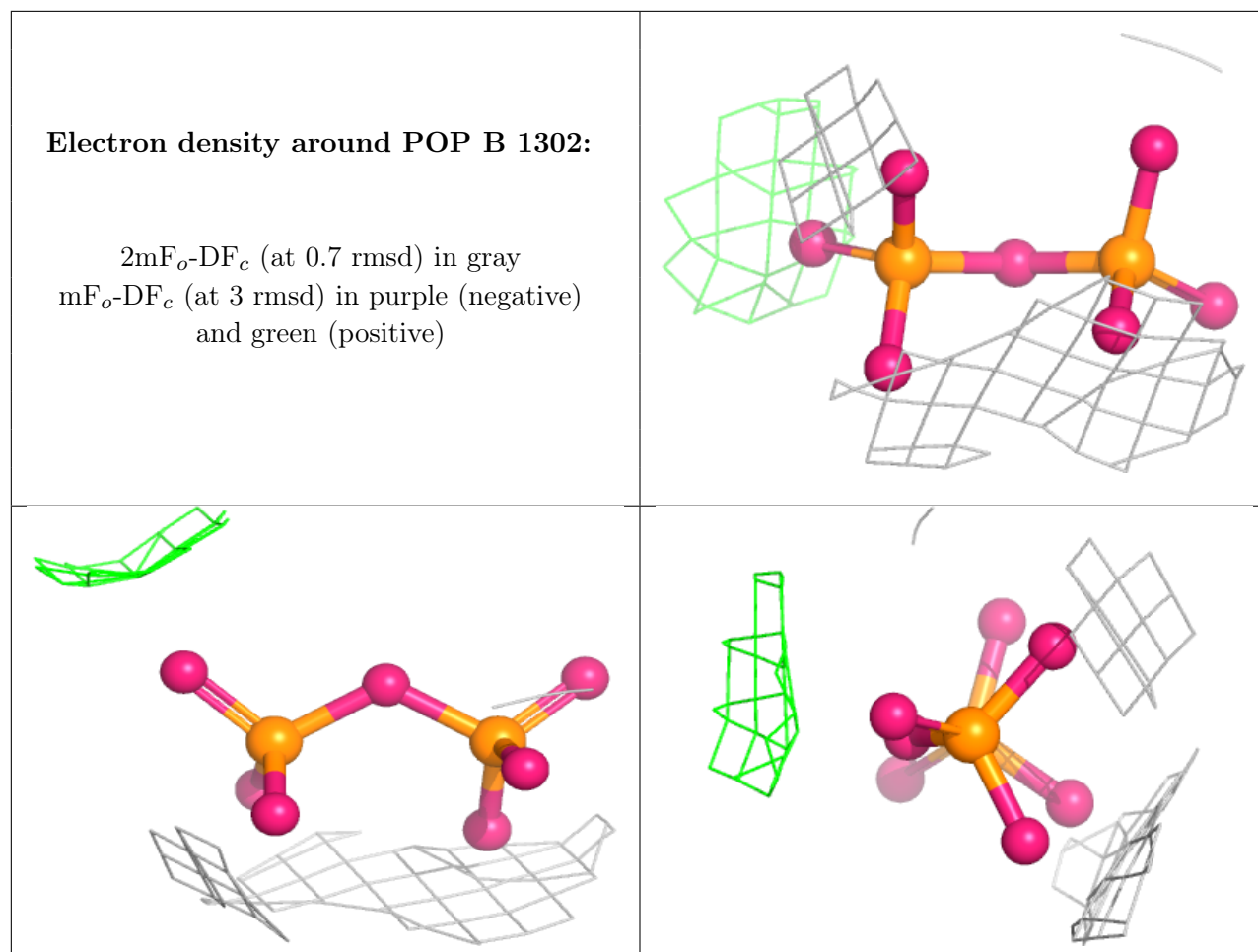
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
16	POP	B	1302	9/9	0.55	0.09	152,187,218,223	0
15	MG	A	1803	1/1	0.85	0.11	184,184,184,184	0
14	ZN	A	1801	1/1	0.91	0.07	348,348,348,348	0
14	ZN	L	101	1/1	0.91	0.07	341,341,341,341	0
14	ZN	A	1802	1/1	0.92	0.08	195,195,195,195	0
14	ZN	I	202	1/1	0.93	0.07	228,228,228,228	0
14	ZN	B	1301	1/1	0.93	0.06	293,293,293,293	0
14	ZN	C	401	1/1	0.97	0.11	253,253,253,253	0
14	ZN	J	101	1/1	0.99	0.03	110,110,110,110	0
14	ZN	I	201	1/1	0.99	0.04	124,124,124,124	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.