



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:02 am GMT

PDB ID : 3KGV
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2009-10-29
Resolution : 6.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

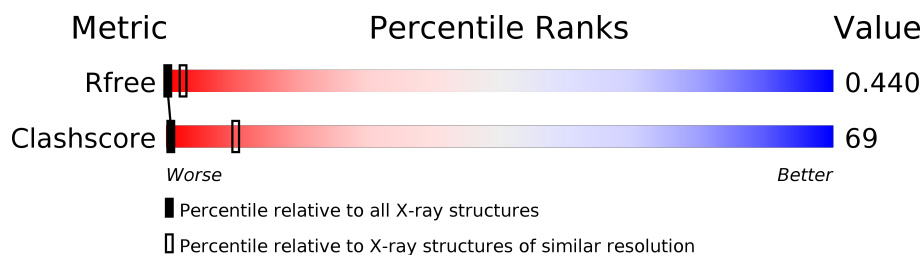
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

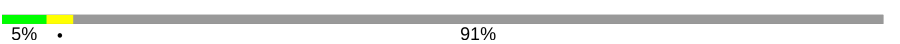
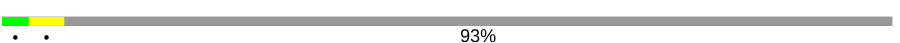







The reported resolution of this entry is 6.60 Å.

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}	100719	1099 (9.50-3.70)
Clashscore	112137	1031 (9.00-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	4128	 91%
1	B	4128	 93%
1	C	4128	 90%
1	D	4128	 96%
1	E	4128	 98%
1	F	4128	 87%
1	O	4128	 91%
1	P	4128	 93%
1	Q	4128	 90%

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Mol	Chain	Length	Quality of chain
1	R	4128	<div><div></div><div></div><div></div></div> 96%
1	S	4128	<div><div></div><div></div><div></div></div> 98%
1	T	4128	<div><div></div><div></div><div></div></div> 87%
1	X	4128	<div><div></div><div></div><div></div></div> 95%
1	Y	4128	<div><div></div><div></div><div></div></div> 95%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20320 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.

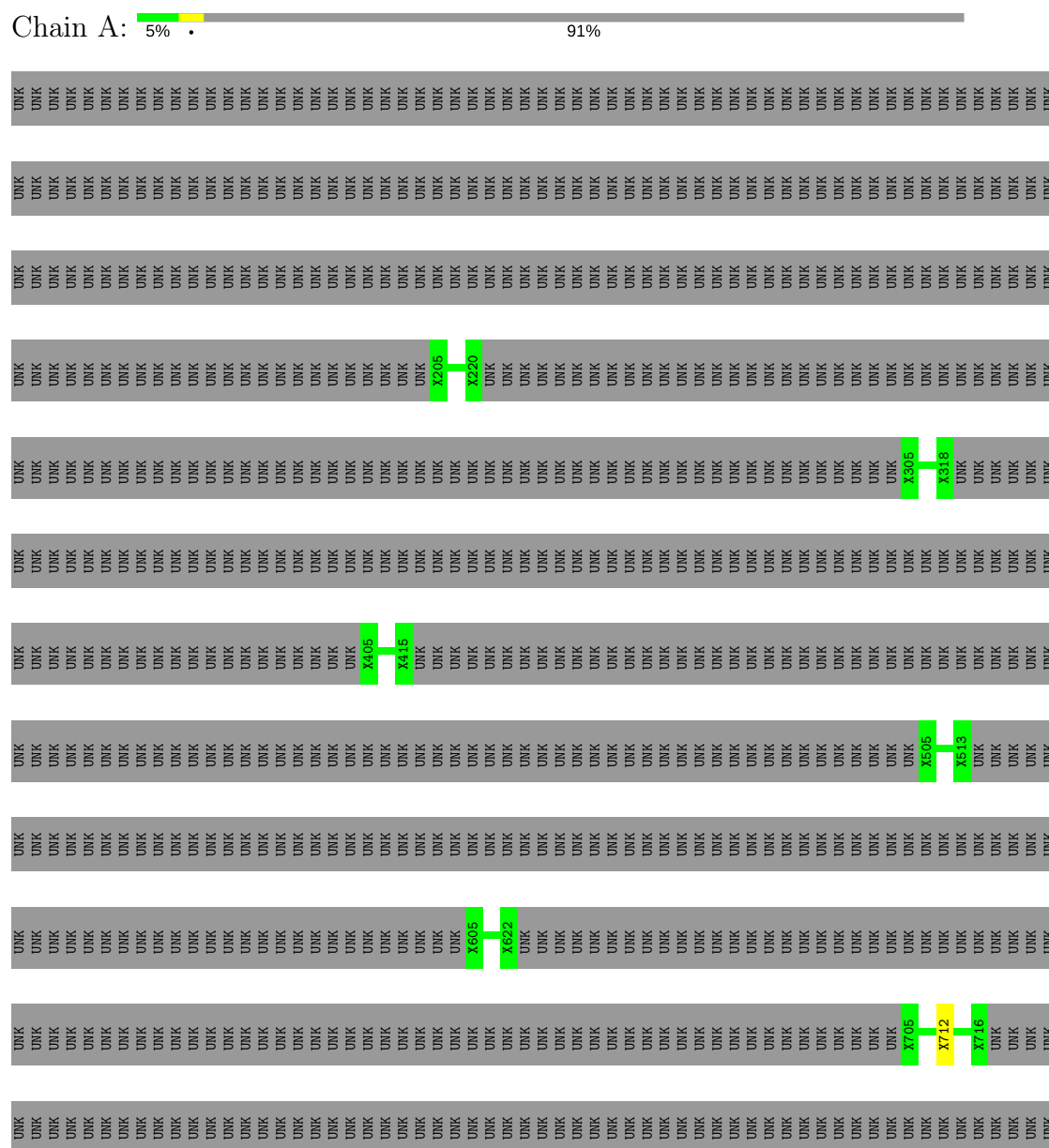
- Molecule 1 is a protein called DNA-dependent Protein Kinase Catalytic Subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	0	0	0
			1770	1062	354	354			
1	B	283	Total	C	N	O	0	0	0
			1415	849	283	283			
1	C	406	Total	C	N	O	0	0	0
			2030	1218	406	406			
1	D	182	Total	C	N	O	0	0	0
			910	546	182	182			
1	E	65	Total	C	N	O	0	0	0
			325	195	65	65			
1	F	531	Total	C	N	O	0	0	0
			2655	1593	531	531			
1	X	211	Total	C	N	O	0	0	0
			1055	633	211	211			
1	O	354	Total	C	N	O	0	0	0
			1770	1062	354	354			
1	P	283	Total	C	N	O	0	0	0
			1415	849	283	283			
1	Q	406	Total	C	N	O	0	0	0
			2030	1218	406	406			
1	R	182	Total	C	N	O	0	0	0
			910	546	182	182			
1	S	65	Total	C	N	O	0	0	0
			325	195	65	65			
1	T	531	Total	C	N	O	0	0	0
			2655	1593	531	531			
1	Y	211	Total	C	N	O	0	0	0
			1055	633	211	211			

3 Residue-property plots [i](#)

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

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



[illegible]

[illegible]

[illegible]

UNK

UNK

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain B: 93%

UNK

[illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible]

X605	X608	X609	X610
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[illegible][illegible][illegible][illegible]

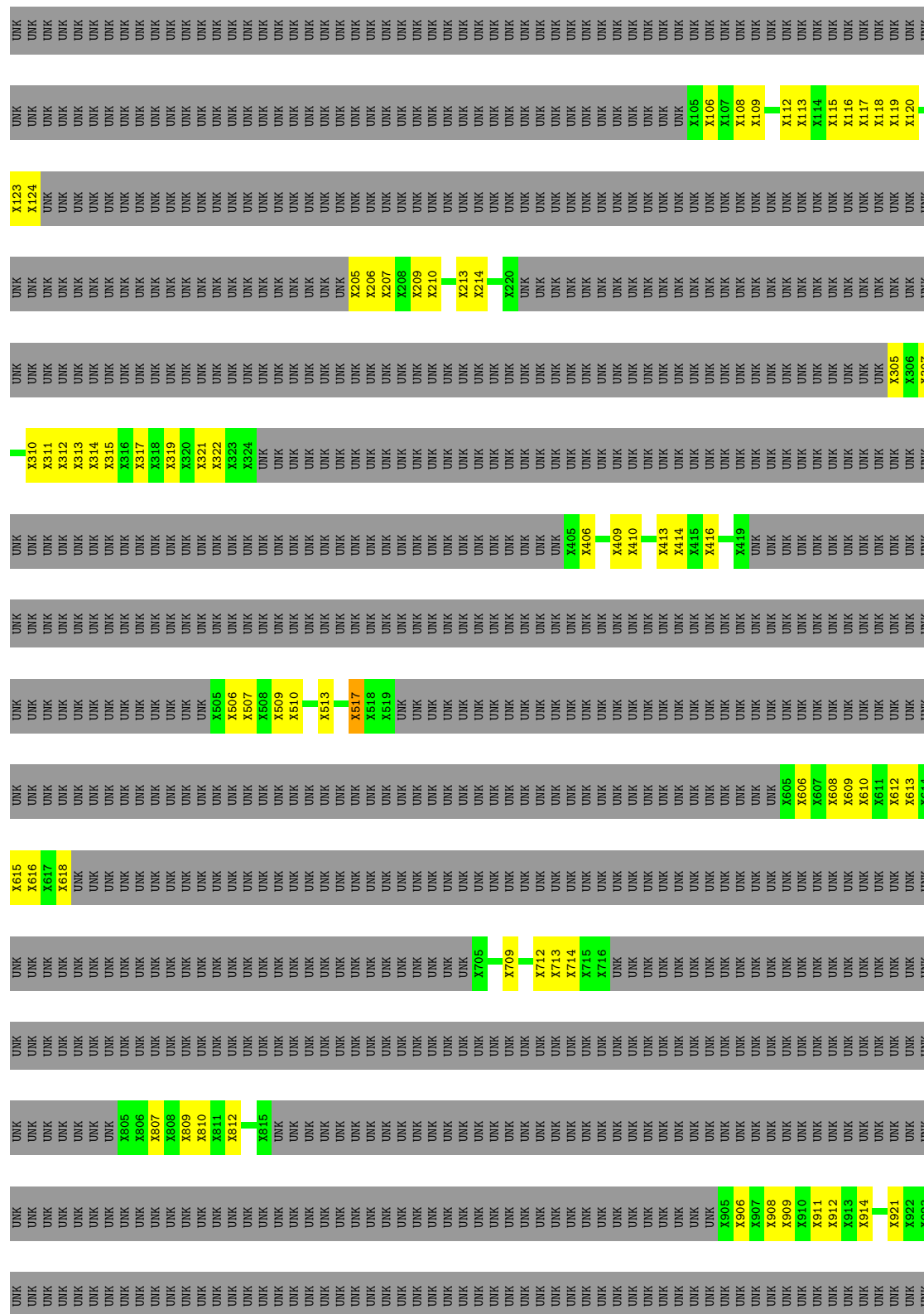


[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain C: 5% 5% 90%

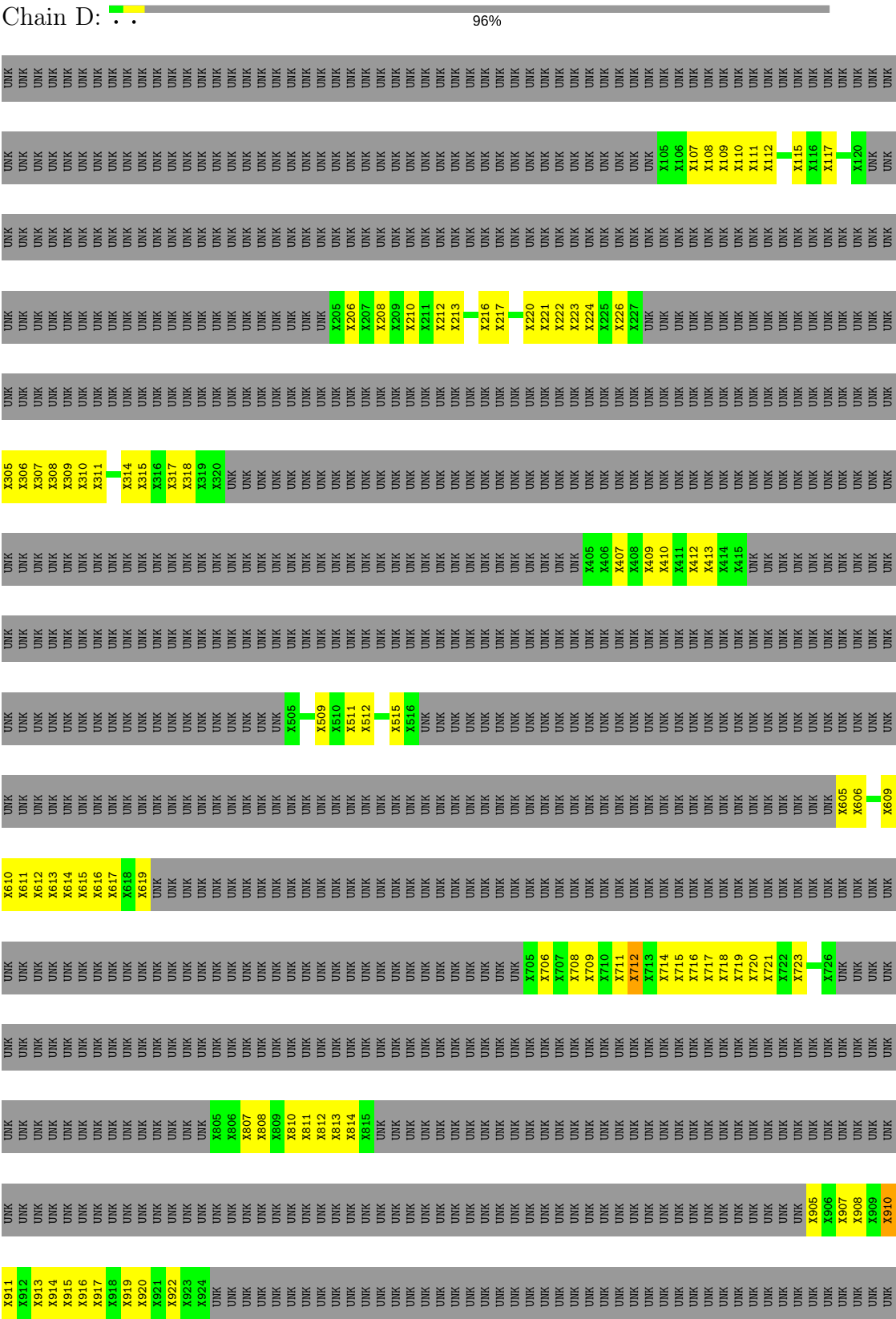


[illegible]

[illegible]

[illegible]

● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain E:  98%

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

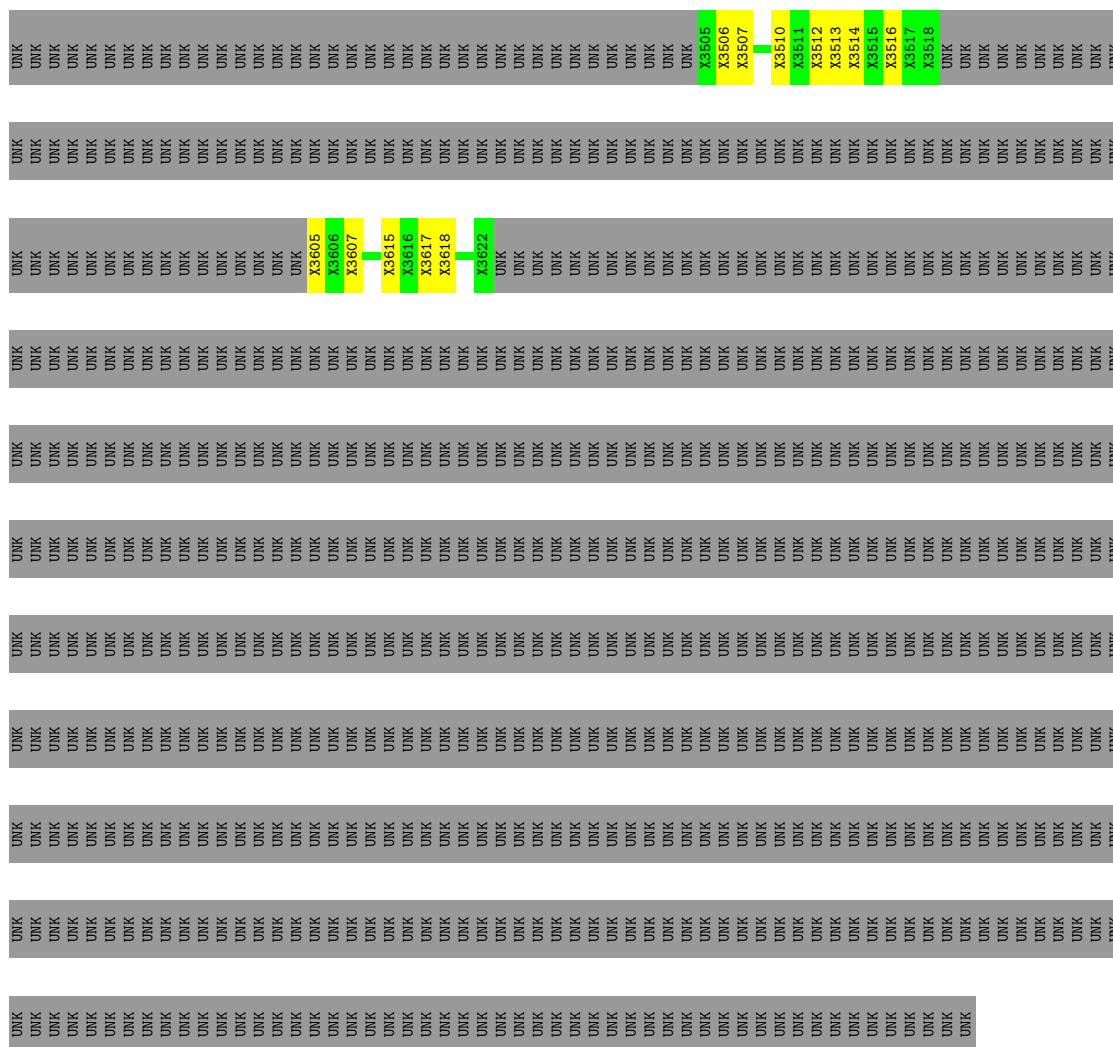
Chain F:  7% 6% 87%

[illegible]



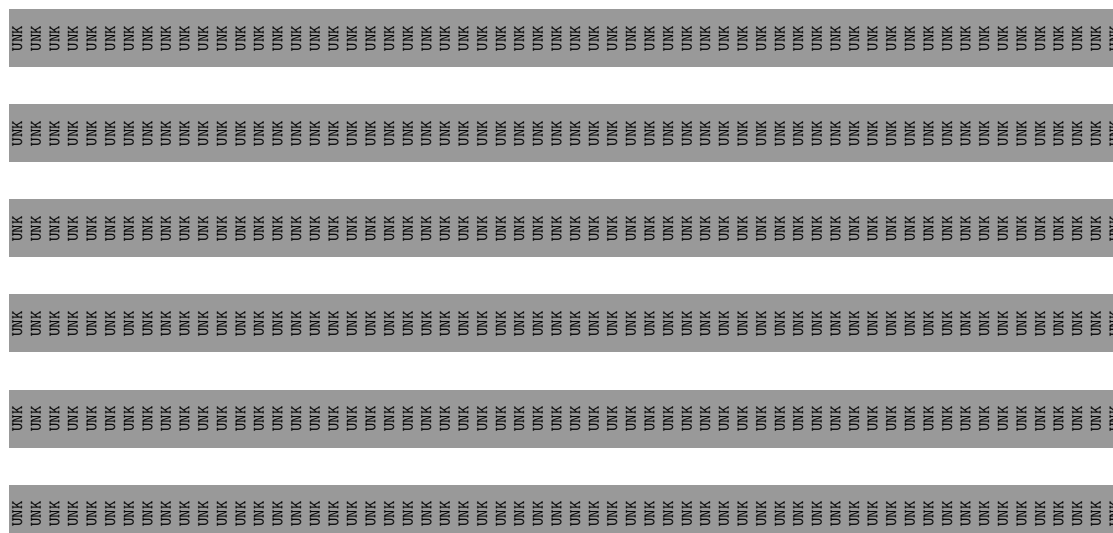
[illegible]

[illegible]



- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

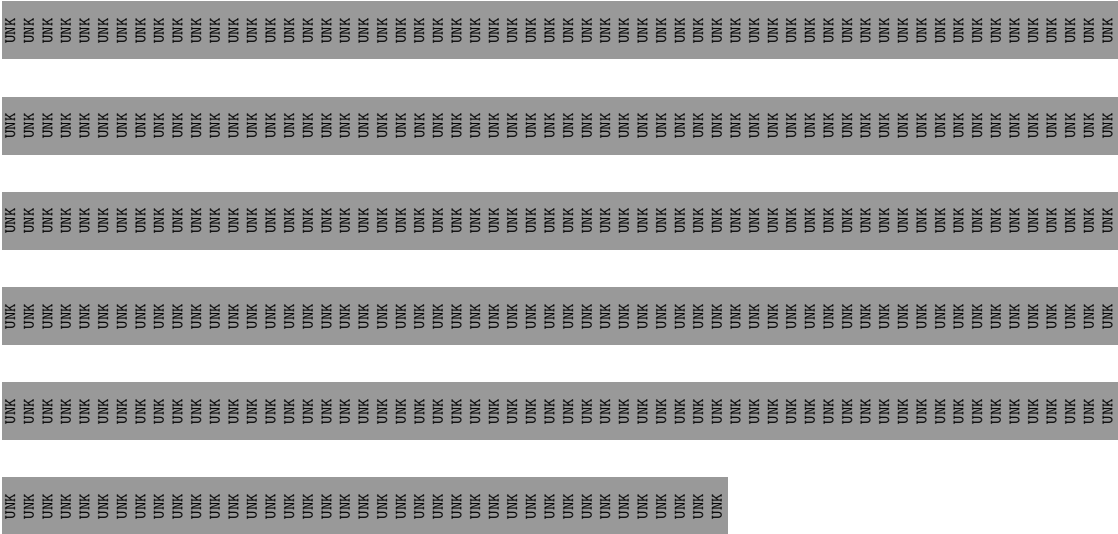
Chain X:  95%



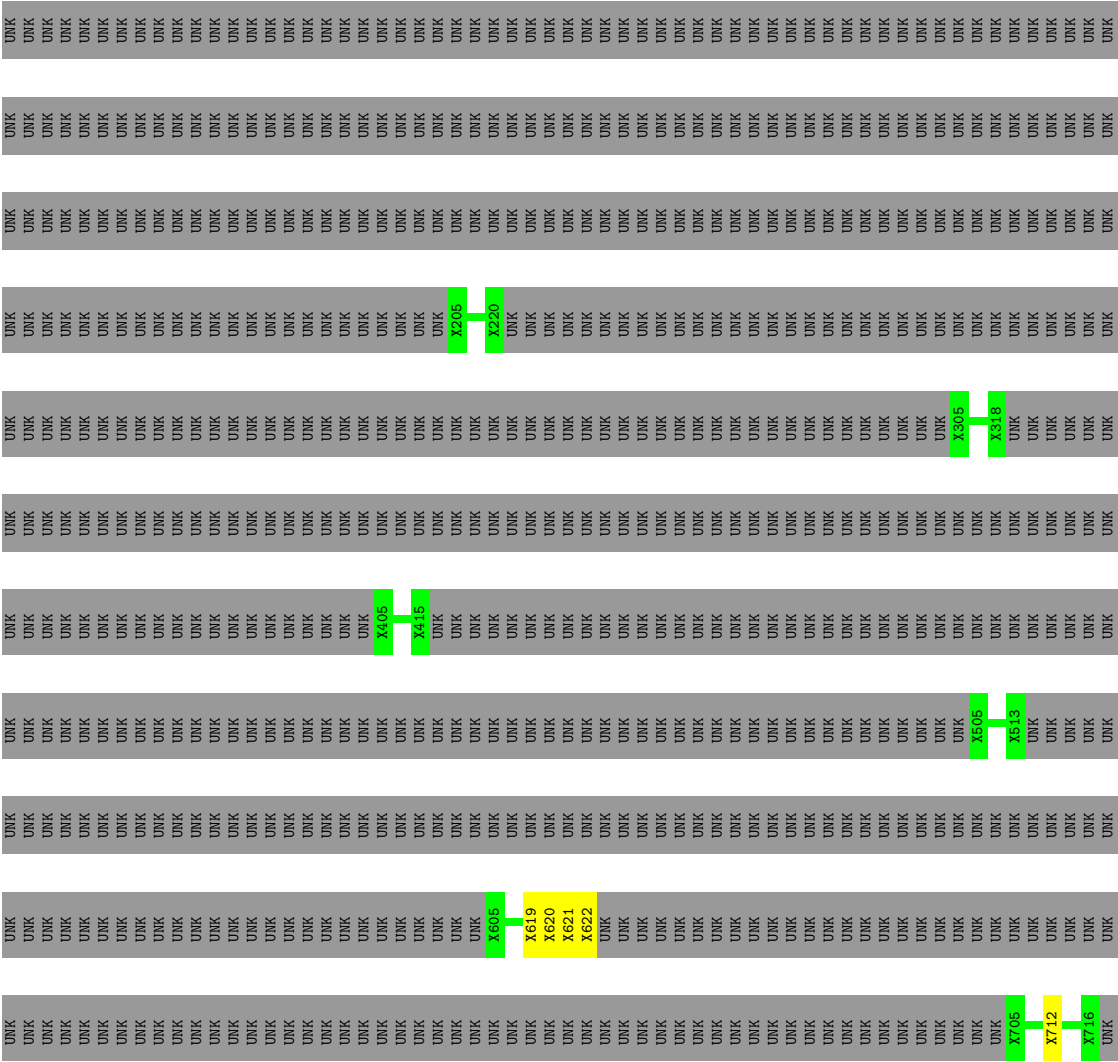


[illegible]

[illegible]



● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



[illegible]

[illegible]

[illegible]

[illegible][illegible][illegible]

UNK UNK

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain P: 93%

[illegible]

X106	X107	X108	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121
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[illegible]

[illegible]

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UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Q: 5% 5% 90%

UNK

[illegible][illegible]

	X206	X207	X208	X209	X210	X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225	X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X244	X245	X246	X247	X248	X249	X250	X251	X252	X253	X254	X255	X256	X257	X258	X259	X260	X261	X262	X263	X264	X265	X266	X267	X268	X269	X270	X271	X272	X273	X274	X275	X276	X277	X278	X279	X280	X281	X282	X283	X284	X285	X286	X287	X288	X289	X290	X291	X292	X293	X294	X295	X296	X297	X298	X299	X300	X301	X302	X303	X304	X305	X306	X307	X308	X309	X310	X311	X312	X313	X314	X315	X316	X317	X318	X319	X320	X321	X322	X323	X324	X325	X326	X327	X328	X329	X330	X331	X332	X333	X334	X335	X336	X337	X338	X339	X340	X341	X342	X343	X344	X345	X346	X347	X348	X349	X350	X351	X352	X353	X354	X355	X356	X357	X358	X359	X360	X361	X362	X363	X364	X365	X366	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565	X566	X567	X568	X569	X570	X571	X572	X573	X574	X575	X576	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X588	X589	X590	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606	X607	X608	X609	X610	X611	X612	X613	X614	X615	X616	X617	X618	X619	X620	X621	X622	X623	X624	X625	X626	X627	X628	X629	X630	X631	X632	X633	X634	X635	X636	X637	X638	X639	X640	X641	X642	X643	X644	X645	X646	X647	X648	X649	X650	X651	X652	X653	X654	X655	X656	X657	X658	X659	X660	X661	X662	X663	X664	X665	X666	X667	X668	X669	X670	X671	X672	X673	X674	X675	X676	X677	X678	X679	X680	X681	X682	X683	X684	X685	X686	X687	X688	X689	X690	X691	X692	X693	X694	X695	X696	X697	X698	X699	X700	X701	X702	X703	X704	X705	X706	X707	X708	X709	X710	X711	X712	X713	X714	X715	X71
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[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain R: 96%

[illegible]

X096	X097	X098	X099	X100	X101	X102	X103	X104	X105	X106	X107	X108	X109	X110	X111	X112	X113	X114	X115	X116	X117	X118	X119	X120	X121	X122	X123	X124	X125	X126	X127	X128	X129	X130	X131	X132	X133	X134	X135	X136	X137	X138	X139	X140	X141	X142	X143	X144	X145	X146	X147	X148	X149	X150	X151	X152	X153	X154	X155	X156	X157	X158	X159	X160	X161	X162	X163	X164	X165	X166	X167	X168	X169	X170	X171	X172	X173	X174	X175	X176	X177	X178	X179	X180	X181	X182	X183	X184	X185	X186	X187	X188	X189	X190	X191	X192	X193	X194	X195	X196	X197	X198	X199	X200	X201	X202	X203	X204	X205	X206	X207	X208	X209	X210	X211	X212	X213	X214	X215	X216	X217	X218	X219	X220	X221	X222	X223	X224	X225	X226	X227	X228	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X244	X245	X246	X247	X248	X249	X250	X251	X252	X253	X254	X255	X256	X257	X258	X259	X260	X261	X262	X263	X264	X265	X266	X267	X268	X269	X270	X271	X272	X273	X274	X275	X276	X277	X278	X279	X280	X281	X282	X283	X284	X285	X286	X287	X288	X289	X290	X291	X292	X293	X294	X295	X296	X297	X298	X299	X300	X301	X302	X303	X304	X305	X306	X307	X308	X309	X310	X311	X312	X313	X314	X315	X316	X317	X318	X319	X320	X321	X322	X323	X324	X325	X326	X327	X328	X329	X330	X331	X332	X333	X334	X335	X336	X337	X338	X339	X340	X341	X342	X343	X344	X345	X346	X347	X348	X349	X350	X351	X352	X353	X354	X355	X356	X357	X358	X359	X360	X361	X362	X363	X364	X365	X366	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	X381	X382	X383	X384	X385	X386	X387	X388	X389	X390	X391	X392	X393	X394	X395	X396	X397	X398	X399	X400	X401	X402	X403	X404	X405	X406	X407	X408	X409	X410	X411	X412	X413	X414	X415	X416	X417	X418	X419	X420	X421	X422	X423	X424	X425	X426	X427	X428	X429	X430	X431	X432	X433	X434	X435	X436	X437	X438	X439	X440	X441	X442	X443	X444	X445	X446	X447	X448	X449	X450	X451	X452	X453	X454	X455	X456	X457	X458	X459	X460	X461	X462	X463	X464	X465	X466	X467	X468	X469	X470	X471	X472	X473	X474	X475	X476	X477	X478	X479	X480	X481	X482	X483	X484	X485	X486	X487	X488	X489	X490	X491	X492	X493	X494	X495	X496	X497	X498	X499	X500	X501	X502	X503	X504	X505	X506	X507	X508	X509	X510	X511	X512	X513	X514	X515	X516	X517	X518	X519	X520	X521	X522	X523	X524	X525	X526	X527	X528	X529	X530	X531	X532	X533	X534	X535	X536	X537	X538	X539	X540	X541	X542	X543	X544	X545	X546	X547	X548	X549	X550	X551	X552	X553	X554	X555	X556	X557	X558	X559	X560	X561	X562	X563	X564	X565	X566	X567	X568	X569	X570	X571	X572	X573	X574	X575	X576	X577	X578	X579	X580	X581	X582	X583	X584	X585	X586	X587	X588	X589	X590	X591	X592	X593	X594	X595	X596	X597	X598	X599	X600	X601	X602	X603	X604	X605	X606
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[illegible][illegible]

UNK

[illegible][illegible]

UNK

[illegible][illegible][illegible]

X706	X707	X708	X709	X710	X711	X712	X713	X714	X715	X716	X717	X718	X719	X720	X721	X722	X723	X724	X725
X726	X727	X728	X729	X730	X731	X732	X733	X734	X735	X736	X737	X738	X739	X740	X741	X742	X743	X744	X745

UNK

[illegible]

	X906	X907	X908	X909	X910
--	------	------	------	------	------

[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain S:

98%

[illegible]

[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

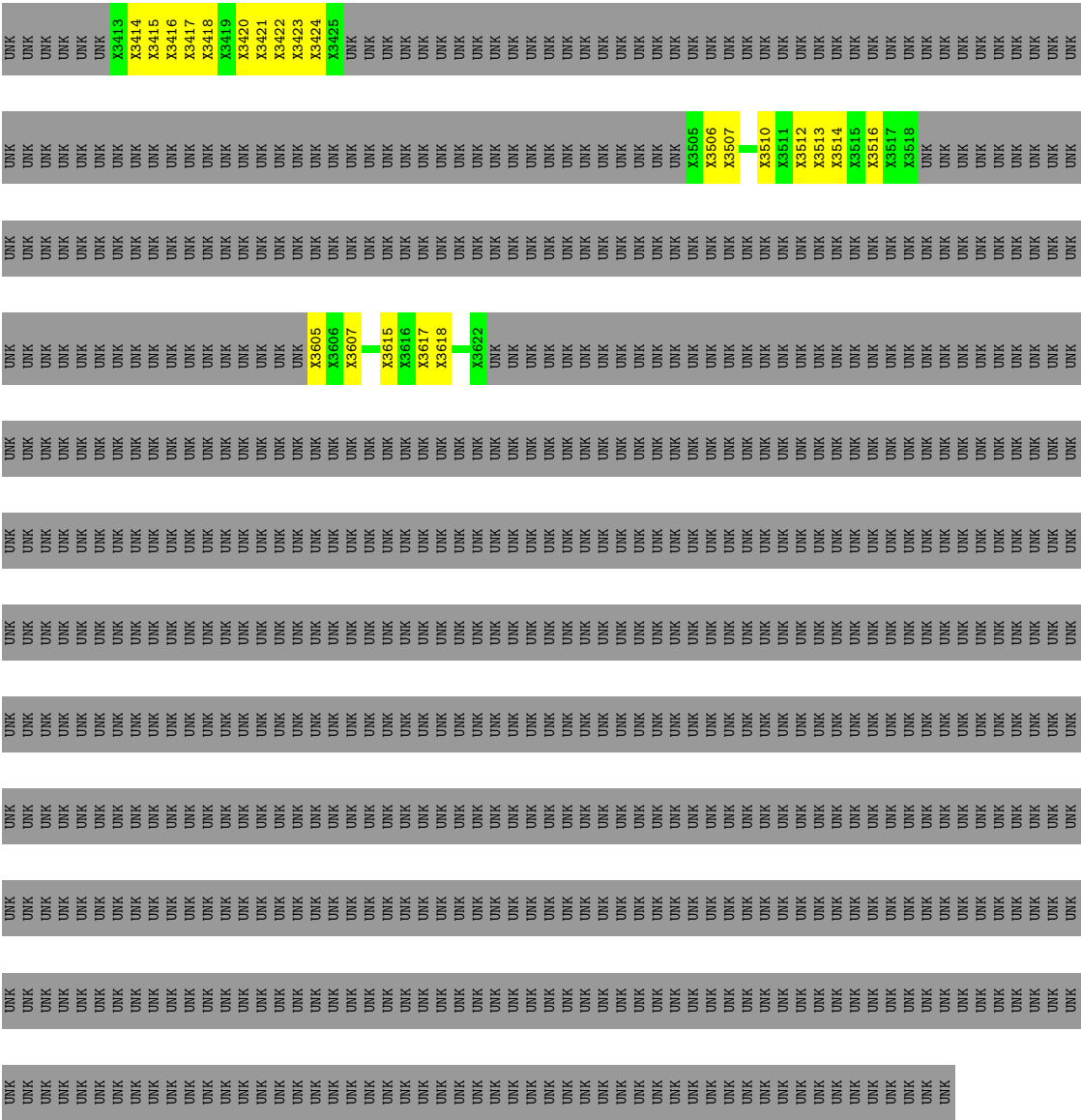
Chain T: 7% 6% 87%

[illegible]

[illegible]

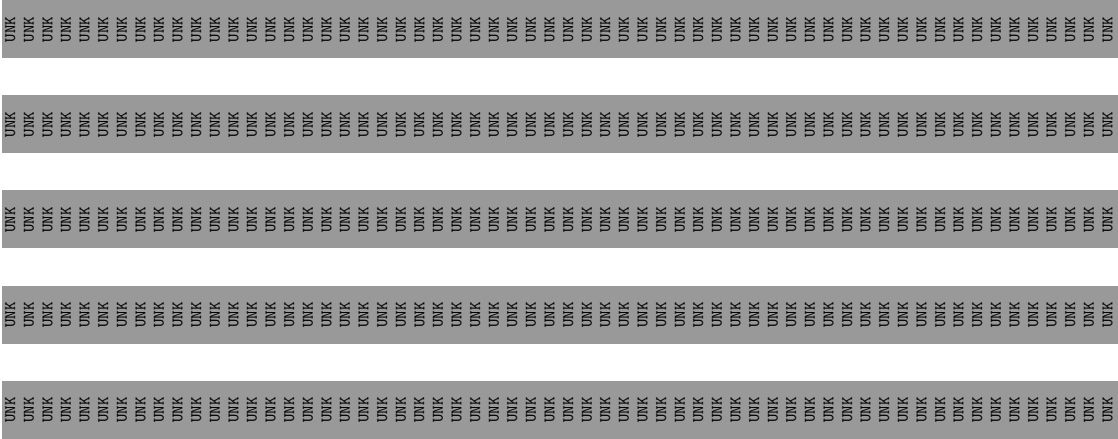
[illegible]





● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Y:  95%



[illegible]

[illegible]

[illegible]

[illegible][illegible][illegible]

UNK

[illegible][illegible][illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.60Å 132.99Å 297.00Å 90.00° 105.58° 90.00°	Depositor
Resolution (Å)	100.00 – 6.60 91.97 – 6.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.00-6.60) 97.6 (91.97-6.58)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.86 (at 6.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.442 , 0.441 0.441 , 0.440	Depositor DCC
R_{free} test set	1214 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	269.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 606.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	20320	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	18
1	C	0	8
1	D	0	8
1	E	0	3
1	F	0	6
1	O	0	2
1	P	0	18
1	Q	0	8
1	R	0	8
1	S	0	3
1	T	0	6
1	X	0	7
1	Y	0	7
All	All	0	104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1214	UNK	Peptide
1	A	2306	UNK	Peptide
1	B	1109	UNK	Peptide
1	B	119	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	B	122	UNK	Peptide
1	B	1309	UNK	Peptide
1	B	1406	UNK	Peptide
1	B	1408	UNK	Peptide
1	B	1411	UNK	Peptide
1	B	1413	UNK	Peptide
1	B	1415	UNK	Peptide
1	B	1417	UNK	Peptide
1	B	1419	UNK	Peptide
1	B	1617	UNK	Peptide
1	B	1618	UNK	Peptide
1	B	1619	UNK	Peptide
1	B	209	UNK	Peptide
1	B	212	UNK	Peptide
1	B	406	UNK	Peptide
1	B	610	UNK	Peptide
1	C	1016	UNK	Peptide
1	C	1812	UNK	Peptide
1	C	2507	UNK	Peptide
1	C	2616	UNK	Peptide
1	C	517	UNK	Peptide
1	C	608	UNK	Peptide
1	C	609	UNK	Peptide
1	C	921	UNK	Peptide
1	D	1013	UNK	Peptide
1	D	1015	UNK	Peptide
1	D	1108	UNK	Peptide
1	D	1111	UNK	Peptide
1	D	1210	UNK	Peptide
1	D	712	UNK	Peptide
1	D	910	UNK	Peptide
1	D	920	UNK	Peptide
1	E	114	UNK	Peptide
1	E	120	UNK	Peptide
1	E	306	UNK	Peptide
1	F	1008	UNK	Peptide
1	F	1509	UNK	Peptide
1	F	222	UNK	Peptide
1	F	2625	UNK	Peptide
1	F	2908	UNK	Peptide
1	F	3212	UNK	Peptide
1	O	1214	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	O	2306	UNK	Peptide
1	P	1109	UNK	Peptide
1	P	119	UNK	Peptide
1	P	122	UNK	Peptide
1	P	1309	UNK	Peptide
1	P	1406	UNK	Peptide
1	P	1408	UNK	Peptide
1	P	1411	UNK	Peptide
1	P	1413	UNK	Peptide
1	P	1415	UNK	Peptide
1	P	1417	UNK	Peptide
1	P	1419	UNK	Peptide
1	P	1617	UNK	Peptide
1	P	1618	UNK	Peptide
1	P	1619	UNK	Peptide
1	P	209	UNK	Peptide
1	P	212	UNK	Peptide
1	P	406	UNK	Peptide
1	P	610	UNK	Peptide
1	Q	1016	UNK	Peptide
1	Q	1812	UNK	Peptide
1	Q	2507	UNK	Peptide
1	Q	2616	UNK	Peptide
1	Q	517	UNK	Peptide
1	Q	608	UNK	Peptide
1	Q	609	UNK	Peptide
1	Q	921	UNK	Peptide
1	R	1013	UNK	Peptide
1	R	1015	UNK	Peptide
1	R	1108	UNK	Peptide
1	R	1111	UNK	Peptide
1	R	1210	UNK	Peptide
1	R	712	UNK	Peptide
1	R	910	UNK	Peptide
1	R	920	UNK	Peptide
1	S	114	UNK	Peptide
1	S	120	UNK	Peptide
1	S	306	UNK	Peptide
1	T	1008	UNK	Peptide
1	T	1509	UNK	Peptide
1	T	222	UNK	Peptide
1	T	2625	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	T	2908	UNK	Peptide
1	T	3212	UNK	Peptide
1	X	1042	UNK	Peptide
1	X	865	UNK	Peptide
1	X	876	UNK	Peptide
1	X	885	UNK	Peptide
1	X	910	UNK	Peptide
1	X	924	UNK	Peptide
1	X	990	UNK	Peptide
1	Y	1042	UNK	Peptide
1	Y	865	UNK	Peptide
1	Y	876	UNK	Peptide
1	Y	885	UNK	Peptide
1	Y	910	UNK	Peptide
1	Y	924	UNK	Peptide
1	Y	990	UNK	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	429	123	0
1	B	1415	0	356	149	0
1	C	2030	0	489	178	0
1	D	910	0	239	117	0
1	E	325	0	78	20	0
1	F	2655	0	648	203	0
1	O	1770	0	429	123	48
1	P	1415	0	358	153	0
1	Q	2030	0	489	180	0
1	R	910	0	239	119	0
1	S	325	0	78	19	0
1	T	2655	0	648	208	48
1	X	1055	0	263	74	0
1	Y	1055	0	264	75	0
All	All	20320	0	5007	1740	48

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 69.

All (1740) 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)
1:B:1412:UNK:CA	1:B:1412:UNK:C	1.75	1.64
1:P:1412:UNK:C	1:P:1412:UNK:CA	1.74	1.58
1:P:1412:UNK:HA	1:P:1415:UNK:CB	1.69	1.22
1:B:1412:UNK:HA	1:B:1415:UNK:CB	1.69	1.20
1:E:116:UNK:O	1:E:118:UNK:N	1.76	1.17
1:S:116:UNK:O	1:S:118:UNK:N	1.76	1.16
1:B:214:UNK:O	1:B:216:UNK:N	1.82	1.13
1:P:1412:UNK:C	1:P:1414:UNK:H	1.59	1.12
1:P:214:UNK:O	1:P:216:UNK:N	1.82	1.12
1:C:906:UNK:O	1:C:908:UNK:N	1.81	1.11
1:Q:906:UNK:O	1:Q:908:UNK:N	1.82	1.11
1:B:1412:UNK:C	1:B:1414:UNK:H	1.59	1.09
1:R:1109:UNK:O	1:R:1111:UNK:N	1.86	1.08
1:O:2606:UNK:O	1:O:2608:UNK:N	1.87	1.08
1:A:2606:UNK:O	1:A:2608:UNK:N	1.87	1.08
1:P:1018:UNK:O	1:P:1020:UNK:N	1.87	1.08
1:B:1018:UNK:O	1:B:1020:UNK:N	1.87	1.07
1:Q:2509:UNK:O	1:Q:2511:UNK:N	1.88	1.06
1:D:1109:UNK:O	1:D:1111:UNK:N	1.86	1.06
1:C:2509:UNK:O	1:C:2511:UNK:N	1.88	1.06
1:Y:838:UNK:O	1:Y:841:UNK:N	1.89	1.06
1:Y:838:UNK:O	1:Y:840:UNK:N	1.88	1.05
1:X:838:UNK:O	1:X:841:UNK:N	1.89	1.05
1:X:838:UNK:O	1:X:840:UNK:N	1.88	1.04
1:A:1514:UNK:O	1:A:1516:UNK:N	1.91	1.04
1:C:315:UNK:O	1:C:317:UNK:N	1.91	1.02
1:Q:315:UNK:O	1:Q:317:UNK:N	1.92	1.02
1:B:1711:UNK:O	1:B:1715:UNK:CB	2.07	1.02
1:P:1711:UNK:O	1:P:1715:UNK:CB	2.07	1.02
1:O:1514:UNK:O	1:O:1516:UNK:N	1.91	1.02
1:D:1012:UNK:O	1:D:1015:UNK:N	1.92	1.02
1:R:1012:UNK:O	1:R:1015:UNK:N	1.92	1.01
1:O:2507:UNK:HA	1:O:2510:UNK:CB	1.89	1.01
1:A:2507:UNK:HA	1:A:2510:UNK:CB	1.89	1.01
1:O:1212:UNK:O	1:O:1215:UNK:N	1.95	0.99
1:C:2513:UNK:O	1:C:2515:UNK:N	1.96	0.99
1:F:2219:UNK:O	1:F:2221:UNK:N	1.96	0.98
1:F:420:UNK:CB	1:F:508:UNK:HA	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:UNK:O	1:A:1215:UNK:N	1.95	0.98
1:R:221:UNK:O	1:R:223:UNK:N	1.96	0.98
1:Q:2513:UNK:O	1:Q:2515:UNK:N	1.96	0.98
1:D:221:UNK:O	1:D:223:UNK:N	1.96	0.98
1:T:420:UNK:CB	1:T:508:UNK:HA	1.92	0.98
1:C:1209:UNK:C	1:C:1211:UNK:H	1.77	0.98
1:C:2010:UNK:O	1:C:2012:UNK:N	1.98	0.97
1:D:407:UNK:O	1:D:409:UNK:N	1.98	0.97
1:F:2215:UNK:O	1:F:2218:UNK:N	1.98	0.97
1:T:2219:UNK:O	1:T:2221:UNK:N	1.96	0.97
1:D:305:UNK:O	1:D:307:UNK:N	1.98	0.97
1:T:2215:UNK:O	1:T:2218:UNK:N	1.98	0.96
1:Y:1034:UNK:HA	1:Y:1038:UNK:CB	1.95	0.96
1:D:509:UNK:C	1:D:511:UNK:H	1.77	0.96
1:R:305:UNK:O	1:R:307:UNK:N	1.98	0.96
1:R:407:UNK:O	1:R:409:UNK:N	1.98	0.96
1:Q:2010:UNK:O	1:Q:2012:UNK:N	1.97	0.95
1:Q:1209:UNK:C	1:Q:1211:UNK:H	1.77	0.95
1:X:1034:UNK:HA	1:X:1038:UNK:CB	1.95	0.95
1:D:1012:UNK:O	1:D:1014:UNK:N	2.00	0.95
1:P:1412:UNK:O	1:P:1414:UNK:N	1.97	0.95
1:R:1012:UNK:O	1:R:1014:UNK:N	2.00	0.95
1:R:509:UNK:C	1:R:511:UNK:H	1.77	0.94
1:Y:1070:UNK:O	1:Y:1073:UNK:N	2.00	0.94
1:Q:615:UNK:HA	1:Q:618:UNK:CB	1.97	0.94
1:O:913:UNK:CB	1:O:1009:UNK:CB	2.46	0.94
1:R:109:UNK:HA	1:R:112:UNK:CB	1.98	0.94
1:X:1070:UNK:O	1:X:1073:UNK:N	2.00	0.94
1:T:317:UNK:C	1:T:319:UNK:H	1.82	0.93
1:C:615:UNK:HA	1:C:618:UNK:CB	1.97	0.93
1:A:913:UNK:CB	1:A:1009:UNK:CB	2.46	0.93
1:B:1412:UNK:O	1:B:1414:UNK:N	1.97	0.93
1:D:109:UNK:HA	1:D:112:UNK:CB	1.98	0.92
1:Q:809:UNK:HA	1:Q:812:UNK:CB	1.99	0.92
1:C:809:UNK:HA	1:C:812:UNK:CB	1.99	0.92
1:A:1608:UNK:HA	1:A:1611:UNK:CB	2.00	0.91
1:F:317:UNK:C	1:F:319:UNK:H	1.82	0.91
1:C:1607:UNK:C	1:C:1609:UNK:H	1.81	0.91
1:O:1514:UNK:C	1:O:1516:UNK:N	2.33	0.91
1:P:1309:UNK:CB	1:P:1405:UNK:O	2.19	0.91
1:Y:873:UNK:O	1:Y:876:UNK:CB	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:838:UNK:C	1:Y:840:UNK:H	1.84	0.91
1:Q:1209:UNK:O	1:Q:1211:UNK:N	2.04	0.90
1:B:1309:UNK:CB	1:B:1405:UNK:O	2.19	0.90
1:O:1608:UNK:HA	1:O:1611:UNK:CB	2.00	0.90
1:X:873:UNK:O	1:X:876:UNK:CB	2.18	0.90
1:C:1412:UNK:C	1:C:1414:UNK:H	1.83	0.90
1:X:838:UNK:C	1:X:840:UNK:H	1.84	0.90
1:A:1514:UNK:C	1:A:1516:UNK:N	2.33	0.90
1:F:415:UNK:O	1:F:418:UNK:N	2.05	0.89
1:Q:1607:UNK:C	1:Q:1609:UNK:H	1.81	0.89
1:T:415:UNK:O	1:T:418:UNK:N	2.05	0.89
1:C:1209:UNK:O	1:C:1211:UNK:N	2.04	0.89
1:Q:1412:UNK:C	1:Q:1414:UNK:H	1.83	0.89
1:D:1012:UNK:C	1:D:1014:UNK:H	1.84	0.89
1:P:1507:UNK:HA	1:P:1510:UNK:CB	2.04	0.88
1:Q:2112:UNK:O	1:Q:2114:UNK:N	2.07	0.88
1:E:313:UNK:C	1:E:315:UNK:H	1.86	0.87
1:F:1312:UNK:C	1:F:1314:UNK:H	1.87	0.87
1:Q:414:UNK:O	1:Q:416:UNK:N	2.08	0.86
1:B:1507:UNK:HA	1:B:1510:UNK:CB	2.03	0.86
1:C:2112:UNK:O	1:C:2114:UNK:N	2.07	0.86
1:T:1312:UNK:C	1:T:1314:UNK:H	1.87	0.86
1:C:312:UNK:O	1:C:314:UNK:N	2.09	0.86
1:S:313:UNK:C	1:S:315:UNK:H	1.87	0.86
1:P:1107:UNK:O	1:P:1109:UNK:N	2.09	0.86
1:R:1012:UNK:C	1:R:1014:UNK:H	1.84	0.85
1:P:1515:UNK:O	1:P:1517:UNK:N	2.09	0.85
1:Q:312:UNK:O	1:Q:314:UNK:N	2.09	0.85
1:C:113:UNK:O	1:C:115:UNK:N	2.09	0.85
1:C:1308:UNK:HA	1:C:1311:UNK:CB	2.06	0.85
1:C:414:UNK:O	1:C:416:UNK:N	2.08	0.85
1:B:1515:UNK:O	1:B:1517:UNK:N	2.09	0.85
1:B:1107:UNK:O	1:B:1109:UNK:N	2.09	0.85
1:T:407:UNK:O	1:T:411:UNK:N	2.10	0.85
1:S:207:UNK:O	1:S:209:UNK:N	2.10	0.85
1:B:615:UNK:O	1:B:617:UNK:N	2.10	0.85
1:F:407:UNK:O	1:F:411:UNK:N	2.10	0.84
1:Q:113:UNK:O	1:Q:115:UNK:N	2.09	0.84
1:E:207:UNK:O	1:E:209:UNK:N	2.10	0.84
1:Q:1308:UNK:HA	1:Q:1311:UNK:CB	2.06	0.84
1:B:415:UNK:O	1:B:417:UNK:N	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:415:UNK:O	1:P:417:UNK:N	2.10	0.84
1:P:615:UNK:O	1:P:617:UNK:N	2.11	0.83
1:F:1010:UNK:HA	1:F:1013:UNK:CB	2.09	0.83
1:Q:1313:UNK:O	1:Q:1316:UNK:N	2.12	0.83
1:R:605:UNK:O	1:R:606:UNK:O	1.96	0.83
1:A:1312:UNK:O	1:A:1316:UNK:N	2.11	0.83
1:C:1313:UNK:O	1:C:1316:UNK:N	2.12	0.83
1:C:1408:UNK:C	1:C:1410:UNK:H	1.90	0.83
1:Q:1408:UNK:C	1:Q:1410:UNK:H	1.90	0.82
1:T:1010:UNK:HA	1:T:1013:UNK:CB	2.09	0.82
1:T:310:UNK:O	1:T:312:UNK:N	2.12	0.82
1:F:310:UNK:O	1:F:312:UNK:N	2.12	0.82
1:X:922:UNK:C	1:X:924:UNK:H	1.92	0.82
1:P:813:UNK:O	1:P:817:UNK:N	2.13	0.82
1:O:1312:UNK:O	1:O:1316:UNK:N	2.11	0.82
1:A:1517:UNK:C	1:A:1519:UNK:H	1.93	0.82
1:B:813:UNK:O	1:B:817:UNK:N	2.13	0.82
1:D:605:UNK:O	1:D:606:UNK:O	1.96	0.82
1:F:3414:UNK:C	1:F:3416:UNK:N	2.38	0.82
1:Q:807:UNK:O	1:Q:809:UNK:N	2.13	0.82
1:T:3414:UNK:C	1:T:3416:UNK:N	2.38	0.82
1:Y:922:UNK:C	1:Y:924:UNK:H	1.92	0.82
1:C:807:UNK:O	1:C:809:UNK:N	2.13	0.82
1:F:2113:UNK:O	1:F:2115:UNK:O	1.99	0.81
1:C:1313:UNK:O	1:C:1315:UNK:N	2.13	0.81
1:P:214:UNK:C	1:P:216:UNK:N	2.43	0.81
1:Q:1408:UNK:O	1:Q:1410:UNK:N	2.14	0.81
1:T:1309:UNK:O	1:T:1311:UNK:N	2.14	0.81
1:C:1408:UNK:O	1:C:1410:UNK:N	2.13	0.81
1:O:1517:UNK:C	1:O:1519:UNK:H	1.93	0.81
1:F:1309:UNK:O	1:F:1311:UNK:N	2.14	0.81
1:T:913:UNK:O	1:T:917:UNK:N	2.15	0.80
1:A:1509:UNK:C	1:A:1511:UNK:H	1.94	0.80
1:Q:1313:UNK:O	1:Q:1315:UNK:N	2.13	0.80
1:B:422:UNK:O	1:B:423:UNK:O	1.99	0.80
1:T:2616:UNK:C	1:T:2618:UNK:H	1.95	0.80
1:F:2616:UNK:C	1:F:2618:UNK:H	1.95	0.80
1:P:422:UNK:O	1:P:423:UNK:O	1.99	0.80
1:R:1205:UNK:O	1:R:1207:UNK:N	2.14	0.80
1:T:2113:UNK:O	1:T:2115:UNK:O	1.98	0.80
1:D:1205:UNK:O	1:D:1207:UNK:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:913:UNK:O	1:F:917:UNK:N	2.15	0.80
1:Q:1209:UNK:C	1:Q:1211:UNK:N	2.41	0.80
1:Q:305:UNK:O	1:Q:307:UNK:N	2.15	0.80
1:C:305:UNK:O	1:C:307:UNK:N	2.15	0.80
1:S:116:UNK:C	1:S:118:UNK:N	2.45	0.79
1:B:1412:UNK:C	1:B:1412:UNK:HA	2.09	0.79
1:C:613:UNK:C	1:C:615:UNK:N	2.42	0.79
1:P:1110:UNK:O	1:P:1112:UNK:N	2.15	0.79
1:B:1110:UNK:O	1:B:1112:UNK:N	2.15	0.79
1:C:1209:UNK:C	1:C:1211:UNK:N	2.41	0.79
1:Q:2509:UNK:C	1:Q:2511:UNK:N	2.46	0.79
1:Q:906:UNK:O	1:Q:909:UNK:N	2.15	0.79
1:O:1509:UNK:C	1:O:1511:UNK:H	1.94	0.79
1:E:116:UNK:C	1:E:118:UNK:N	2.45	0.79
1:R:1109:UNK:C	1:R:1111:UNK:H	1.96	0.79
1:B:214:UNK:C	1:B:216:UNK:N	2.43	0.78
1:Q:613:UNK:C	1:Q:615:UNK:N	2.42	0.78
1:T:516:UNK:O	1:T:605:UNK:N	2.16	0.78
1:F:418:UNK:C	1:F:420:UNK:H	1.96	0.78
1:Q:206:UNK:O	1:Q:210:UNK:CB	2.32	0.78
1:C:406:UNK:HA	1:C:409:UNK:CB	2.13	0.78
1:Q:406:UNK:HA	1:Q:409:UNK:CB	2.13	0.78
1:T:810:UNK:O	1:T:812:UNK:N	2.16	0.78
1:C:206:UNK:O	1:C:210:UNK:CB	2.32	0.78
1:P:1412:UNK:HA	1:P:1412:UNK:C	2.09	0.78
1:F:810:UNK:O	1:F:812:UNK:N	2.16	0.78
1:D:1109:UNK:C	1:D:1111:UNK:H	1.96	0.77
1:F:516:UNK:O	1:F:605:UNK:N	2.17	0.77
1:P:608:UNK:C	1:P:610:UNK:H	1.97	0.77
1:Q:1919:UNK:O	1:Q:1921:UNK:N	2.18	0.77
1:T:418:UNK:C	1:T:420:UNK:H	1.96	0.77
1:P:1420:UNK:O	1:P:1421:UNK:C	2.32	0.77
1:C:1919:UNK:O	1:C:1921:UNK:N	2.18	0.77
1:C:906:UNK:O	1:C:909:UNK:N	2.15	0.77
1:O:1421:UNK:C	1:O:1423:UNK:H	1.98	0.77
1:C:307:UNK:O	1:C:311:UNK:CB	2.32	0.77
1:P:1507:UNK:C	1:P:1509:UNK:H	1.97	0.77
1:Q:1415:UNK:O	1:Q:1418:UNK:N	2.17	0.77
1:A:2113:UNK:O	1:A:2116:UNK:N	2.18	0.77
1:B:608:UNK:C	1:B:610:UNK:H	1.97	0.77
1:Q:307:UNK:O	1:Q:311:UNK:CB	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2113:UNK:O	1:O:2116:UNK:N	2.18	0.77
1:C:1415:UNK:O	1:C:1418:UNK:N	2.17	0.77
1:F:105:UNK:O	1:F:109:UNK:N	2.18	0.76
1:A:1310:UNK:C	1:A:1312:UNK:N	2.45	0.76
1:A:1421:UNK:C	1:A:1423:UNK:H	1.98	0.76
1:C:2010:UNK:C	1:C:2012:UNK:H	1.98	0.76
1:C:2509:UNK:C	1:C:2511:UNK:N	2.46	0.76
1:B:1507:UNK:C	1:B:1509:UNK:H	1.97	0.76
1:B:1420:UNK:O	1:B:1421:UNK:C	2.32	0.76
1:C:1010:UNK:O	1:C:1012:UNK:N	2.19	0.76
1:D:908:UNK:O	1:D:910:UNK:N	2.19	0.76
1:F:505:UNK:O	1:F:507:UNK:N	2.19	0.76
1:T:2814:UNK:O	1:T:2816:UNK:N	2.18	0.76
1:B:207:UNK:HA	1:B:210:UNK:CB	2.17	0.76
1:T:105:UNK:O	1:T:109:UNK:N	2.18	0.75
1:P:207:UNK:HA	1:P:210:UNK:CB	2.16	0.75
1:R:107:UNK:O	1:R:111:UNK:N	2.19	0.75
1:D:107:UNK:O	1:D:111:UNK:N	2.19	0.75
1:Q:1010:UNK:O	1:Q:1012:UNK:N	2.19	0.75
1:Q:2010:UNK:C	1:Q:2012:UNK:H	1.98	0.75
1:B:1613:UNK:O	1:B:1615:UNK:N	2.20	0.75
1:F:2814:UNK:O	1:F:2816:UNK:N	2.18	0.75
1:O:2109:UNK:HA	1:O:2112:UNK:CB	2.16	0.75
1:Q:906:UNK:C	1:Q:908:UNK:N	2.50	0.75
1:P:1613:UNK:O	1:P:1615:UNK:N	2.20	0.75
1:T:3420:UNK:O	1:T:3423:UNK:O	2.05	0.75
1:C:2207:UNK:O	1:C:2210:UNK:N	2.20	0.75
1:T:505:UNK:O	1:T:507:UNK:N	2.19	0.75
1:A:2109:UNK:HA	1:A:2112:UNK:CB	2.16	0.74
1:F:3420:UNK:O	1:F:3423:UNK:O	2.05	0.74
1:Q:1320:UNK:O	1:Q:1322:UNK:N	2.21	0.74
1:B:1110:UNK:O	1:B:1113:UNK:N	2.21	0.74
1:O:2106:UNK:C	1:O:2108:UNK:H	2.00	0.74
1:F:2515:UNK:C	1:F:2517:UNK:N	2.48	0.74
1:R:908:UNK:O	1:R:910:UNK:N	2.19	0.74
1:A:2106:UNK:C	1:A:2108:UNK:H	2.00	0.73
1:Q:2207:UNK:O	1:Q:2210:UNK:N	2.20	0.73
1:C:1320:UNK:O	1:C:1322:UNK:N	2.21	0.73
1:D:610:UNK:O	1:D:612:UNK:N	2.21	0.73
1:C:906:UNK:C	1:C:908:UNK:N	2.50	0.73
1:P:1614:UNK:HA	1:P:1617:UNK:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1014:UNK:C	1:F:1016:UNK:N	2.49	0.73
1:R:610:UNK:O	1:R:612:UNK:N	2.21	0.73
1:D:716:UNK:O	1:D:720:UNK:N	2.22	0.73
1:P:1110:UNK:O	1:P:1113:UNK:N	2.21	0.73
1:T:1309:UNK:C	1:T:1311:UNK:N	2.52	0.73
1:C:106:UNK:O	1:C:109:UNK:N	2.21	0.73
1:Q:106:UNK:O	1:Q:109:UNK:N	2.21	0.73
1:F:1309:UNK:C	1:F:1311:UNK:N	2.52	0.73
1:O:2209:UNK:O	1:O:2213:UNK:CB	2.36	0.73
1:Q:2216:UNK:C	1:Q:2218:UNK:H	2.01	0.73
1:D:914:UNK:HA	1:D:917:UNK:CB	2.19	0.73
1:O:1310:UNK:C	1:O:1312:UNK:N	2.45	0.73
1:R:1214:UNK:C	1:R:1216:UNK:N	2.50	0.73
1:R:716:UNK:O	1:R:720:UNK:N	2.22	0.73
1:T:2515:UNK:C	1:T:2517:UNK:N	2.48	0.73
1:B:112:UNK:O	1:B:115:UNK:N	2.22	0.73
1:T:123:UNK:C	1:T:125:UNK:H	2.01	0.73
1:B:1614:UNK:HA	1:B:1617:UNK:CB	2.19	0.73
1:T:3208:UNK:C	1:T:3210:UNK:N	2.51	0.73
1:S:225:UNK:O	1:S:227:UNK:N	2.22	0.72
1:F:1211:UNK:O	1:F:1212:UNK:C	2.38	0.72
1:R:1005:UNK:O	1:R:1007:UNK:N	2.22	0.72
1:F:1014:UNK:O	1:F:1017:UNK:N	2.22	0.72
1:F:123:UNK:C	1:F:125:UNK:H	2.01	0.72
1:T:715:UNK:C	1:T:717:UNK:H	2.01	0.72
1:A:2209:UNK:O	1:A:2213:UNK:CB	2.36	0.72
1:C:2216:UNK:C	1:C:2218:UNK:H	2.01	0.72
1:E:225:UNK:O	1:E:227:UNK:N	2.22	0.72
1:F:715:UNK:C	1:F:717:UNK:H	2.01	0.72
1:R:307:UNK:O	1:R:308:UNK:C	2.37	0.72
1:T:1014:UNK:C	1:T:1016:UNK:N	2.49	0.72
1:D:1005:UNK:O	1:D:1007:UNK:N	2.22	0.72
1:P:1311:UNK:O	1:P:1315:UNK:N	2.22	0.72
1:R:914:UNK:HA	1:R:917:UNK:CB	2.19	0.72
1:F:2005:UNK:C	1:F:2007:UNK:N	2.51	0.72
1:A:1114:UNK:O	1:A:1117:UNK:N	2.23	0.72
1:X:1030:UNK:O	1:X:1031:UNK:C	2.38	0.72
1:C:1906:UNK:O	1:C:1909:UNK:N	2.23	0.72
1:F:913:UNK:C	1:F:915:UNK:N	2.52	0.72
1:T:1014:UNK:O	1:T:1017:UNK:N	2.22	0.72
1:B:1412:UNK:CA	1:B:1415:UNK:CB	2.62	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:407:UNK:O	1:P:410:UNK:N	2.23	0.71
1:T:913:UNK:C	1:T:915:UNK:N	2.52	0.71
1:B:1311:UNK:O	1:B:1315:UNK:N	2.22	0.71
1:B:407:UNK:O	1:B:410:UNK:N	2.23	0.71
1:Q:1906:UNK:O	1:Q:1909:UNK:N	2.23	0.71
1:X:1029:UNK:O	1:X:1030:UNK:C	2.38	0.71
1:F:120:UNK:O	1:F:122:UNK:N	2.23	0.71
1:P:112:UNK:O	1:P:115:UNK:N	2.22	0.71
1:D:307:UNK:O	1:D:308:UNK:C	2.37	0.71
1:T:3207:UNK:O	1:T:3211:UNK:CB	2.39	0.71
1:X:847:UNK:C	1:X:849:UNK:H	2.03	0.71
1:A:1810:UNK:O	1:A:1814:UNK:N	2.23	0.71
1:O:1114:UNK:O	1:O:1117:UNK:N	2.23	0.71
1:F:3207:UNK:O	1:F:3211:UNK:CB	2.39	0.71
1:F:3414:UNK:O	1:F:3416:UNK:N	2.24	0.71
1:O:2115:UNK:O	1:O:2118:UNK:CB	2.39	0.71
1:T:3414:UNK:O	1:T:3416:UNK:N	2.24	0.71
1:R:221:UNK:C	1:R:223:UNK:N	2.53	0.71
1:A:2115:UNK:O	1:A:2118:UNK:CB	2.39	0.71
1:Y:804:UNK:C	1:Y:806:UNK:N	2.51	0.71
1:D:609:UNK:O	1:D:610:UNK:O	2.08	0.71
1:O:1810:UNK:O	1:O:1814:UNK:N	2.23	0.71
1:T:120:UNK:O	1:T:122:UNK:N	2.23	0.71
1:Y:1029:UNK:O	1:Y:1030:UNK:C	2.38	0.71
1:F:1312:UNK:HA	1:F:1315:UNK:CB	2.21	0.70
1:S:309:UNK:O	1:S:311:UNK:N	2.24	0.70
1:D:221:UNK:C	1:D:223:UNK:N	2.53	0.70
1:P:118:UNK:O	1:P:121:UNK:CB	2.40	0.70
1:T:1312:UNK:HA	1:T:1315:UNK:CB	2.21	0.70
1:X:804:UNK:C	1:X:806:UNK:N	2.51	0.70
1:F:3208:UNK:C	1:F:3210:UNK:N	2.51	0.70
1:T:2005:UNK:C	1:T:2007:UNK:N	2.51	0.70
1:Q:2207:UNK:O	1:Q:2208:UNK:C	2.39	0.70
1:E:309:UNK:O	1:E:311:UNK:N	2.24	0.70
1:T:2620:UNK:O	1:T:2623:UNK:N	2.25	0.70
1:X:1048:UNK:O	1:X:1050:UNK:N	2.25	0.70
1:Y:1048:UNK:O	1:Y:1050:UNK:N	2.25	0.70
1:T:120:UNK:C	1:T:122:UNK:N	2.55	0.69
1:C:2211:UNK:C	1:C:2213:UNK:H	2.06	0.69
1:P:605:UNK:CB	1:P:905:UNK:H	2.05	0.69
1:F:120:UNK:C	1:F:122:UNK:N	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2620:UNK:O	1:F:2623:UNK:N	2.25	0.69
1:P:1107:UNK:O	1:P:1110:UNK:N	2.26	0.69
1:Y:847:UNK:C	1:Y:849:UNK:H	2.03	0.69
1:Q:709:UNK:O	1:Q:713:UNK:N	2.25	0.69
1:T:1211:UNK:O	1:T:1212:UNK:C	2.38	0.69
1:C:2207:UNK:O	1:C:2208:UNK:C	2.39	0.69
1:C:709:UNK:O	1:C:713:UNK:N	2.25	0.69
1:D:1214:UNK:C	1:D:1216:UNK:N	2.50	0.69
1:R:609:UNK:O	1:R:610:UNK:O	2.08	0.69
1:Q:1209:UNK:O	1:Q:1212:UNK:N	2.26	0.69
1:T:1908:UNK:C	1:T:1910:UNK:N	2.52	0.69
1:Y:1030:UNK:O	1:Y:1031:UNK:C	2.38	0.69
1:B:1210:UNK:O	1:B:1211:UNK:C	2.41	0.69
1:B:1608:UNK:HA	1:B:1611:UNK:CB	2.23	0.69
1:C:1209:UNK:O	1:C:1212:UNK:N	2.26	0.69
1:B:118:UNK:O	1:B:121:UNK:CB	2.40	0.69
1:B:1107:UNK:O	1:B:1110:UNK:N	2.26	0.69
1:C:2208:UNK:C	1:C:2210:UNK:H	2.06	0.69
1:F:1417:UNK:O	1:F:1418:UNK:C	2.41	0.69
1:F:1908:UNK:C	1:F:1910:UNK:N	2.52	0.69
1:Y:873:UNK:O	1:Y:874:UNK:C	2.41	0.69
1:B:605:UNK:CB	1:B:905:UNK:H	2.05	0.68
1:D:115:UNK:C	1:D:117:UNK:N	2.54	0.68
1:P:1608:UNK:C	1:P:1610:UNK:H	2.05	0.68
1:Q:2208:UNK:C	1:Q:2210:UNK:H	2.06	0.68
1:T:3308:UNK:C	1:T:3310:UNK:N	2.56	0.68
1:P:1608:UNK:HA	1:P:1611:UNK:CB	2.23	0.68
1:Q:2211:UNK:C	1:Q:2213:UNK:H	2.06	0.68
1:X:873:UNK:O	1:X:874:UNK:C	2.41	0.68
1:A:2110:UNK:O	1:A:2114:UNK:N	2.27	0.68
1:B:611:UNK:O	1:B:613:UNK:N	2.26	0.68
1:O:2110:UNK:O	1:O:2114:UNK:N	2.27	0.68
1:A:1212:UNK:O	1:A:1214:UNK:N	2.27	0.68
1:A:2606:UNK:O	1:A:2609:UNK:N	2.27	0.68
1:O:1212:UNK:O	1:O:1214:UNK:N	2.27	0.68
1:P:1412:UNK:CA	1:P:1415:UNK:CB	2.62	0.68
1:D:709:UNK:C	1:D:711:UNK:H	2.08	0.68
1:O:2606:UNK:O	1:O:2609:UNK:N	2.27	0.68
1:P:1210:UNK:O	1:P:1211:UNK:C	2.41	0.68
1:P:1511:UNK:C	1:P:1513:UNK:N	2.55	0.68
1:R:509:UNK:O	1:R:512:UNK:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:922:UNK:C	1:X:924:UNK:N	2.56	0.68
1:C:315:UNK:C	1:C:317:UNK:N	2.56	0.67
1:D:509:UNK:O	1:D:512:UNK:N	2.27	0.67
1:F:3308:UNK:C	1:F:3310:UNK:N	2.56	0.67
1:F:2817:UNK:O	1:F:2820:UNK:CB	2.43	0.67
1:P:611:UNK:O	1:P:613:UNK:N	2.26	0.67
1:F:418:UNK:O	1:F:421:UNK:N	2.28	0.67
1:B:1010:UNK:O	1:B:1011:UNK:C	2.43	0.67
1:D:911:UNK:O	1:D:913:UNK:N	2.28	0.67
1:Q:315:UNK:C	1:Q:317:UNK:N	2.56	0.67
1:T:2817:UNK:O	1:T:2820:UNK:CB	2.43	0.67
1:D:224:UNK:O	1:D:226:UNK:N	2.24	0.67
1:O:2111:UNK:HA	1:O:2114:UNK:CB	2.24	0.67
1:T:2319:UNK:O	1:T:2321:UNK:N	2.28	0.67
1:A:2111:UNK:HA	1:A:2114:UNK:CB	2.24	0.67
1:R:115:UNK:C	1:R:117:UNK:N	2.54	0.67
1:R:212:UNK:O	1:R:213:UNK:C	2.43	0.67
1:R:224:UNK:C	1:R:226:UNK:H	2.08	0.67
1:T:418:UNK:O	1:T:421:UNK:N	2.28	0.67
1:A:1820:UNK:CB	1:A:2012:UNK:CB	2.73	0.66
1:F:2219:UNK:C	1:F:2221:UNK:N	2.58	0.66
1:F:2319:UNK:O	1:F:2321:UNK:N	2.28	0.66
1:D:315:UNK:HA	1:D:318:UNK:CB	2.25	0.66
1:D:315:UNK:HA	1:D:318:UNK:CA	2.25	0.66
1:R:709:UNK:C	1:R:711:UNK:H	2.08	0.66
1:T:1417:UNK:O	1:T:1418:UNK:C	2.41	0.66
1:D:224:UNK:C	1:D:226:UNK:H	2.08	0.66
1:F:1521:UNK:O	1:F:1523:UNK:N	2.28	0.66
1:T:3206:UNK:O	1:T:3210:UNK:CB	2.44	0.66
1:P:1010:UNK:O	1:P:1011:UNK:C	2.43	0.66
1:C:117:UNK:C	1:C:119:UNK:N	2.58	0.66
1:C:2112:UNK:C	1:C:2114:UNK:N	2.59	0.66
1:C:2305:UNK:O	1:C:2307:UNK:N	2.28	0.66
1:O:1820:UNK:CB	1:O:2012:UNK:CB	2.73	0.66
1:Q:2305:UNK:O	1:Q:2307:UNK:N	2.29	0.66
1:R:911:UNK:O	1:R:913:UNK:N	2.28	0.66
1:Y:917:UNK:C	1:Y:919:UNK:H	2.09	0.66
1:R:208:UNK:C	1:R:210:UNK:N	2.55	0.66
1:T:1521:UNK:O	1:T:1523:UNK:N	2.28	0.66
1:O:1317:UNK:O	1:O:1318:UNK:C	2.44	0.66
1:P:1213:UNK:C	1:P:1215:UNK:H	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:315:UNK:HA	1:R:318:UNK:CB	2.25	0.66
1:P:711:UNK:C	1:P:713:UNK:H	2.09	0.66
1:A:2121:UNK:C	1:A:2123:UNK:H	2.09	0.66
1:T:2219:UNK:C	1:T:2221:UNK:N	2.58	0.66
1:F:3206:UNK:O	1:F:3210:UNK:CB	2.44	0.65
1:Q:117:UNK:C	1:Q:119:UNK:N	2.57	0.65
1:R:315:UNK:HA	1:R:318:UNK:CA	2.25	0.65
1:A:1418:UNK:O	1:A:1420:UNK:N	2.29	0.65
1:B:707:UNK:C	1:B:709:UNK:N	2.58	0.65
1:O:1114:UNK:C	1:O:1116:UNK:N	2.56	0.65
1:O:2121:UNK:C	1:O:2123:UNK:H	2.09	0.65
1:A:2415:UNK:O	1:A:2417:UNK:N	2.30	0.65
1:C:2112:UNK:O	1:C:2115:UNK:N	2.29	0.65
1:B:1511:UNK:C	1:B:1513:UNK:N	2.55	0.65
1:Q:2112:UNK:O	1:Q:2115:UNK:N	2.30	0.65
1:C:1320:UNK:O	1:C:1321:UNK:C	2.45	0.65
1:C:613:UNK:O	1:C:615:UNK:N	2.30	0.65
1:F:3305:UNK:O	1:F:3307:UNK:N	2.30	0.65
1:O:1418:UNK:O	1:O:1420:UNK:N	2.30	0.65
1:O:2415:UNK:O	1:O:2417:UNK:N	2.30	0.65
1:T:3305:UNK:O	1:T:3307:UNK:N	2.29	0.65
1:B:1213:UNK:C	1:B:1215:UNK:H	2.09	0.65
1:E:112:UNK:C	1:E:114:UNK:H	2.10	0.65
1:Q:1320:UNK:O	1:Q:1321:UNK:C	2.45	0.65
1:T:2006:UNK:O	1:T:2007:UNK:C	2.45	0.65
1:A:1317:UNK:O	1:A:1318:UNK:C	2.44	0.65
1:D:208:UNK:C	1:D:210:UNK:N	2.55	0.65
1:F:2215:UNK:O	1:F:2216:UNK:C	2.45	0.65
1:X:917:UNK:C	1:X:919:UNK:H	2.09	0.65
1:D:212:UNK:O	1:D:213:UNK:C	2.43	0.65
1:P:615:UNK:C	1:P:617:UNK:H	2.07	0.65
1:Q:1005:UNK:HA	1:Q:1120:UNK:CB	2.26	0.65
1:T:1208:UNK:O	1:T:1210:UNK:N	2.30	0.65
1:T:2215:UNK:O	1:T:2216:UNK:C	2.45	0.65
1:A:1114:UNK:C	1:A:1116:UNK:N	2.56	0.65
1:C:2408:UNK:O	1:C:2409:UNK:C	2.45	0.65
1:C:113:UNK:C	1:C:115:UNK:N	2.60	0.65
1:F:2006:UNK:O	1:F:2007:UNK:C	2.45	0.65
1:F:316:UNK:O	1:F:320:UNK:N	2.30	0.65
1:Q:513:UNK:O	1:Q:517:UNK:N	2.31	0.65
1:T:316:UNK:O	1:T:320:UNK:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:UNK:HA	1:C:1120:UNK:CB	2.26	0.64
1:C:117:UNK:O	1:C:119:UNK:N	2.29	0.64
1:C:513:UNK:O	1:C:517:UNK:N	2.31	0.64
1:F:1208:UNK:O	1:F:1210:UNK:N	2.30	0.64
1:R:308:UNK:O	1:R:310:UNK:N	2.30	0.64
1:Y:922:UNK:C	1:Y:924:UNK:N	2.56	0.64
1:B:711:UNK:C	1:B:713:UNK:H	2.09	0.64
1:O:1209:UNK:HA	1:O:1212:UNK:CB	2.28	0.64
1:Q:117:UNK:O	1:Q:119:UNK:N	2.29	0.64
1:D:808:UNK:O	1:D:812:UNK:N	2.31	0.64
1:Y:1048:UNK:C	1:Y:1050:UNK:N	2.60	0.64
1:A:1209:UNK:HA	1:A:1212:UNK:CB	2.28	0.64
1:Q:912:UNK:O	1:Q:914:UNK:N	2.30	0.64
1:P:1015:UNK:O	1:P:1017:UNK:N	2.31	0.64
1:R:808:UNK:O	1:R:812:UNK:N	2.31	0.64
1:B:615:UNK:C	1:B:617:UNK:H	2.07	0.64
1:F:415:UNK:O	1:F:417:UNK:N	2.31	0.64
1:C:912:UNK:O	1:C:914:UNK:N	2.30	0.64
1:F:2814:UNK:O	1:F:2817:UNK:N	2.31	0.64
1:C:1806:UNK:C	1:C:1808:UNK:N	2.61	0.64
1:P:818:UNK:C	1:P:820:UNK:N	2.59	0.64
1:B:818:UNK:C	1:B:820:UNK:N	2.59	0.64
1:D:308:UNK:O	1:D:310:UNK:N	2.31	0.64
1:Q:613:UNK:O	1:Q:615:UNK:N	2.30	0.64
1:R:1009:UNK:O	1:R:1013:UNK:N	2.31	0.64
1:A:2108:UNK:O	1:A:2112:UNK:N	2.31	0.64
1:A:2406:UNK:O	1:A:2407:UNK:O	2.16	0.64
1:P:306:UNK:O	1:P:310:UNK:N	2.31	0.64
1:Q:2112:UNK:C	1:Q:2114:UNK:N	2.59	0.64
1:A:1221:UNK:O	1:A:1307:UNK:HA	1.99	0.63
1:B:1015:UNK:O	1:B:1017:UNK:N	2.31	0.63
1:C:2409:UNK:O	1:C:2410:UNK:O	2.16	0.63
1:C:807:UNK:C	1:C:809:UNK:N	2.61	0.63
1:S:112:UNK:C	1:S:114:UNK:H	2.10	0.63
1:D:1009:UNK:O	1:D:1013:UNK:N	2.31	0.63
1:P:211:UNK:HA	1:P:214:UNK:CB	2.27	0.63
1:T:415:UNK:O	1:T:417:UNK:N	2.31	0.63
1:B:306:UNK:O	1:B:310:UNK:N	2.31	0.63
1:C:2121:UNK:O	1:C:2125:UNK:N	2.31	0.63
1:Q:2121:UNK:O	1:Q:2125:UNK:N	2.31	0.63
1:Q:2409:UNK:O	1:Q:2410:UNK:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3007:UNK:C	1:F:3009:UNK:N	2.60	0.63
1:O:2406:UNK:O	1:O:2407:UNK:O	2.16	0.63
1:Q:2408:UNK:O	1:Q:2409:UNK:C	2.45	0.63
1:P:707:UNK:C	1:P:709:UNK:N	2.58	0.63
1:T:2006:UNK:O	1:T:2010:UNK:N	2.32	0.63
1:C:2305:UNK:C	1:C:2307:UNK:N	2.61	0.63
1:P:716:UNK:O	1:P:718:UNK:N	2.32	0.63
1:Q:1818:UNK:O	1:Q:1820:UNK:N	2.32	0.63
1:B:211:UNK:HA	1:B:214:UNK:CB	2.27	0.63
1:A:2406:UNK:O	1:A:2407:UNK:C	2.47	0.63
1:B:716:UNK:O	1:B:718:UNK:N	2.32	0.63
1:A:2411:UNK:C	1:A:2413:UNK:N	2.60	0.63
1:F:2109:UNK:C	1:F:2111:UNK:N	2.60	0.63
1:O:1008:UNK:C	1:O:1010:UNK:N	2.60	0.63
1:P:1313:UNK:O	1:P:1317:UNK:N	2.32	0.63
1:P:210:UNK:C	1:P:212:UNK:H	2.11	0.63
1:Q:113:UNK:C	1:Q:115:UNK:N	2.60	0.63
1:T:3414:UNK:O	1:T:3417:UNK:N	2.32	0.63
1:X:1048:UNK:C	1:X:1050:UNK:N	2.60	0.63
1:Y:924:UNK:O	1:Y:928:UNK:N	2.32	0.63
1:O:2406:UNK:O	1:O:2407:UNK:C	2.47	0.62
1:Q:1411:UNK:O	1:Q:1415:UNK:N	2.32	0.62
1:Q:807:UNK:C	1:Q:809:UNK:N	2.61	0.62
1:C:1013:UNK:O	1:C:1015:UNK:N	2.32	0.62
1:C:1305:UNK:O	1:C:1307:UNK:N	2.32	0.62
1:F:3414:UNK:O	1:F:3417:UNK:N	2.32	0.62
1:O:2307:UNK:O	1:O:2310:UNK:N	2.32	0.62
1:Q:1415:UNK:C	1:Q:1417:UNK:N	2.61	0.62
1:A:1418:UNK:O	1:A:1421:UNK:N	2.32	0.62
1:B:1313:UNK:O	1:B:1317:UNK:N	2.32	0.62
1:D:714:UNK:O	1:D:716:UNK:N	2.33	0.62
1:F:2817:UNK:O	1:F:2820:UNK:N	2.32	0.62
1:F:512:UNK:C	1:F:514:UNK:N	2.61	0.62
1:O:1221:UNK:O	1:O:1307:UNK:HA	1.98	0.62
1:O:2108:UNK:O	1:O:2112:UNK:N	2.31	0.62
1:R:509:UNK:C	1:R:511:UNK:N	2.52	0.62
1:X:924:UNK:O	1:X:928:UNK:N	2.32	0.62
1:D:919:UNK:HA	1:D:922:UNK:CB	2.30	0.62
1:F:512:UNK:O	1:F:514:UNK:N	2.33	0.62
1:Y:1025:UNK:HA	1:Y:1028:UNK:CB	2.30	0.62
1:A:1418:UNK:C	1:A:1420:UNK:N	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:706:UNK:O	1:D:708:UNK:N	2.33	0.62
1:T:2109:UNK:C	1:T:2111:UNK:N	2.60	0.62
1:Y:1066:UNK:HA	1:Y:1069:UNK:CB	2.30	0.62
1:C:1415:UNK:C	1:C:1417:UNK:N	2.61	0.62
1:O:2411:UNK:C	1:O:2413:UNK:N	2.61	0.62
1:Q:1412:UNK:O	1:Q:1414:UNK:N	2.31	0.62
1:R:919:UNK:HA	1:R:922:UNK:CB	2.30	0.62
1:T:512:UNK:O	1:T:514:UNK:N	2.33	0.62
1:C:1411:UNK:O	1:C:1415:UNK:N	2.32	0.62
1:Q:1806:UNK:C	1:Q:1808:UNK:N	2.61	0.62
1:Q:506:UNK:HA	1:Q:509:UNK:CB	2.30	0.62
1:A:1008:UNK:C	1:A:1010:UNK:N	2.60	0.62
1:O:1418:UNK:O	1:O:1421:UNK:N	2.32	0.62
1:T:2814:UNK:O	1:T:2817:UNK:N	2.31	0.62
1:T:317:UNK:O	1:T:321:UNK:N	2.33	0.62
1:B:1015:UNK:C	1:B:1017:UNK:N	2.60	0.62
1:B:1310:UNK:O	1:B:1314:UNK:N	2.33	0.62
1:F:2207:UNK:O	1:F:2210:UNK:N	2.33	0.62
1:R:706:UNK:O	1:R:708:UNK:N	2.33	0.62
1:T:1517:UNK:O	1:T:1521:UNK:N	2.33	0.62
1:B:911:UNK:C	1:B:913:UNK:N	2.61	0.62
1:C:1818:UNK:O	1:C:1820:UNK:N	2.32	0.62
1:F:220:UNK:C	1:F:222:UNK:N	2.60	0.62
1:P:1015:UNK:C	1:P:1017:UNK:N	2.61	0.62
1:A:1712:UNK:O	1:A:1715:UNK:N	2.33	0.61
1:P:1310:UNK:O	1:P:1314:UNK:N	2.33	0.61
1:R:719:UNK:C	1:R:721:UNK:N	2.61	0.61
1:A:2307:UNK:O	1:A:2310:UNK:N	2.32	0.61
1:C:1919:UNK:C	1:C:1921:UNK:N	2.63	0.61
1:F:1517:UNK:O	1:F:1521:UNK:N	2.33	0.61
1:F:708:UNK:O	1:F:710:UNK:N	2.33	0.61
1:T:220:UNK:C	1:T:222:UNK:N	2.60	0.61
1:X:855:UNK:O	1:X:858:UNK:C	2.48	0.61
1:C:506:UNK:HA	1:C:509:UNK:CB	2.30	0.61
1:D:717:UNK:HA	1:D:720:UNK:CB	2.30	0.61
1:P:1708:UNK:O	1:P:1709:UNK:C	2.48	0.61
1:Q:1305:UNK:O	1:Q:1307:UNK:N	2.32	0.61
1:Q:1919:UNK:C	1:Q:1921:UNK:N	2.63	0.61
1:T:2207:UNK:O	1:T:2210:UNK:N	2.33	0.61
1:X:1025:UNK:HA	1:X:1028:UNK:CB	2.30	0.61
1:C:1507:UNK:O	1:C:1510:UNK:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2006:UNK:O	1:F:2010:UNK:N	2.32	0.61
1:R:717:UNK:HA	1:R:720:UNK:CB	2.30	0.61
1:D:509:UNK:C	1:D:511:UNK:N	2.52	0.61
1:O:1712:UNK:O	1:O:1715:UNK:N	2.33	0.61
1:Q:1814:UNK:O	1:Q:1815:UNK:C	2.49	0.61
1:T:2817:UNK:O	1:T:2820:UNK:N	2.32	0.61
1:F:1514:UNK:O	1:F:1518:UNK:N	2.33	0.61
1:C:1505:UNK:O	1:C:1507:UNK:N	2.33	0.61
1:D:709:UNK:O	1:D:711:UNK:N	2.33	0.61
1:F:418:UNK:C	1:F:420:UNK:N	2.60	0.61
1:O:1418:UNK:C	1:O:1420:UNK:N	2.62	0.61
1:Q:2010:UNK:C	1:Q:2012:UNK:N	2.60	0.61
1:R:224:UNK:O	1:R:226:UNK:N	2.24	0.61
1:C:1309:UNK:O	1:C:1312:UNK:N	2.34	0.61
1:C:2513:UNK:C	1:C:2515:UNK:N	2.64	0.61
1:P:1515:UNK:C	1:P:1517:UNK:N	2.63	0.61
1:P:615:UNK:C	1:P:617:UNK:N	2.64	0.61
1:Q:1505:UNK:O	1:Q:1507:UNK:N	2.33	0.61
1:R:714:UNK:O	1:R:716:UNK:N	2.33	0.61
1:T:119:UNK:HA	1:T:122:UNK:CB	2.31	0.61
1:A:1406:UNK:C	1:A:1408:UNK:H	2.14	0.61
1:B:1708:UNK:O	1:B:1709:UNK:C	2.48	0.61
1:B:210:UNK:C	1:B:212:UNK:H	2.11	0.61
1:T:1514:UNK:O	1:T:1518:UNK:N	2.34	0.61
1:X:1066:UNK:HA	1:X:1069:UNK:CB	2.30	0.61
1:A:2406:UNK:O	1:A:2410:UNK:N	2.34	0.60
1:B:210:UNK:O	1:B:213:UNK:N	2.34	0.60
1:F:317:UNK:O	1:F:321:UNK:N	2.33	0.60
1:P:911:UNK:C	1:P:913:UNK:N	2.61	0.60
1:R:709:UNK:O	1:R:711:UNK:N	2.33	0.60
1:C:1814:UNK:O	1:C:1815:UNK:C	2.49	0.60
1:Y:806:UNK:C	1:Y:808:UNK:H	2.14	0.60
1:Y:855:UNK:O	1:Y:858:UNK:C	2.48	0.60
1:A:1206:UNK:C	1:A:1208:UNK:N	2.64	0.60
1:Q:1507:UNK:O	1:Q:1510:UNK:N	2.33	0.60
1:R:610:UNK:O	1:R:611:UNK:C	2.49	0.60
1:B:615:UNK:C	1:B:617:UNK:N	2.64	0.60
1:C:2010:UNK:C	1:C:2012:UNK:N	2.60	0.60
1:C:2309:UNK:C	1:C:2311:UNK:N	2.64	0.60
1:D:905:UNK:C	1:D:907:UNK:N	2.62	0.60
1:F:2814:UNK:C	1:F:2816:UNK:N	2.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1307:UNK:O	1:P:1309:UNK:N	2.35	0.60
1:Q:2305:UNK:C	1:Q:2307:UNK:N	2.61	0.60
1:R:1211:UNK:O	1:R:1213:UNK:N	2.35	0.60
1:D:719:UNK:C	1:D:721:UNK:N	2.62	0.60
1:P:210:UNK:O	1:P:213:UNK:N	2.34	0.60
1:T:310:UNK:C	1:T:312:UNK:N	2.63	0.60
1:X:834:UNK:O	1:X:835:UNK:CB	2.49	0.60
1:D:407:UNK:C	1:D:409:UNK:N	2.64	0.60
1:R:407:UNK:C	1:R:409:UNK:N	2.65	0.60
1:T:418:UNK:C	1:T:420:UNK:N	2.60	0.60
1:C:2216:UNK:C	1:C:2218:UNK:N	2.64	0.60
1:D:1211:UNK:O	1:D:1213:UNK:N	2.34	0.60
1:Q:1309:UNK:O	1:Q:1312:UNK:N	2.34	0.60
1:Q:2211:UNK:C	1:Q:2213:UNK:N	2.62	0.60
1:Y:920:UNK:O	1:Y:923:UNK:N	2.35	0.60
1:B:1307:UNK:O	1:B:1309:UNK:N	2.35	0.60
1:D:107:UNK:HA	1:D:110:UNK:CB	2.32	0.60
1:T:1417:UNK:O	1:T:1420:UNK:N	2.35	0.60
1:T:512:UNK:C	1:T:514:UNK:N	2.61	0.60
1:D:610:UNK:O	1:D:611:UNK:C	2.49	0.60
1:Y:843:UNK:O	1:Y:846:UNK:N	2.35	0.60
1:D:1112:UNK:O	1:D:1114:UNK:N	2.35	0.59
1:F:119:UNK:HA	1:F:122:UNK:CB	2.31	0.59
1:Q:2309:UNK:C	1:Q:2311:UNK:N	2.64	0.59
1:R:1112:UNK:O	1:R:1114:UNK:N	2.35	0.59
1:T:1906:UNK:O	1:T:1910:UNK:N	2.35	0.59
1:O:2406:UNK:O	1:O:2410:UNK:N	2.34	0.59
1:R:107:UNK:HA	1:R:110:UNK:CB	2.32	0.59
1:R:721:UNK:C	1:R:723:UNK:N	2.65	0.59
1:T:3007:UNK:C	1:T:3009:UNK:N	2.60	0.59
1:T:708:UNK:O	1:T:710:UNK:N	2.33	0.59
1:A:2005:UNK:C	1:A:2007:UNK:N	2.63	0.59
1:O:1206:UNK:C	1:O:1208:UNK:N	2.65	0.59
1:O:1406:UNK:C	1:O:1408:UNK:H	2.13	0.59
1:T:2616:UNK:C	1:T:2618:UNK:N	2.59	0.59
1:O:2305:UNK:O	1:O:2308:UNK:CB	2.50	0.59
1:P:508:UNK:O	1:P:511:UNK:N	2.35	0.59
1:T:3305:UNK:C	1:T:3307:UNK:N	2.64	0.59
1:C:911:UNK:O	1:C:914:UNK:CB	2.51	0.59
1:O:2507:UNK:CA	1:O:2510:UNK:CB	2.75	0.59
1:Q:117:UNK:O	1:Q:120:UNK:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:709:UNK:HA	1:T:712:UNK:CB	2.33	0.59
1:A:712:UNK:CB	1:A:905:UNK:CB	2.81	0.59
1:B:508:UNK:O	1:B:511:UNK:N	2.35	0.59
1:F:3308:UNK:O	1:F:3310:UNK:N	2.36	0.59
1:Q:2118:UNK:O	1:Q:2122:UNK:N	2.36	0.59
1:T:3308:UNK:O	1:T:3310:UNK:N	2.36	0.59
1:X:920:UNK:O	1:X:923:UNK:N	2.35	0.59
1:C:1313:UNK:C	1:C:1315:UNK:N	2.64	0.59
1:F:3308:UNK:O	1:F:3311:UNK:N	2.36	0.59
1:O:2005:UNK:C	1:O:2007:UNK:N	2.63	0.59
1:T:2814:UNK:C	1:T:2816:UNK:N	2.63	0.59
1:X:803:UNK:HA	1:X:810:UNK:O	2.03	0.59
1:B:1515:UNK:C	1:B:1517:UNK:N	2.63	0.59
1:F:3305:UNK:C	1:F:3307:UNK:N	2.64	0.59
1:X:1050:UNK:O	1:X:1053:UNK:CB	2.51	0.59
1:Y:834:UNK:O	1:Y:835:UNK:CB	2.50	0.59
1:A:2305:UNK:O	1:A:2308:UNK:CB	2.50	0.59
1:C:1013:UNK:C	1:C:1015:UNK:H	2.16	0.59
1:C:2118:UNK:O	1:C:2122:UNK:N	2.36	0.59
1:F:2616:UNK:C	1:F:2618:UNK:N	2.59	0.59
1:X:843:UNK:O	1:X:846:UNK:N	2.35	0.59
1:C:117:UNK:O	1:C:120:UNK:N	2.36	0.59
1:F:1417:UNK:O	1:F:1420:UNK:N	2.35	0.59
1:F:3421:UNK:C	1:F:3423:UNK:N	2.61	0.59
1:T:3308:UNK:O	1:T:3311:UNK:N	2.36	0.59
1:T:1309:UNK:O	1:T:1313:UNK:N	2.36	0.58
1:X:880:UNK:O	1:X:881:UNK:C	2.50	0.58
1:D:908:UNK:O	1:D:911:UNK:N	2.37	0.58
1:O:712:UNK:CB	1:O:905:UNK:CB	2.81	0.58
1:Q:911:UNK:O	1:Q:914:UNK:CB	2.51	0.58
1:Y:1050:UNK:O	1:Y:1053:UNK:CB	2.51	0.58
1:Y:803:UNK:HA	1:Y:810:UNK:O	2.03	0.58
1:A:2106:UNK:C	1:A:2108:UNK:N	2.64	0.58
1:D:907:UNK:O	1:D:908:UNK:C	2.51	0.58
1:F:310:UNK:C	1:F:312:UNK:N	2.64	0.58
1:D:221:UNK:O	1:D:222:UNK:C	2.52	0.58
1:F:1005:UNK:C	1:F:1007:UNK:N	2.62	0.58
1:Q:109:UNK:O	1:Q:112:UNK:N	2.37	0.58
1:Q:2513:UNK:C	1:Q:2515:UNK:N	2.64	0.58
1:Y:880:UNK:O	1:Y:881:UNK:C	2.50	0.58
1:C:2505:UNK:HA	1:C:2508:UNK:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:UNK:O	1:C:313:UNK:C	2.51	0.58
1:F:1309:UNK:O	1:F:1313:UNK:N	2.36	0.58
1:Q:2512:UNK:O	1:Q:2513:UNK:O	2.22	0.58
1:Y:874:UNK:O	1:Y:875:UNK:C	2.50	0.58
1:D:721:UNK:C	1:D:723:UNK:N	2.65	0.58
1:Q:1010:UNK:O	1:Q:1013:UNK:N	2.37	0.58
1:T:3421:UNK:C	1:T:3423:UNK:N	2.61	0.58
1:F:1906:UNK:O	1:F:1910:UNK:N	2.35	0.58
1:P:507:UNK:O	1:P:511:UNK:N	2.37	0.58
1:R:108:UNK:O	1:R:112:UNK:N	2.37	0.58
1:X:1067:UNK:O	1:X:1071:UNK:N	2.37	0.58
1:O:2207:UNK:O	1:O:2210:UNK:N	2.37	0.58
1:Q:2505:UNK:HA	1:Q:2508:UNK:CB	2.33	0.58
1:R:1205:UNK:C	1:R:1207:UNK:N	2.67	0.58
1:D:1205:UNK:C	1:D:1207:UNK:N	2.67	0.58
1:F:1420:UNK:O	1:F:1423:UNK:N	2.37	0.58
1:F:2212:UNK:C	1:F:2214:UNK:N	2.67	0.58
1:B:1614:UNK:HA	1:B:1617:UNK:CA	2.34	0.57
1:D:108:UNK:O	1:D:112:UNK:N	2.37	0.57
1:F:2113:UNK:C	1:F:2115:UNK:N	2.66	0.57
1:E:225:UNK:C	1:E:227:UNK:N	2.67	0.57
1:Y:1067:UNK:O	1:Y:1071:UNK:N	2.37	0.57
1:A:1008:UNK:O	1:A:1011:UNK:N	2.38	0.57
1:C:2612:UNK:HA	1:C:2615:UNK:CB	2.34	0.57
1:S:225:UNK:C	1:S:227:UNK:N	2.67	0.57
1:A:1509:UNK:O	1:A:1513:UNK:N	2.37	0.57
1:C:109:UNK:O	1:C:112:UNK:N	2.37	0.57
1:C:2512:UNK:O	1:C:2513:UNK:O	2.22	0.57
1:Q:1013:UNK:O	1:Q:1015:UNK:N	2.32	0.57
1:Q:2612:UNK:HA	1:Q:2615:UNK:CB	2.34	0.57
1:R:221:UNK:O	1:R:222:UNK:C	2.52	0.57
1:R:905:UNK:C	1:R:907:UNK:N	2.62	0.57
1:A:2207:UNK:O	1:A:2210:UNK:N	2.37	0.57
1:C:1010:UNK:O	1:C:1013:UNK:N	2.37	0.57
1:F:3510:UNK:O	1:F:3512:UNK:N	2.38	0.57
1:O:1509:UNK:O	1:O:1513:UNK:N	2.37	0.57
1:P:1311:UNK:C	1:P:1313:UNK:N	2.67	0.57
1:Q:1013:UNK:C	1:Q:1015:UNK:H	2.16	0.57
1:Q:312:UNK:O	1:Q:313:UNK:C	2.51	0.57
1:R:907:UNK:O	1:R:908:UNK:C	2.52	0.57
1:Y:843:UNK:O	1:Y:844:UNK:C	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:224:UNK:C	1:R:226:UNK:N	2.68	0.57
1:B:1711:UNK:HA	1:B:1714:UNK:CB	2.35	0.57
1:B:507:UNK:O	1:B:511:UNK:N	2.37	0.57
1:F:709:UNK:HA	1:F:712:UNK:CB	2.33	0.57
1:D:605:UNK:O	1:D:606:UNK:C	2.53	0.57
1:T:1420:UNK:O	1:T:1423:UNK:N	2.37	0.57
1:T:2512:UNK:O	1:T:2515:UNK:N	2.37	0.57
1:B:513:UNK:O	1:B:517:UNK:N	2.37	0.57
1:F:2512:UNK:O	1:F:2515:UNK:N	2.37	0.57
1:P:1614:UNK:HA	1:P:1617:UNK:CA	2.34	0.57
1:Q:1313:UNK:C	1:Q:1315:UNK:N	2.65	0.57
1:C:912:UNK:C	1:C:914:UNK:N	2.67	0.57
1:R:908:UNK:O	1:R:911:UNK:N	2.37	0.57
1:C:1412:UNK:O	1:C:1414:UNK:N	2.31	0.56
1:T:2005:UNK:O	1:T:2006:UNK:C	2.53	0.56
1:T:2113:UNK:C	1:T:2115:UNK:N	2.66	0.56
1:A:1713:UNK:C	1:A:1715:UNK:N	2.67	0.56
1:P:1613:UNK:O	1:P:1616:UNK:N	2.38	0.56
1:R:611:UNK:CB	1:R:813:UNK:CB	2.83	0.56
1:T:512:UNK:O	1:T:515:UNK:N	2.38	0.56
1:T:3510:UNK:O	1:T:3512:UNK:N	2.38	0.56
1:C:2119:UNK:O	1:C:2123:UNK:N	2.38	0.56
1:D:611:UNK:CB	1:D:813:UNK:CB	2.83	0.56
1:E:214:UNK:O	1:E:215:UNK:C	2.53	0.56
1:O:1008:UNK:O	1:O:1011:UNK:N	2.38	0.56
1:P:115:UNK:C	1:P:117:UNK:N	2.68	0.56
1:P:513:UNK:O	1:P:517:UNK:N	2.37	0.56
1:Q:1412:UNK:O	1:Q:1415:UNK:N	2.39	0.56
1:A:1305:UNK:O	1:A:1308:UNK:N	2.39	0.56
1:C:1412:UNK:O	1:C:1415:UNK:N	2.39	0.56
1:Q:2119:UNK:O	1:Q:2123:UNK:N	2.38	0.56
1:R:605:UNK:O	1:R:606:UNK:C	2.53	0.56
1:Y:908:UNK:O	1:Y:910:UNK:N	2.39	0.56
1:D:1006:UNK:O	1:D:1007:UNK:C	2.52	0.56
1:F:2316:UNK:O	1:F:2320:UNK:N	2.38	0.56
1:P:1711:UNK:HA	1:P:1714:UNK:CB	2.35	0.56
1:X:908:UNK:O	1:X:909:UNK:C	2.53	0.56
1:X:908:UNK:O	1:X:910:UNK:N	2.39	0.56
1:F:512:UNK:O	1:F:515:UNK:N	2.38	0.56
1:O:1908:UNK:C	1:O:1910:UNK:N	2.65	0.56
1:X:874:UNK:O	1:X:875:UNK:C	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:319:UNK:O	1:Q:322:UNK:N	2.39	0.56
1:T:2316:UNK:O	1:T:2320:UNK:N	2.38	0.56
1:O:2307:UNK:O	1:O:2311:UNK:N	2.39	0.56
1:S:214:UNK:O	1:S:215:UNK:C	2.53	0.56
1:X:843:UNK:O	1:X:844:UNK:C	2.53	0.56
1:F:1517:UNK:O	1:F:1520:UNK:N	2.39	0.56
1:Y:908:UNK:O	1:Y:909:UNK:C	2.53	0.56
1:T:1913:UNK:O	1:T:1917:UNK:N	2.39	0.56
1:T:3510:UNK:C	1:T:3512:UNK:N	2.68	0.56
1:B:1713:UNK:C	1:B:1715:UNK:N	2.64	0.55
1:C:319:UNK:O	1:C:322:UNK:N	2.39	0.55
1:Q:1010:UNK:C	1:Q:1012:UNK:N	2.69	0.55
1:B:1709:UNK:O	1:B:1712:UNK:CB	2.54	0.55
1:B:1613:UNK:O	1:B:1616:UNK:N	2.38	0.55
1:P:1709:UNK:O	1:P:1712:UNK:CB	2.54	0.55
1:Q:912:UNK:C	1:Q:914:UNK:N	2.67	0.55
1:Y:1070:UNK:O	1:Y:1071:UNK:C	2.54	0.55
1:C:2313:UNK:C	1:C:2315:UNK:N	2.69	0.55
1:R:1006:UNK:O	1:R:1007:UNK:C	2.52	0.55
1:T:1005:UNK:C	1:T:1007:UNK:N	2.62	0.55
1:Y:1068:UNK:HA	1:Y:1071:UNK:CB	2.37	0.55
1:O:1517:UNK:O	1:O:1519:UNK:N	2.40	0.55
1:O:1713:UNK:C	1:O:1715:UNK:N	2.67	0.55
1:Q:2313:UNK:C	1:Q:2315:UNK:N	2.69	0.55
1:T:3208:UNK:O	1:T:3211:UNK:N	2.39	0.55
1:X:1068:UNK:HA	1:X:1071:UNK:CB	2.37	0.55
1:Y:838:UNK:C	1:Y:840:UNK:N	2.52	0.55
1:A:2008:UNK:O	1:A:2010:UNK:N	2.40	0.55
1:B:1311:UNK:C	1:B:1313:UNK:N	2.67	0.55
1:O:1305:UNK:O	1:O:1308:UNK:N	2.39	0.55
1:P:1013:UNK:O	1:P:1014:UNK:C	2.55	0.55
1:C:1607:UNK:HA	1:C:1610:UNK:CB	2.36	0.55
1:E:118:UNK:O	1:E:121:UNK:N	2.40	0.55
1:F:1913:UNK:O	1:F:1917:UNK:N	2.39	0.55
1:T:1517:UNK:O	1:T:1520:UNK:N	2.39	0.55
1:T:2109:UNK:O	1:T:2112:UNK:N	2.39	0.55
1:B:1713:UNK:O	1:B:1714:UNK:C	2.53	0.55
1:C:2211:UNK:C	1:C:2213:UNK:N	2.62	0.55
1:F:205:UNK:O	1:F:207:UNK:N	2.40	0.55
1:F:3510:UNK:C	1:F:3512:UNK:N	2.68	0.55
1:B:1107:UNK:C	1:B:1109:UNK:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2109:UNK:O	1:F:2112:UNK:N	2.39	0.55
1:F:3208:UNK:O	1:F:3211:UNK:N	2.39	0.55
1:Q:1607:UNK:HA	1:Q:1610:UNK:CB	2.36	0.55
1:Y:1024:UNK:O	1:Y:1026:UNK:N	2.39	0.55
1:D:315:UNK:HA	1:D:318:UNK:N	2.22	0.55
1:Q:1922:UNK:C	1:Q:1924:UNK:N	2.69	0.55
1:Q:2216:UNK:C	1:Q:2218:UNK:N	2.64	0.55
1:Q:2313:UNK:O	1:Q:2315:UNK:N	2.40	0.55
1:R:220:UNK:HA	1:R:223:UNK:CB	2.37	0.55
1:S:118:UNK:O	1:S:121:UNK:N	2.40	0.55
1:T:2415:UNK:O	1:T:2419:UNK:CB	2.55	0.55
1:Y:906:UNK:C	1:Y:908:UNK:N	2.70	0.55
1:A:2307:UNK:O	1:A:2311:UNK:N	2.39	0.54
1:B:1013:UNK:O	1:B:1014:UNK:C	2.55	0.54
1:B:818:UNK:O	1:B:820:UNK:N	2.40	0.54
1:C:2313:UNK:O	1:C:2315:UNK:N	2.40	0.54
1:C:410:UNK:O	1:C:413:UNK:CB	2.55	0.54
1:P:818:UNK:O	1:P:820:UNK:N	2.40	0.54
1:T:2212:UNK:C	1:T:2214:UNK:N	2.67	0.54
1:X:1024:UNK:O	1:X:1026:UNK:N	2.39	0.54
1:B:316:UNK:O	1:B:317:UNK:C	2.55	0.54
1:F:3007:UNK:O	1:F:3009:UNK:N	2.40	0.54
1:Q:410:UNK:O	1:Q:413:UNK:CB	2.55	0.54
1:X:1070:UNK:O	1:X:1071:UNK:C	2.54	0.54
1:A:1908:UNK:C	1:A:1910:UNK:N	2.65	0.54
1:B:210:UNK:O	1:B:213:UNK:CB	2.56	0.54
1:A:1517:UNK:O	1:A:1519:UNK:N	2.40	0.54
1:O:2008:UNK:O	1:O:2010:UNK:N	2.40	0.54
1:P:1110:UNK:C	1:P:1112:UNK:N	2.70	0.54
1:R:107:UNK:O	1:R:108:UNK:C	2.55	0.54
1:S:225:UNK:O	1:S:228:UNK:N	2.41	0.54
1:X:838:UNK:C	1:X:840:UNK:N	2.52	0.54
1:B:605:UNK:CB	1:B:905:UNK:N	2.71	0.54
1:C:1922:UNK:C	1:C:1924:UNK:N	2.69	0.54
1:E:225:UNK:O	1:E:228:UNK:N	2.41	0.54
1:F:1208:UNK:O	1:F:1209:UNK:C	2.55	0.54
1:F:3418:UNK:O	1:F:3422:UNK:CB	2.55	0.54
1:R:811:UNK:O	1:R:814:UNK:N	2.41	0.54
1:X:906:UNK:C	1:X:908:UNK:N	2.70	0.54
1:B:115:UNK:C	1:B:117:UNK:N	2.68	0.54
1:D:1005:UNK:C	1:D:1007:UNK:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:UNK:O	1:D:814:UNK:N	2.41	0.54
1:F:2005:UNK:O	1:F:2006:UNK:C	2.53	0.54
1:F:2112:UNK:O	1:F:2115:UNK:C	2.56	0.54
1:P:605:UNK:CB	1:P:905:UNK:N	2.71	0.54
1:X:911:UNK:O	1:X:915:UNK:O	2.26	0.54
1:O:1707:UNK:C	1:O:1709:UNK:N	2.68	0.54
1:T:2112:UNK:O	1:T:2115:UNK:C	2.56	0.54
1:T:3007:UNK:O	1:T:3009:UNK:N	2.40	0.54
1:A:1707:UNK:C	1:A:1709:UNK:N	2.68	0.54
1:A:2110:UNK:O	1:A:2113:UNK:N	2.41	0.54
1:F:2415:UNK:O	1:F:2419:UNK:CB	2.55	0.54
1:R:315:UNK:HA	1:R:318:UNK:N	2.22	0.54
1:S:308:UNK:HA	1:S:311:UNK:CB	2.38	0.54
1:A:1305:UNK:O	1:A:1309:UNK:N	2.41	0.54
1:B:1110:UNK:C	1:B:1112:UNK:N	2.70	0.54
1:P:210:UNK:O	1:P:213:UNK:CB	2.56	0.54
1:Q:1813:UNK:O	1:Q:1817:UNK:CB	2.56	0.54
1:R:1005:UNK:C	1:R:1007:UNK:N	2.71	0.54
1:Y:804:UNK:O	1:Y:806:UNK:N	2.41	0.54
1:D:220:UNK:HA	1:D:223:UNK:CB	2.37	0.54
1:F:810:UNK:O	1:F:811:UNK:C	2.55	0.54
1:O:2110:UNK:O	1:O:2113:UNK:N	2.41	0.54
1:R:915:UNK:C	1:R:917:UNK:N	2.71	0.54
1:X:804:UNK:O	1:X:806:UNK:N	2.41	0.54
1:A:2407:UNK:O	1:A:2408:UNK:C	2.56	0.53
1:F:1413:UNK:O	1:F:1417:UNK:CB	2.56	0.53
1:F:418:UNK:O	1:F:420:UNK:N	2.25	0.53
1:O:1812:UNK:O	1:O:1816:UNK:N	2.41	0.53
1:O:2407:UNK:O	1:O:2408:UNK:C	2.56	0.53
1:Q:911:UNK:O	1:Q:912:UNK:C	2.57	0.53
1:T:3418:UNK:O	1:T:3422:UNK:CB	2.55	0.53
1:A:1812:UNK:O	1:A:1816:UNK:N	2.41	0.53
1:D:107:UNK:O	1:D:108:UNK:C	2.55	0.53
1:T:205:UNK:O	1:T:207:UNK:N	2.40	0.53
1:T:218:UNK:C	1:T:220:UNK:N	2.70	0.53
1:X:813:UNK:O	1:X:814:UNK:C	2.56	0.53
1:O:1305:UNK:O	1:O:1309:UNK:N	2.41	0.53
1:T:1208:UNK:O	1:T:1209:UNK:C	2.55	0.53
1:Y:911:UNK:O	1:Y:915:UNK:O	2.26	0.53
1:A:2005:UNK:O	1:A:2007:UNK:N	2.42	0.53
1:D:224:UNK:C	1:D:226:UNK:N	2.68	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2011:UNK:O	1:O:2015:UNK:N	2.41	0.53
1:P:611:UNK:O	1:P:614:UNK:N	2.42	0.53
1:A:2011:UNK:O	1:A:2015:UNK:N	2.42	0.53
1:O:2005:UNK:O	1:O:2007:UNK:N	2.42	0.53
1:P:716:UNK:O	1:P:717:UNK:C	2.56	0.53
1:T:3109:UNK:C	1:T:3111:UNK:N	2.69	0.53
1:B:407:UNK:O	1:B:409:UNK:N	2.42	0.53
1:B:611:UNK:O	1:B:614:UNK:N	2.42	0.53
1:C:1813:UNK:O	1:C:1817:UNK:CB	2.56	0.53
1:C:911:UNK:O	1:C:912:UNK:C	2.56	0.53
1:P:1713:UNK:O	1:P:1714:UNK:C	2.53	0.53
1:Y:813:UNK:O	1:Y:814:UNK:C	2.56	0.53
1:A:2609:UNK:O	1:A:2611:UNK:N	2.42	0.53
1:B:508:UNK:O	1:B:512:UNK:N	2.42	0.53
1:D:715:UNK:HA	1:D:718:UNK:CB	2.39	0.53
1:D:915:UNK:O	1:D:916:UNK:C	2.56	0.53
1:F:2414:UNK:HA	1:F:2417:UNK:CB	2.39	0.53
1:F:3109:UNK:C	1:F:3111:UNK:N	2.69	0.53
1:Q:2313:UNK:O	1:Q:2315:UNK:O	2.27	0.53
1:T:3506:UNK:O	1:T:3507:UNK:C	2.57	0.53
1:C:2515:UNK:C	1:C:2517:UNK:N	2.72	0.53
1:P:1107:UNK:C	1:P:1109:UNK:N	2.69	0.53
1:P:1313:UNK:C	1:P:1315:UNK:N	2.72	0.53
1:P:316:UNK:O	1:P:317:UNK:C	2.55	0.53
1:Q:1511:UNK:C	1:Q:1513:UNK:N	2.70	0.53
1:Q:1919:UNK:O	1:Q:1920:UNK:C	2.57	0.53
1:R:915:UNK:O	1:R:916:UNK:C	2.56	0.53
1:T:1413:UNK:O	1:T:1417:UNK:CB	2.56	0.53
1:T:3210:UNK:CB	1:T:3316:UNK:CB	2.87	0.53
1:A:1114:UNK:O	1:A:1116:UNK:N	2.42	0.53
1:A:2507:UNK:CA	1:A:2510:UNK:CB	2.75	0.53
1:C:1511:UNK:C	1:C:1513:UNK:N	2.70	0.53
1:P:1713:UNK:C	1:P:1715:UNK:N	2.64	0.53
1:T:512:UNK:HA	1:T:515:UNK:CB	2.39	0.53
1:E:308:UNK:HA	1:E:311:UNK:CB	2.38	0.53
1:F:2207:UNK:O	1:F:2208:UNK:C	2.57	0.53
1:O:1114:UNK:O	1:O:1116:UNK:N	2.42	0.53
1:R:305:UNK:C	1:R:307:UNK:N	2.72	0.53
1:D:609:UNK:O	1:D:610:UNK:C	2.57	0.52
1:F:3615:UNK:C	1:F:3617:UNK:N	2.70	0.52
1:P:112:UNK:C	1:P:114:UNK:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:608:UNK:C	1:P:610:UNK:N	2.67	0.52
1:R:614:UNK:O	1:R:617:UNK:CB	2.57	0.52
1:T:2414:UNK:HA	1:T:2417:UNK:CB	2.39	0.52
1:T:2714:UNK:C	1:T:2716:UNK:H	2.22	0.52
1:T:3421:UNK:HA	1:T:3424:UNK:CB	2.39	0.52
1:A:2110:UNK:O	1:A:2113:UNK:CB	2.57	0.52
1:C:319:UNK:C	1:C:321:UNK:N	2.72	0.52
1:P:1507:UNK:O	1:P:1511:UNK:N	2.43	0.52
1:R:715:UNK:HA	1:R:718:UNK:CB	2.39	0.52
1:T:2111:UNK:O	1:T:2115:UNK:CB	2.57	0.52
1:C:2313:UNK:O	1:C:2315:UNK:O	2.27	0.52
1:F:213:UNK:HA	1:F:216:UNK:CB	2.39	0.52
1:R:807:UNK:O	1:R:808:UNK:C	2.57	0.52
1:T:407:UNK:C	1:T:409:UNK:H	2.22	0.52
1:T:810:UNK:O	1:T:811:UNK:C	2.56	0.52
1:B:407:UNK:C	1:B:409:UNK:N	2.72	0.52
1:B:716:UNK:O	1:B:717:UNK:C	2.56	0.52
1:F:2111:UNK:O	1:F:2115:UNK:CB	2.57	0.52
1:O:2110:UNK:O	1:O:2113:UNK:CB	2.57	0.52
1:O:2416:UNK:O	1:O:2417:UNK:C	2.57	0.52
1:C:1919:UNK:O	1:C:1920:UNK:C	2.57	0.52
1:F:108:UNK:C	1:F:110:UNK:N	2.68	0.52
1:F:3210:UNK:CB	1:F:3316:UNK:CB	2.87	0.52
1:P:216:UNK:O	1:P:218:UNK:N	2.42	0.52
1:D:111:UNK:O	1:D:115:UNK:CB	2.58	0.52
1:F:2714:UNK:C	1:F:2716:UNK:H	2.22	0.52
1:O:2609:UNK:O	1:O:2611:UNK:N	2.42	0.52
1:Q:2515:UNK:C	1:Q:2517:UNK:N	2.72	0.52
1:T:607:UNK:C	1:T:609:UNK:N	2.71	0.52
1:C:1010:UNK:C	1:C:1012:UNK:N	2.69	0.52
1:C:809:UNK:CA	1:C:812:UNK:CB	2.83	0.52
1:D:614:UNK:O	1:D:617:UNK:CB	2.57	0.52
1:F:2006:UNK:O	1:F:2007:UNK:O	2.28	0.52
1:Y:880:UNK:O	1:Y:881:UNK:O	2.27	0.52
1:F:1017:UNK:HA	1:F:1020:UNK:CB	2.40	0.52
1:F:407:UNK:C	1:F:409:UNK:H	2.22	0.52
1:P:407:UNK:O	1:P:409:UNK:N	2.42	0.52
1:R:609:UNK:O	1:R:610:UNK:C	2.57	0.52
1:A:2416:UNK:O	1:A:2417:UNK:C	2.57	0.52
1:F:305:UNK:O	1:F:306:UNK:C	2.57	0.52
1:P:407:UNK:C	1:P:409:UNK:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:2006:UNK:O	1:T:2007:UNK:O	2.28	0.52
1:T:213:UNK:HA	1:T:216:UNK:CB	2.39	0.52
1:T:305:UNK:O	1:T:306:UNK:C	2.57	0.52
1:B:1506:UNK:O	1:B:1510:UNK:N	2.43	0.52
1:F:3421:UNK:HA	1:F:3424:UNK:CB	2.39	0.52
1:O:1817:UNK:O	1:O:1819:UNK:N	2.43	0.52
1:O:2008:UNK:C	1:O:2010:UNK:N	2.72	0.52
1:A:1908:UNK:O	1:A:1909:UNK:C	2.58	0.51
1:A:2008:UNK:C	1:A:2010:UNK:N	2.72	0.51
1:B:1313:UNK:C	1:B:1315:UNK:N	2.72	0.51
1:B:1507:UNK:O	1:B:1511:UNK:N	2.43	0.51
1:F:607:UNK:C	1:F:609:UNK:N	2.71	0.51
1:P:508:UNK:O	1:P:512:UNK:N	2.42	0.51
1:B:1307:UNK:O	1:B:1308:UNK:C	2.58	0.51
1:C:1214:UNK:C	1:C:1216:UNK:N	2.73	0.51
1:F:3210:UNK:C	1:F:3212:UNK:N	2.71	0.51
1:P:1506:UNK:O	1:P:1510:UNK:N	2.43	0.51
1:R:721:UNK:O	1:R:723:UNK:N	2.43	0.51
1:T:1017:UNK:HA	1:T:1020:UNK:CB	2.40	0.51
1:B:216:UNK:O	1:B:218:UNK:N	2.42	0.51
1:F:310:UNK:O	1:F:313:UNK:N	2.44	0.51
1:F:3506:UNK:O	1:F:3507:UNK:C	2.57	0.51
1:F:512:UNK:HA	1:F:515:UNK:CB	2.39	0.51
1:P:1307:UNK:O	1:P:1308:UNK:C	2.58	0.51
1:F:1012:UNK:HA	1:F:1015:UNK:CB	2.41	0.51
1:O:1416:UNK:O	1:O:1420:UNK:CB	2.59	0.51
1:Q:1708:UNK:O	1:Q:1712:UNK:N	2.43	0.51
1:R:306:UNK:O	1:R:309:UNK:N	2.44	0.51
1:A:1811:UNK:O	1:A:1815:UNK:CB	2.59	0.51
1:B:1018:UNK:C	1:B:1020:UNK:N	2.70	0.51
1:B:1620:UNK:O	1:B:1621:UNK:CB	2.58	0.51
1:B:220:UNK:O	1:B:221:UNK:C	2.59	0.51
1:P:415:UNK:C	1:P:417:UNK:N	2.74	0.51
1:Q:319:UNK:C	1:Q:321:UNK:N	2.72	0.51
1:R:709:UNK:O	1:R:712:UNK:N	2.44	0.51
1:T:1012:UNK:HA	1:T:1015:UNK:CB	2.41	0.51
1:A:1315:UNK:O	1:A:1318:UNK:N	2.43	0.51
1:B:415:UNK:C	1:B:417:UNK:N	2.73	0.51
1:D:305:UNK:C	1:D:307:UNK:N	2.72	0.51
1:D:807:UNK:O	1:D:808:UNK:C	2.57	0.51
1:T:3615:UNK:C	1:T:3617:UNK:N	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1078:UNK:O	1:Y:1079:UNK:CB	2.59	0.51
1:D:306:UNK:O	1:D:309:UNK:N	2.44	0.51
1:T:2714:UNK:C	1:T:2716:UNK:N	2.74	0.51
1:D:721:UNK:O	1:D:723:UNK:N	2.43	0.51
1:F:2714:UNK:C	1:F:2716:UNK:N	2.74	0.51
1:O:1421:UNK:O	1:O:1423:UNK:N	2.35	0.51
1:Q:809:UNK:CA	1:Q:812:UNK:CB	2.83	0.51
1:T:2207:UNK:O	1:T:2208:UNK:C	2.57	0.51
1:A:1416:UNK:O	1:A:1420:UNK:CB	2.59	0.51
1:A:2312:UNK:O	1:A:2314:UNK:N	2.44	0.51
1:R:610:UNK:C	1:R:612:UNK:N	2.74	0.51
1:A:1809:UNK:O	1:A:1810:UNK:C	2.57	0.51
1:B:206:UNK:O	1:B:207:UNK:C	2.59	0.51
1:C:1708:UNK:O	1:C:1712:UNK:N	2.43	0.51
1:F:2109:UNK:O	1:F:2111:UNK:N	2.44	0.51
1:O:1206:UNK:O	1:O:1208:UNK:N	2.44	0.51
1:O:1811:UNK:O	1:O:1815:UNK:CB	2.59	0.51
1:P:206:UNK:O	1:P:207:UNK:C	2.59	0.51
1:R:111:UNK:O	1:R:115:UNK:CB	2.58	0.51
1:O:1221:UNK:HA	1:O:1306:UNK:O	2.11	0.50
1:O:1315:UNK:O	1:O:1318:UNK:N	2.43	0.50
1:O:1813:UNK:O	1:O:1817:UNK:N	2.44	0.50
1:T:310:UNK:O	1:T:313:UNK:N	2.44	0.50
1:X:1078:UNK:O	1:X:1079:UNK:CB	2.59	0.50
1:X:940:UNK:O	1:X:1054:UNK:CB	2.59	0.50
1:P:310:UNK:O	1:P:311:UNK:C	2.59	0.50
1:T:3605:UNK:O	1:T:3607:UNK:N	2.45	0.50
1:X:812:UNK:C	1:X:814:UNK:H2	2.22	0.50
1:B:516:UNK:O	1:B:517:UNK:C	2.59	0.50
1:D:610:UNK:C	1:D:612:UNK:N	2.74	0.50
1:O:1809:UNK:O	1:O:1810:UNK:C	2.57	0.50
1:O:2106:UNK:C	1:O:2108:UNK:N	2.64	0.50
1:Q:911:UNK:O	1:Q:914:UNK:N	2.44	0.50
1:X:880:UNK:O	1:X:881:UNK:O	2.27	0.50
1:Y:940:UNK:O	1:Y:1054:UNK:CB	2.59	0.50
1:B:1113:UNK:O	1:B:1114:UNK:C	2.59	0.50
1:D:509:UNK:HA	1:D:512:UNK:CB	2.41	0.50
1:E:205:UNK:O	1:E:206:UNK:O	2.30	0.50
1:F:2411:UNK:O	1:F:2414:UNK:N	2.45	0.50
1:Q:115:UNK:O	1:Q:119:UNK:N	2.45	0.50
1:A:1012:UNK:O	1:A:1015:UNK:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1009:UNK:O	1:F:1013:UNK:N	2.44	0.50
1:F:3605:UNK:O	1:F:3607:UNK:N	2.45	0.50
1:O:2312:UNK:O	1:O:2314:UNK:N	2.44	0.50
1:P:1210:UNK:O	1:P:1213:UNK:N	2.44	0.50
1:Q:2309:UNK:O	1:Q:2311:UNK:N	2.45	0.50
1:T:3210:UNK:C	1:T:3212:UNK:N	2.71	0.50
1:A:1817:UNK:O	1:A:1819:UNK:N	2.44	0.50
1:A:2121:UNK:C	1:A:2123:UNK:N	2.72	0.50
1:B:310:UNK:O	1:B:311:UNK:C	2.59	0.50
1:Q:312:UNK:C	1:Q:314:UNK:N	2.75	0.50
1:R:1008:UNK:O	1:R:1011:UNK:N	2.45	0.50
1:T:1009:UNK:O	1:T:1013:UNK:N	2.44	0.50
1:T:1908:UNK:N	1:T:1911:UNK:N	2.60	0.50
1:A:1206:UNK:O	1:A:1208:UNK:N	2.44	0.50
1:A:1906:UNK:C	1:A:1908:UNK:N	2.74	0.50
1:C:115:UNK:O	1:C:119:UNK:N	2.45	0.50
1:C:1818:UNK:C	1:C:1820:UNK:N	2.74	0.50
1:C:312:UNK:C	1:C:314:UNK:N	2.75	0.50
1:D:709:UNK:O	1:D:712:UNK:N	2.44	0.50
1:P:1113:UNK:O	1:P:1114:UNK:C	2.59	0.50
1:P:516:UNK:O	1:P:517:UNK:C	2.59	0.50
1:Q:1607:UNK:C	1:Q:1609:UNK:N	2.59	0.50
1:Q:1910:UNK:O	1:Q:1913:UNK:N	2.45	0.50
1:S:205:UNK:O	1:S:206:UNK:O	2.30	0.50
1:T:319:UNK:O	1:T:322:UNK:N	2.45	0.50
1:B:1210:UNK:O	1:B:1213:UNK:N	2.44	0.50
1:B:1712:UNK:O	1:B:1716:UNK:N	2.45	0.50
1:B:507:UNK:O	1:B:511:UNK:CB	2.60	0.50
1:C:2309:UNK:O	1:C:2311:UNK:N	2.45	0.50
1:F:1908:UNK:N	1:F:1911:UNK:N	2.60	0.50
1:O:1008:UNK:O	1:O:1010:UNK:N	2.45	0.50
1:P:1620:UNK:O	1:P:1621:UNK:CB	2.58	0.50
1:P:711:UNK:C	1:P:713:UNK:N	2.75	0.50
1:A:1813:UNK:O	1:A:1817:UNK:N	2.44	0.50
1:C:911:UNK:O	1:C:914:UNK:N	2.44	0.50
1:D:1211:UNK:C	1:D:1213:UNK:N	2.75	0.50
1:O:1906:UNK:C	1:O:1908:UNK:N	2.74	0.50
1:Q:1214:UNK:C	1:Q:1216:UNK:N	2.73	0.50
1:A:2506:UNK:O	1:A:2510:UNK:N	2.45	0.49
1:C:1910:UNK:O	1:C:1913:UNK:N	2.45	0.49
1:F:1911:UNK:O	1:F:1912:UNK:C	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:UNK:O	1:F:322:UNK:N	2.45	0.49
1:O:2506:UNK:O	1:O:2510:UNK:N	2.45	0.49
1:R:509:UNK:HA	1:R:512:UNK:CB	2.41	0.49
1:X:924:UNK:HA	1:X:927:UNK:CB	2.42	0.49
1:Y:1073:UNK:O	1:Y:1076:UNK:N	2.45	0.49
1:A:1221:UNK:HA	1:A:1306:UNK:O	2.11	0.49
1:F:3615:UNK:O	1:F:3618:UNK:N	2.46	0.49
1:P:220:UNK:O	1:P:221:UNK:C	2.59	0.49
1:Q:1706:UNK:C	1:Q:1708:UNK:N	2.74	0.49
1:X:1073:UNK:O	1:X:1076:UNK:N	2.45	0.49
1:Y:920:UNK:C	1:Y:922:UNK:N	2.74	0.49
1:F:1915:UNK:O	1:F:1918:UNK:CB	2.61	0.49
1:O:1012:UNK:O	1:O:1015:UNK:N	2.45	0.49
1:O:1212:UNK:C	1:O:1214:UNK:N	2.75	0.49
1:R:913:UNK:C	1:R:915:UNK:N	2.75	0.49
1:T:123:UNK:O	1:T:126:UNK:N	2.46	0.49
1:T:1915:UNK:O	1:T:1918:UNK:CB	2.61	0.49
1:A:1611:UNK:O	1:A:1615:UNK:N	2.45	0.49
1:D:915:UNK:C	1:D:917:UNK:N	2.71	0.49
1:F:407:UNK:O	1:F:410:UNK:N	2.46	0.49
1:O:1908:UNK:O	1:O:1909:UNK:C	2.58	0.49
1:Q:1818:UNK:C	1:Q:1820:UNK:N	2.74	0.49
1:T:2109:UNK:O	1:T:2111:UNK:N	2.44	0.49
1:C:1508:UNK:O	1:C:1512:UNK:CB	2.60	0.49
1:F:218:UNK:C	1:F:220:UNK:N	2.70	0.49
1:Q:1508:UNK:O	1:Q:1512:UNK:CB	2.60	0.49
1:T:2411:UNK:O	1:T:2414:UNK:N	2.45	0.49
1:T:412:UNK:O	1:T:416:UNK:N	2.46	0.49
1:Y:924:UNK:HA	1:Y:927:UNK:CB	2.42	0.49
1:C:1305:UNK:O	1:C:1309:UNK:N	2.46	0.49
1:O:1514:UNK:O	1:O:1515:UNK:C	2.59	0.49
1:P:507:UNK:O	1:P:511:UNK:CB	2.60	0.49
1:T:511:UNK:O	1:T:512:UNK:C	2.60	0.49
1:Y:812:UNK:C	1:Y:814:UNK:H2	2.22	0.49
1:Y:873:UNK:O	1:Y:874:UNK:O	2.30	0.49
1:B:1417:UNK:C	1:B:1419:UNK:H	2.26	0.49
1:O:1611:UNK:O	1:O:1615:UNK:N	2.45	0.49
1:Q:310:UNK:HA	1:Q:313:UNK:CB	2.43	0.49
1:R:1012:UNK:O	1:R:1014:UNK:C	2.58	0.49
1:T:3615:UNK:O	1:T:3618:UNK:N	2.46	0.49
1:A:2113:UNK:HA	1:A:2116:UNK:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:UNK:O	1:F:512:UNK:C	2.60	0.49
1:O:2113:UNK:HA	1:O:2116:UNK:CB	2.43	0.49
1:P:206:UNK:O	1:P:210:UNK:N	2.46	0.49
1:Q:1305:UNK:O	1:Q:1309:UNK:N	2.46	0.49
1:Q:610:UNK:C	1:Q:612:UNK:N	2.75	0.49
1:X:873:UNK:O	1:X:874:UNK:O	2.30	0.49
1:B:1007:UNK:C	1:B:1009:UNK:N	2.74	0.49
1:B:206:UNK:O	1:B:210:UNK:N	2.46	0.49
1:D:720:UNK:HA	1:D:723:UNK:CB	2.43	0.49
1:F:123:UNK:O	1:F:126:UNK:N	2.46	0.49
1:P:1712:UNK:O	1:P:1716:UNK:N	2.45	0.49
1:Q:2305:UNK:O	1:Q:2308:UNK:N	2.46	0.49
1:R:1211:UNK:C	1:R:1213:UNK:N	2.75	0.49
1:T:1208:UNK:O	1:T:1211:UNK:N	2.46	0.49
1:X:1014:UNK:CB	1:X:1065:UNK:CB	2.91	0.49
1:A:1212:UNK:C	1:A:1214:UNK:N	2.75	0.49
1:C:2305:UNK:O	1:C:2308:UNK:N	2.46	0.49
1:C:310:UNK:HA	1:C:313:UNK:CB	2.43	0.49
1:D:1008:UNK:O	1:D:1011:UNK:N	2.45	0.49
1:R:720:UNK:HA	1:R:723:UNK:CB	2.43	0.49
1:X:917:UNK:C	1:X:919:UNK:N	2.69	0.49
1:A:2012:UNK:O	1:A:2013:UNK:CB	2.61	0.48
1:C:712:UNK:C	1:C:714:UNK:H	2.26	0.48
1:A:1406:UNK:HA	1:A:1409:UNK:CB	2.43	0.48
1:A:2411:UNK:O	1:A:2413:UNK:N	2.46	0.48
1:F:1007:UNK:O	1:F:1009:UNK:N	2.47	0.48
1:T:407:UNK:O	1:T:410:UNK:N	2.46	0.48
1:A:1008:UNK:O	1:A:1010:UNK:N	2.45	0.48
1:A:1607:UNK:O	1:A:1611:UNK:N	2.47	0.48
1:D:310:UNK:O	1:D:314:UNK:N	2.47	0.48
1:F:2627:UNK:C	1:F:2629:UNK:N	2.75	0.48
1:O:2012:UNK:O	1:O:2013:UNK:CB	2.61	0.48
1:B:112:UNK:C	1:B:114:UNK:N	2.72	0.48
1:F:1208:UNK:O	1:F:1211:UNK:N	2.46	0.48
1:F:1305:UNK:O	1:F:1306:UNK:C	2.62	0.48
1:F:412:UNK:O	1:F:416:UNK:N	2.46	0.48
1:T:418:UNK:O	1:T:420:UNK:N	2.25	0.48
1:D:913:UNK:C	1:D:915:UNK:N	2.75	0.48
1:F:319:UNK:O	1:F:320:UNK:C	2.61	0.48
1:O:1107:UNK:O	1:O:1110:UNK:CB	2.61	0.48
1:T:1007:UNK:O	1:T:1009:UNK:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1911:UNK:O	1:T:1912:UNK:C	2.59	0.48
1:T:319:UNK:O	1:T:320:UNK:C	2.61	0.48
1:X:1073:UNK:O	1:X:1074:UNK:C	2.61	0.48
1:Y:1073:UNK:O	1:Y:1074:UNK:C	2.61	0.48
1:Y:808:UNK:O	1:Y:809:UNK:C	2.62	0.48
1:P:1417:UNK:C	1:P:1419:UNK:H	2.26	0.48
1:X:920:UNK:C	1:X:922:UNK:N	2.74	0.48
1:C:1212:UNK:O	1:C:1216:UNK:N	2.46	0.48
1:D:807:UNK:O	1:D:811:UNK:N	2.46	0.48
1:O:1607:UNK:O	1:O:1611:UNK:N	2.47	0.48
1:Q:2411:UNK:C	1:Q:2413:UNK:N	2.76	0.48
1:A:1107:UNK:O	1:A:1110:UNK:CB	2.61	0.48
1:D:719:UNK:O	1:D:721:UNK:N	2.47	0.48
1:F:1014:UNK:O	1:F:1016:UNK:N	2.46	0.48
1:F:205:UNK:O	1:F:208:UNK:N	2.47	0.48
1:R:1006:UNK:C	1:R:1008:UNK:N	2.75	0.48
1:T:613:UNK:O	1:T:615:UNK:N	2.47	0.48
1:C:1305:UNK:O	1:C:1306:UNK:C	2.62	0.48
1:C:2411:UNK:C	1:C:2413:UNK:N	2.76	0.48
1:C:2610:UNK:C	1:C:2612:UNK:N	2.77	0.48
1:O:2411:UNK:O	1:O:2413:UNK:N	2.46	0.48
1:Q:414:UNK:C	1:Q:416:UNK:H	2.21	0.48
1:X:1033:UNK:C	1:X:1035:UNK:H	2.26	0.48
1:A:1214:UNK:HA	1:A:1217:UNK:CB	2.44	0.48
1:D:1012:UNK:O	1:D:1014:UNK:C	2.58	0.48
1:F:2512:UNK:C	1:F:2514:UNK:N	2.77	0.48
1:O:1414:UNK:O	1:O:1417:UNK:N	2.47	0.48
1:P:1007:UNK:C	1:P:1009:UNK:N	2.74	0.48
1:Q:1212:UNK:O	1:Q:1216:UNK:N	2.46	0.48
1:Q:2610:UNK:C	1:Q:2612:UNK:N	2.77	0.48
1:T:108:UNK:C	1:T:110:UNK:N	2.68	0.48
1:T:205:UNK:O	1:T:208:UNK:N	2.47	0.48
1:Y:1033:UNK:C	1:Y:1035:UNK:H	2.26	0.48
1:Y:1014:UNK:CB	1:Y:1065:UNK:CB	2.91	0.48
1:C:414:UNK:C	1:C:416:UNK:H	2.21	0.47
1:C:610:UNK:C	1:C:612:UNK:N	2.75	0.47
1:D:1008:UNK:O	1:D:1009:UNK:C	2.62	0.47
1:Q:1808:UNK:O	1:Q:1809:UNK:C	2.60	0.47
1:Y:917:UNK:C	1:Y:919:UNK:N	2.69	0.47
1:B:1511:UNK:O	1:B:1515:UNK:N	2.47	0.47
1:B:608:UNK:C	1:B:610:UNK:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1808:UNK:O	1:C:1809:UNK:C	2.60	0.47
1:O:1406:UNK:HA	1:O:1409:UNK:CB	2.43	0.47
1:B:1107:UNK:O	1:B:1108:UNK:C	2.62	0.47
1:F:2007:UNK:O	1:F:2008:UNK:C	2.62	0.47
1:Q:712:UNK:C	1:Q:714:UNK:H	2.26	0.47
1:R:807:UNK:O	1:R:810:UNK:N	2.47	0.47
1:T:1014:UNK:O	1:T:1016:UNK:N	2.46	0.47
1:Q:1309:UNK:C	1:Q:1311:UNK:N	2.76	0.47
1:R:1008:UNK:O	1:R:1009:UNK:C	2.62	0.47
1:R:719:UNK:O	1:R:721:UNK:N	2.47	0.47
1:S:207:UNK:C	1:S:209:UNK:N	2.76	0.47
1:C:1706:UNK:C	1:C:1708:UNK:N	2.74	0.47
1:F:1424:UNK:C	1:F:1426:UNK:H	2.27	0.47
1:O:2121:UNK:C	1:O:2123:UNK:N	2.72	0.47
1:P:718:UNK:CB	1:P:1019:UNK:O	2.62	0.47
1:R:310:UNK:O	1:R:314:UNK:N	2.47	0.47
1:R:807:UNK:O	1:R:811:UNK:N	2.46	0.47
1:T:1424:UNK:C	1:T:1426:UNK:H	2.27	0.47
1:A:1414:UNK:O	1:A:1417:UNK:N	2.47	0.47
1:C:1320:UNK:C	1:C:1322:UNK:N	2.78	0.47
1:T:1305:UNK:O	1:T:1306:UNK:C	2.62	0.47
1:T:1312:UNK:C	1:T:1314:UNK:N	2.63	0.47
1:X:808:UNK:O	1:X:809:UNK:C	2.62	0.47
1:E:207:UNK:C	1:E:209:UNK:N	2.76	0.47
1:F:317:UNK:O	1:F:320:UNK:N	2.47	0.47
1:F:607:UNK:O	1:F:609:UNK:N	2.48	0.47
1:F:613:UNK:O	1:F:615:UNK:N	2.47	0.47
1:P:613:UNK:O	1:P:617:UNK:CB	2.63	0.47
1:Q:1910:UNK:C	1:Q:1912:UNK:N	2.78	0.47
1:T:2512:UNK:C	1:T:2514:UNK:N	2.77	0.47
1:B:317:UNK:O	1:B:319:UNK:N	2.48	0.47
1:C:1910:UNK:C	1:C:1912:UNK:N	2.78	0.47
1:F:3106:UNK:C	1:F:3108:UNK:N	2.76	0.47
1:P:106:UNK:O	1:P:110:UNK:N	2.48	0.47
1:P:317:UNK:O	1:P:319:UNK:N	2.48	0.47
1:T:2627:UNK:C	1:T:2629:UNK:N	2.75	0.47
1:B:310:UNK:O	1:B:313:UNK:N	2.48	0.47
1:C:213:UNK:O	1:C:214:UNK:C	2.62	0.47
1:P:1511:UNK:O	1:P:1515:UNK:N	2.47	0.47
1:P:310:UNK:O	1:P:313:UNK:N	2.48	0.47
1:T:3106:UNK:C	1:T:3108:UNK:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:317:UNK:O	1:T:320:UNK:N	2.47	0.47
1:B:106:UNK:O	1:B:110:UNK:N	2.48	0.47
1:B:718:UNK:CB	1:B:1019:UNK:O	2.62	0.47
1:C:1309:UNK:C	1:C:1311:UNK:N	2.76	0.47
1:D:807:UNK:O	1:D:810:UNK:N	2.47	0.47
1:Y:851:UNK:O	1:Y:855:UNK:CB	2.63	0.47
1:B:613:UNK:O	1:B:617:UNK:CB	2.63	0.47
1:C:1115:UNK:C	1:C:1117:UNK:N	2.76	0.47
1:O:1605:UNK:O	1:O:1609:UNK:CB	2.63	0.47
1:T:2609:UNK:C	1:T:2611:UNK:N	2.78	0.47
1:A:2013:UNK:O	1:A:2014:UNK:C	2.61	0.46
1:D:717:UNK:O	1:D:721:UNK:N	2.48	0.46
1:F:2319:UNK:C	1:F:2321:UNK:N	2.78	0.46
1:P:1613:UNK:C	1:P:1615:UNK:N	2.78	0.46
1:T:2007:UNK:O	1:T:2008:UNK:C	2.62	0.46
1:T:2319:UNK:C	1:T:2321:UNK:N	2.78	0.46
1:T:3208:UNK:O	1:T:3212:UNK:N	2.48	0.46
1:B:106:UNK:O	1:B:109:UNK:N	2.48	0.46
1:B:611:UNK:C	1:B:613:UNK:N	2.79	0.46
1:O:1214:UNK:HA	1:O:1217:UNK:CB	2.44	0.46
1:P:1107:UNK:O	1:P:1108:UNK:C	2.62	0.46
1:Q:1115:UNK:C	1:Q:1117:UNK:N	2.76	0.46
1:R:610:UNK:O	1:R:613:UNK:N	2.48	0.46
1:C:1817:UNK:O	1:C:1820:UNK:CB	2.64	0.46
1:F:3208:UNK:O	1:F:3212:UNK:N	2.48	0.46
1:P:106:UNK:O	1:P:109:UNK:N	2.48	0.46
1:P:115:UNK:O	1:P:119:UNK:N	2.48	0.46
1:B:127:UNK:CB	1:B:1019:UNK:CB	2.93	0.46
1:P:411:UNK:O	1:P:412:UNK:C	2.63	0.46
1:T:2814:UNK:O	1:T:2815:UNK:C	2.64	0.46
1:B:1608:UNK:C	1:B:1610:UNK:N	2.79	0.46
1:D:615:UNK:C	1:D:617:UNK:N	2.76	0.46
1:P:127:UNK:CB	1:P:1019:UNK:CB	2.93	0.46
1:Q:1320:UNK:C	1:Q:1322:UNK:N	2.78	0.46
1:R:512:UNK:O	1:R:515:UNK:CB	2.64	0.46
1:R:717:UNK:O	1:R:721:UNK:N	2.48	0.46
1:A:1605:UNK:O	1:A:1609:UNK:CB	2.63	0.46
1:B:1708:UNK:O	1:B:1711:UNK:N	2.48	0.46
1:B:411:UNK:O	1:B:412:UNK:C	2.63	0.46
1:B:605:UNK:HA	1:B:608:UNK:CB	2.46	0.46
1:C:2411:UNK:O	1:C:2414:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1018:UNK:C	1:P:1020:UNK:N	2.71	0.46
1:X:806:UNK:O	1:X:808:UNK:N	2.48	0.46
1:X:851:UNK:O	1:X:855:UNK:CB	2.63	0.46
1:D:610:UNK:O	1:D:613:UNK:N	2.49	0.46
1:D:611:UNK:O	1:D:615:UNK:CB	2.64	0.46
1:P:1708:UNK:O	1:P:1711:UNK:N	2.48	0.46
1:S:106:UNK:O	1:S:108:UNK:N	2.49	0.46
1:T:2620:UNK:O	1:T:2623:UNK:CA	2.63	0.46
1:T:2620:UNK:O	1:T:2623:UNK:CB	2.64	0.46
1:T:607:UNK:O	1:T:609:UNK:N	2.48	0.46
1:X:838:UNK:CB	1:X:871:UNK:HA	2.46	0.46
1:P:605:UNK:HA	1:P:608:UNK:CB	2.46	0.46
1:P:611:UNK:C	1:P:613:UNK:N	2.79	0.46
1:Q:2411:UNK:O	1:Q:2414:UNK:N	2.49	0.46
1:R:107:UNK:O	1:R:108:UNK:O	2.34	0.46
1:R:315:UNK:C	1:R:317:UNK:N	2.78	0.46
1:R:611:UNK:O	1:R:615:UNK:CB	2.64	0.46
1:T:1908:UNK:O	1:T:1912:UNK:N	2.49	0.46
1:D:512:UNK:O	1:D:515:UNK:CB	2.64	0.46
1:F:2620:UNK:O	1:F:2623:UNK:CA	2.63	0.46
1:Y:920:UNK:O	1:Y:923:UNK:CB	2.64	0.46
1:B:115:UNK:O	1:B:119:UNK:N	2.48	0.46
1:B:1613:UNK:C	1:B:1615:UNK:N	2.78	0.46
1:X:847:UNK:C	1:X:849:UNK:N	2.75	0.46
1:D:1216:UNK:C	1:D:1218:UNK:H	2.27	0.45
1:F:1908:UNK:O	1:F:1912:UNK:N	2.49	0.45
1:F:2814:UNK:O	1:F:2815:UNK:C	2.64	0.45
1:P:311:UNK:O	1:P:315:UNK:N	2.49	0.45
1:D:107:UNK:O	1:D:108:UNK:O	2.34	0.45
1:F:913:UNK:O	1:F:916:UNK:N	2.50	0.45
1:Q:1214:UNK:O	1:Q:1217:UNK:N	2.49	0.45
1:Q:606:UNK:O	1:Q:610:UNK:N	2.49	0.45
1:R:615:UNK:C	1:R:617:UNK:N	2.76	0.45
1:A:1814:UNK:HA	1:A:1817:UNK:CB	2.46	0.45
1:B:414:UNK:O	1:B:415:UNK:C	2.64	0.45
1:C:205:UNK:C	1:C:207:UNK:N	2.78	0.45
1:C:606:UNK:O	1:C:610:UNK:N	2.49	0.45
1:Q:1817:UNK:O	1:Q:1820:UNK:CB	2.64	0.45
1:Q:213:UNK:O	1:Q:214:UNK:C	2.62	0.45
1:Y:838:UNK:CB	1:Y:871:UNK:HA	2.46	0.45
1:A:1514:UNK:O	1:A:1515:UNK:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2609:UNK:C	1:F:2611:UNK:N	2.78	0.45
1:F:3414:UNK:O	1:F:3415:UNK:C	2.64	0.45
1:F:3510:UNK:O	1:F:3513:UNK:N	2.50	0.45
1:P:115:UNK:O	1:P:118:UNK:N	2.50	0.45
1:P:216:UNK:C	1:P:218:UNK:N	2.79	0.45
1:Q:1417:UNK:C	1:Q:1419:UNK:H	2.30	0.45
1:X:920:UNK:O	1:X:923:UNK:CB	2.64	0.45
1:A:2609:UNK:C	1:A:2611:UNK:N	2.80	0.45
1:C:1214:UNK:O	1:C:1217:UNK:N	2.49	0.45
1:D:308:UNK:O	1:D:311:UNK:N	2.49	0.45
1:F:209:UNK:O	1:F:210:UNK:C	2.65	0.45
1:O:1814:UNK:HA	1:O:1817:UNK:CB	2.46	0.45
1:Q:1305:UNK:O	1:Q:1306:UNK:C	2.62	0.45
1:R:1216:UNK:C	1:R:1218:UNK:H	2.27	0.45
1:R:308:UNK:O	1:R:311:UNK:N	2.49	0.45
1:S:307:UNK:O	1:S:310:UNK:N	2.50	0.45
1:T:2213:UNK:HA	1:T:2216:UNK:CB	2.47	0.45
1:C:116:UNK:HA	1:C:119:UNK:CB	2.47	0.45
1:F:1007:UNK:O	1:F:1008:UNK:C	2.65	0.45
1:P:414:UNK:O	1:P:415:UNK:C	2.64	0.45
1:T:2605:UNK:O	1:T:2607:UNK:N	2.50	0.45
1:X:811:UNK:N	1:X:832:UNK:O	2.50	0.45
1:B:1612:UNK:O	1:B:1613:UNK:C	2.62	0.45
1:T:1417:UNK:C	1:T:1419:UNK:N	2.79	0.45
1:C:1408:UNK:C	1:C:1410:UNK:N	2.64	0.45
1:E:313:UNK:C	1:E:315:UNK:N	2.65	0.45
1:F:2620:UNK:O	1:F:2623:UNK:CB	2.64	0.45
1:T:1007:UNK:O	1:T:1008:UNK:C	2.65	0.45
1:B:1608:UNK:O	1:B:1610:UNK:N	2.50	0.45
1:T:3510:UNK:O	1:T:3513:UNK:N	2.50	0.45
1:T:515:UNK:O	1:T:605:UNK:N	2.50	0.45
1:T:913:UNK:O	1:T:916:UNK:N	2.50	0.45
1:Y:811:UNK:N	1:Y:832:UNK:O	2.50	0.45
1:C:1417:UNK:C	1:C:1419:UNK:H	2.29	0.45
1:C:1907:UNK:C	1:C:1909:UNK:N	2.77	0.45
1:P:1708:UNK:C	1:P:1710:UNK:N	2.80	0.45
1:Q:1007:UNK:C	1:Q:1009:UNK:N	2.80	0.45
1:T:209:UNK:O	1:T:210:UNK:C	2.65	0.45
1:X:872:UNK:CB	1:X:876:UNK:O	2.65	0.45
1:A:2307:UNK:O	1:A:2309:UNK:N	2.50	0.44
1:B:311:UNK:O	1:B:315:UNK:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:2520:UNK:O	1:Q:2521:UNK:O	2.35	0.44
1:B:216:UNK:C	1:B:218:UNK:N	2.79	0.44
1:C:123:UNK:O	1:C:124:UNK:C	2.66	0.44
1:C:507:UNK:C	1:C:509:UNK:N	2.80	0.44
1:E:106:UNK:O	1:E:108:UNK:N	2.49	0.44
1:F:2213:UNK:HA	1:F:2216:UNK:CB	2.46	0.44
1:P:1213:UNK:C	1:P:1215:UNK:N	2.78	0.44
1:P:1612:UNK:O	1:P:1613:UNK:C	2.62	0.44
1:Q:1708:UNK:O	1:Q:1709:UNK:C	2.65	0.44
1:T:415:UNK:C	1:T:417:UNK:N	2.80	0.44
1:B:1708:UNK:C	1:B:1710:UNK:N	2.80	0.44
1:C:1007:UNK:C	1:C:1009:UNK:N	2.80	0.44
1:F:2605:UNK:O	1:F:2607:UNK:N	2.50	0.44
1:O:2606:UNK:C	1:O:2608:UNK:N	2.67	0.44
1:Q:1910:UNK:O	1:Q:1914:UNK:N	2.51	0.44
1:S:112:UNK:C	1:S:114:UNK:N	2.76	0.44
1:T:3207:UNK:HA	1:T:3316:UNK:CB	2.47	0.44
1:X:829:UNK:O	1:X:880:UNK:HA	2.17	0.44
1:E:307:UNK:O	1:E:310:UNK:N	2.50	0.44
1:O:2307:UNK:O	1:O:2309:UNK:N	2.51	0.44
1:O:2315:UNK:C	1:O:2317:UNK:N	2.79	0.44
1:Q:116:UNK:HA	1:Q:119:UNK:CB	2.47	0.44
1:F:2609:UNK:O	1:F:2612:UNK:N	2.51	0.44
1:O:1305:UNK:C	1:O:1307:UNK:N	2.80	0.44
1:O:2013:UNK:O	1:O:2014:UNK:C	2.61	0.44
1:T:910:UNK:C	1:T:912:UNK:N	2.79	0.44
1:X:1014:UNK:HA	1:X:1017:UNK:CB	2.48	0.44
1:A:1315:UNK:O	1:A:1318:UNK:CB	2.66	0.44
1:B:115:UNK:O	1:B:118:UNK:N	2.50	0.44
1:D:206:UNK:O	1:D:208:UNK:N	2.51	0.44
1:F:320:UNK:O	1:F:323:UNK:N	2.51	0.44
1:F:415:UNK:C	1:F:417:UNK:N	2.80	0.44
1:O:2115:UNK:O	1:O:2118:UNK:N	2.51	0.44
1:P:1113:UNK:O	1:P:1116:UNK:N	2.51	0.44
1:P:1608:UNK:O	1:P:1610:UNK:N	2.50	0.44
1:T:2609:UNK:O	1:T:2612:UNK:N	2.51	0.44
1:Y:872:UNK:CB	1:Y:876:UNK:O	2.66	0.44
1:B:206:UNK:O	1:B:209:UNK:N	2.51	0.44
1:C:1708:UNK:O	1:C:1709:UNK:C	2.65	0.44
1:C:1910:UNK:O	1:C:1914:UNK:N	2.51	0.44
1:E:309:UNK:C	1:E:311:UNK:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3207:UNK:HA	1:F:3316:UNK:CB	2.47	0.44
1:D:306:UNK:O	1:D:309:UNK:CB	2.66	0.44
1:F:2810:UNK:C	1:F:2812:UNK:H	2.31	0.44
1:F:515:UNK:O	1:F:605:UNK:N	2.50	0.44
1:F:910:UNK:C	1:F:912:UNK:N	2.79	0.44
1:Q:1115:UNK:O	1:Q:1118:UNK:N	2.51	0.44
1:Q:1505:UNK:C	1:Q:1507:UNK:N	2.81	0.44
1:Q:1907:UNK:C	1:Q:1909:UNK:N	2.77	0.44
1:R:206:UNK:O	1:R:208:UNK:N	2.51	0.44
1:T:1521:UNK:C	1:T:1523:UNK:N	2.81	0.44
1:X:922:UNK:O	1:X:926:UNK:N	2.51	0.44
1:Y:1014:UNK:HA	1:Y:1017:UNK:CB	2.48	0.44
1:A:2115:UNK:O	1:A:2118:UNK:N	2.51	0.44
1:B:818:UNK:O	1:B:821:UNK:N	2.51	0.44
1:C:1505:UNK:C	1:C:1507:UNK:N	2.81	0.44
1:O:2013:UNK:N	1:O:2015:UNK:O	2.51	0.44
1:O:2609:UNK:C	1:O:2611:UNK:N	2.80	0.44
1:Q:1922:UNK:O	1:Q:1924:UNK:N	2.51	0.44
1:Q:507:UNK:C	1:Q:509:UNK:N	2.80	0.44
1:Y:802:UNK:O	1:Y:811:UNK:HA	2.18	0.44
1:B:813:UNK:HA	1:B:816:UNK:CB	2.48	0.43
1:C:2520:UNK:O	1:C:2521:UNK:O	2.36	0.43
1:C:509:UNK:O	1:C:510:UNK:C	2.66	0.43
1:D:616:UNK:O	1:D:619:UNK:C	2.66	0.43
1:D:917:UNK:C	1:D:919:UNK:H	2.31	0.43
1:O:1315:UNK:O	1:O:1318:UNK:CB	2.66	0.43
1:X:802:UNK:O	1:X:812:UNK:N	2.51	0.43
1:Y:1043:UNK:O	1:Y:1044:UNK:CB	2.65	0.43
1:Y:829:UNK:O	1:Y:880:UNK:HA	2.17	0.43
1:O:1421:UNK:C	1:O:1423:UNK:N	2.68	0.43
1:Q:2410:UNK:C	1:Q:2412:UNK:N	2.81	0.43
1:T:1208:UNK:C	1:T:1210:UNK:N	2.81	0.43
1:T:507:UNK:HA	1:T:510:UNK:CB	2.48	0.43
1:X:1043:UNK:O	1:X:1044:UNK:CB	2.65	0.43
1:Y:856:UNK:C	1:Y:858:UNK:H	2.31	0.43
1:B:1113:UNK:O	1:B:1116:UNK:N	2.51	0.43
1:C:117:UNK:O	1:C:118:UNK:C	2.67	0.43
1:F:1521:UNK:C	1:F:1523:UNK:N	2.81	0.43
1:P:206:UNK:O	1:P:209:UNK:N	2.51	0.43
1:P:818:UNK:O	1:P:821:UNK:N	2.51	0.43
1:Q:117:UNK:O	1:Q:118:UNK:C	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:856:UNK:C	1:X:858:UNK:H	2.31	0.43
1:Y:922:UNK:O	1:Y:926:UNK:N	2.51	0.43
1:A:2013:UNK:N	1:A:2015:UNK:O	2.51	0.43
1:B:1307:UNK:C	1:B:1309:UNK:N	2.82	0.43
1:D:308:UNK:C	1:D:310:UNK:N	2.81	0.43
1:O:2110:UNK:O	1:O:2113:UNK:CA	2.67	0.43
1:O:2313:UNK:CB	1:T:1414:UNK:CB	2.97	0.43
1:O:2612:UNK:O	1:O:2614:UNK:N	2.51	0.43
1:R:306:UNK:O	1:R:309:UNK:CB	2.66	0.43
1:X:802:UNK:O	1:X:811:UNK:HA	2.18	0.43
1:C:2410:UNK:C	1:C:2412:UNK:N	2.81	0.43
1:D:315:UNK:C	1:D:317:UNK:N	2.78	0.43
1:Q:509:UNK:O	1:Q:510:UNK:C	2.66	0.43
1:R:616:UNK:O	1:R:619:UNK:C	2.66	0.43
1:R:715:UNK:C	1:R:718:UNK:N	2.82	0.43
1:T:320:UNK:O	1:T:323:UNK:N	2.51	0.43
1:B:1619:UNK:C	1:B:1621:UNK:H	2.31	0.43
1:C:1206:UNK:C	1:C:1208:UNK:N	2.81	0.43
1:C:1922:UNK:O	1:C:1924:UNK:N	2.51	0.43
1:O:1209:UNK:C	1:O:1211:UNK:N	2.80	0.43
1:P:1117:UNK:C	1:P:1118:UNK:O	2.67	0.43
1:Q:1305:UNK:O	1:Q:1308:UNK:N	2.52	0.43
1:Q:1305:UNK:C	1:Q:1307:UNK:N	2.81	0.43
1:Y:802:UNK:O	1:Y:812:UNK:N	2.51	0.43
1:A:2612:UNK:O	1:A:2614:UNK:N	2.51	0.43
1:B:1007:UNK:O	1:B:1010:UNK:N	2.52	0.43
1:C:1115:UNK:O	1:C:1118:UNK:N	2.51	0.43
1:O:1414:UNK:C	1:O:1416:UNK:N	2.82	0.43
1:O:1616:UNK:O	1:O:1617:UNK:C	2.67	0.43
1:P:207:UNK:O	1:P:208:UNK:C	2.67	0.43
1:Q:123:UNK:O	1:Q:124:UNK:C	2.66	0.43
1:Q:909:UNK:C	1:Q:911:UNK:N	2.82	0.43
1:R:509:UNK:O	1:R:511:UNK:N	2.30	0.43
1:B:1117:UNK:C	1:B:1118:UNK:O	2.67	0.43
1:C:1511:UNK:O	1:C:1514:UNK:N	2.52	0.43
1:F:1208:UNK:C	1:F:1210:UNK:N	2.81	0.43
1:F:3514:UNK:O	1:F:3516:UNK:N	2.51	0.43
1:F:507:UNK:HA	1:F:510:UNK:CB	2.48	0.43
1:P:218:UNK:C	1:P:220:UNK:N	2.78	0.43
1:T:2106:UNK:O	1:T:2107:UNK:CB	2.66	0.43
1:B:711:UNK:C	1:B:713:UNK:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:UNK:O	1:D:721:UNK:CB	2.67	0.43
1:F:2221:UNK:C	1:F:2223:UNK:N	2.80	0.43
1:P:1619:UNK:C	1:P:1621:UNK:H	2.31	0.43
1:Q:1206:UNK:C	1:Q:1208:UNK:N	2.81	0.43
1:R:719:UNK:O	1:R:723:UNK:N	2.52	0.43
1:C:1305:UNK:C	1:C:1307:UNK:N	2.81	0.43
1:C:205:UNK:O	1:C:209:UNK:N	2.52	0.43
1:D:715:UNK:C	1:D:718:UNK:N	2.82	0.43
1:F:117:UNK:HA	1:F:120:UNK:CB	2.49	0.43
1:F:317:UNK:C	1:F:319:UNK:N	2.66	0.43
1:R:605:UNK:C	1:R:606:UNK:O	2.66	0.43
1:T:2810:UNK:C	1:T:2812:UNK:H	2.31	0.43
1:T:418:UNK:HA	1:T:421:UNK:CB	2.49	0.43
1:X:1030:UNK:O	1:X:1032:UNK:N	2.52	0.43
1:Y:804:UNK:N	1:Y:810:UNK:O	2.52	0.43
1:Y:838:UNK:CB	1:Y:871:UNK:CA	2.97	0.43
1:B:207:UNK:O	1:B:208:UNK:C	2.67	0.42
1:P:1315:UNK:C	1:P:1317:UNK:N	2.82	0.42
1:R:216:UNK:O	1:R:217:UNK:C	2.67	0.42
1:B:1406:UNK:O	1:B:1407:UNK:CB	2.67	0.42
1:C:106:UNK:O	1:C:108:UNK:N	2.53	0.42
1:C:909:UNK:C	1:C:911:UNK:N	2.82	0.42
1:F:1405:UNK:C	1:F:1407:UNK:H	2.32	0.42
1:P:1307:UNK:C	1:P:1309:UNK:N	2.82	0.42
1:P:1515:UNK:O	1:P:1517:UNK:C	2.67	0.42
1:P:813:UNK:HA	1:P:816:UNK:CB	2.49	0.42
1:Q:1309:UNK:O	1:Q:1312:UNK:CB	2.67	0.42
1:R:718:UNK:O	1:R:721:UNK:CB	2.67	0.42
1:S:309:UNK:C	1:S:311:UNK:N	2.81	0.42
1:T:3514:UNK:O	1:T:3516:UNK:N	2.51	0.42
1:X:804:UNK:N	1:X:810:UNK:O	2.52	0.42
1:C:1412:UNK:C	1:C:1414:UNK:N	2.62	0.42
1:C:807:UNK:O	1:C:810:UNK:N	2.52	0.42
1:D:1006:UNK:C	1:D:1008:UNK:N	2.75	0.42
1:D:216:UNK:O	1:D:217:UNK:C	2.67	0.42
1:F:613:UNK:C	1:F:615:UNK:N	2.83	0.42
1:O:1414:UNK:O	1:O:1416:UNK:N	2.52	0.42
1:P:1007:UNK:O	1:P:1010:UNK:N	2.52	0.42
1:P:1406:UNK:O	1:P:1407:UNK:CB	2.67	0.42
1:P:214:UNK:O	1:P:216:UNK:C	2.68	0.42
1:Q:205:UNK:C	1:Q:207:UNK:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:125:UNK:C	1:T:127:UNK:N	2.82	0.42
1:A:1414:UNK:O	1:A:1416:UNK:N	2.52	0.42
1:A:2110:UNK:O	1:A:2113:UNK:CA	2.67	0.42
1:C:1309:UNK:O	1:C:1312:UNK:CB	2.67	0.42
1:D:811:UNK:O	1:D:812:UNK:C	2.68	0.42
1:F:2106:UNK:O	1:F:2107:UNK:CB	2.66	0.42
1:F:418:UNK:HA	1:F:421:UNK:CB	2.49	0.42
1:Q:2205:UNK:C	1:Q:2207:UNK:N	2.83	0.42
1:A:1005:UNK:C	1:A:1007:UNK:N	2.83	0.42
1:A:2306:UNK:O	1:A:2307:UNK:C	2.62	0.42
1:P:1317:UNK:O	1:P:1318:UNK:C	2.68	0.42
1:Q:106:UNK:O	1:Q:108:UNK:N	2.52	0.42
1:Q:109:UNK:O	1:Q:112:UNK:CB	2.67	0.42
1:R:308:UNK:C	1:R:310:UNK:N	2.81	0.42
1:A:2506:UNK:C	1:A:2508:UNK:N	2.82	0.42
1:B:1515:UNK:O	1:B:1517:UNK:C	2.67	0.42
1:F:1521:UNK:O	1:F:1524:UNK:N	2.53	0.42
1:O:1005:UNK:O	1:O:1007:UNK:N	2.53	0.42
1:O:2506:UNK:C	1:O:2508:UNK:N	2.82	0.42
1:Q:1511:UNK:O	1:Q:1514:UNK:N	2.52	0.42
1:Q:205:UNK:O	1:Q:209:UNK:N	2.52	0.42
1:Q:909:UNK:O	1:Q:911:UNK:N	2.53	0.42
1:T:1430:UNK:O	1:T:1431:UNK:C	2.67	0.42
1:T:1521:UNK:O	1:T:1524:UNK:N	2.53	0.42
1:T:812:UNK:HA	1:T:815:UNK:CB	2.50	0.42
1:A:1616:UNK:O	1:A:1617:UNK:C	2.67	0.42
1:B:214:UNK:O	1:B:216:UNK:C	2.68	0.42
1:B:317:UNK:O	1:B:318:UNK:C	2.68	0.42
1:C:109:UNK:O	1:C:112:UNK:CB	2.67	0.42
1:D:410:UNK:O	1:D:413:UNK:N	2.53	0.42
1:D:412:UNK:O	1:D:413:UNK:C	2.67	0.42
1:F:1430:UNK:O	1:F:1431:UNK:C	2.67	0.42
1:F:812:UNK:HA	1:F:815:UNK:CB	2.50	0.42
1:F:810:UNK:C	1:F:812:UNK:N	2.82	0.42
1:R:410:UNK:O	1:R:413:UNK:N	2.53	0.42
1:R:917:UNK:C	1:R:919:UNK:H	2.31	0.42
1:T:117:UNK:HA	1:T:120:UNK:CB	2.49	0.42
1:T:317:UNK:C	1:T:319:UNK:N	2.66	0.42
1:Y:811:UNK:O	1:Y:813:UNK:N	2.53	0.42
1:A:1005:UNK:O	1:A:1007:UNK:N	2.53	0.42
1:A:1209:UNK:C	1:A:1211:UNK:N	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1305:UNK:O	1:C:1308:UNK:N	2.52	0.42
1:F:2507:UNK:O	1:F:2511:UNK:CB	2.68	0.42
1:P:1311:UNK:HA	1:P:1314:UNK:CB	2.50	0.42
1:P:1715:UNK:O	1:P:1716:UNK:O	2.38	0.42
1:R:412:UNK:O	1:R:413:UNK:C	2.67	0.42
1:R:908:UNK:C	1:R:910:UNK:N	2.82	0.42
1:T:1517:UNK:O	1:T:1518:UNK:C	2.68	0.42
1:Y:917:UNK:O	1:Y:918:UNK:C	2.67	0.42
1:A:1415:UNK:HA	1:A:1418:UNK:CB	2.49	0.42
1:B:1315:UNK:C	1:B:1317:UNK:N	2.82	0.42
1:C:613:UNK:O	1:C:616:UNK:N	2.53	0.42
1:D:719:UNK:O	1:D:723:UNK:N	2.52	0.42
1:P:514:UNK:O	1:P:515:UNK:C	2.68	0.42
1:Q:1415:UNK:O	1:Q:1418:UNK:CB	2.68	0.42
1:T:1405:UNK:C	1:T:1407:UNK:H	2.33	0.42
1:T:613:UNK:C	1:T:615:UNK:N	2.83	0.42
1:X:811:UNK:O	1:X:813:UNK:N	2.53	0.42
1:X:838:UNK:CB	1:X:871:UNK:CA	2.97	0.42
1:Y:1013:UNK:O	1:Y:1017:UNK:CB	2.68	0.42
1:Y:1030:UNK:O	1:Y:1032:UNK:N	2.52	0.42
1:A:1108:UNK:O	1:A:1109:UNK:C	2.66	0.42
1:B:1311:UNK:HA	1:B:1314:UNK:CB	2.50	0.42
1:B:1317:UNK:O	1:B:1318:UNK:C	2.68	0.42
1:D:908:UNK:C	1:D:910:UNK:N	2.82	0.42
1:F:1507:UNK:O	1:F:1511:UNK:N	2.53	0.42
1:P:811:UNK:C	1:P:813:UNK:N	2.82	0.42
1:T:1507:UNK:O	1:T:1511:UNK:N	2.53	0.42
1:T:410:UNK:O	1:T:413:UNK:N	2.53	0.42
1:A:1414:UNK:C	1:A:1416:UNK:N	2.82	0.41
1:A:1521:UNK:C	1:A:1523:UNK:N	2.83	0.41
1:B:1712:UNK:O	1:B:1715:UNK:CB	2.68	0.41
1:F:125:UNK:C	1:F:127:UNK:N	2.82	0.41
1:F:2809:UNK:O	1:F:2813:UNK:N	2.53	0.41
1:Q:1412:UNK:C	1:Q:1414:UNK:N	2.62	0.41
1:R:706:UNK:C	1:R:708:UNK:N	2.83	0.41
1:B:520:UNK:C	1:B:522:UNK:N	2.83	0.41
1:F:817:UNK:O	1:F:818:UNK:C	2.68	0.41
1:O:1005:UNK:C	1:O:1007:UNK:N	2.83	0.41
1:Q:613:UNK:O	1:Q:616:UNK:N	2.53	0.41
1:B:514:UNK:O	1:B:515:UNK:C	2.68	0.41
1:B:514:UNK:O	1:B:517:UNK:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1415:UNK:O	1:C:1418:UNK:CB	2.68	0.41
1:O:1415:UNK:HA	1:O:1418:UNK:CB	2.49	0.41
1:P:1412:UNK:HA	1:P:1415:UNK:CA	2.44	0.41
1:P:1712:UNK:O	1:P:1715:UNK:CB	2.68	0.41
1:Q:1214:UNK:O	1:Q:1216:UNK:N	2.53	0.41
1:Q:807:UNK:O	1:Q:810:UNK:N	2.52	0.41
1:T:2809:UNK:O	1:T:2813:UNK:N	2.53	0.41
1:X:1013:UNK:O	1:X:1017:UNK:CB	2.68	0.41
1:A:1305:UNK:C	1:A:1307:UNK:N	2.80	0.41
1:A:1312:UNK:O	1:A:1315:UNK:N	2.54	0.41
1:C:507:UNK:O	1:C:509:UNK:N	2.54	0.41
1:F:1417:UNK:C	1:F:1419:UNK:N	2.79	0.41
1:Q:1115:UNK:O	1:Q:1117:UNK:N	2.54	0.41
1:R:1109:UNK:C	1:R:1111:UNK:N	2.67	0.41
1:R:811:UNK:O	1:R:812:UNK:C	2.68	0.41
1:T:1911:UNK:C	1:T:1913:UNK:N	2.83	0.41
1:T:209:UNK:O	1:T:211:UNK:N	2.54	0.41
1:T:2507:UNK:O	1:T:2511:UNK:CB	2.68	0.41
1:T:2618:UNK:C	1:T:2620:UNK:N	2.83	0.41
1:Y:1033:UNK:O	1:Y:1037:UNK:N	2.54	0.41
1:Y:908:UNK:C	1:Y:910:UNK:N	2.83	0.41
1:P:1113:UNK:C	1:P:1115:UNK:N	2.84	0.41
1:P:317:UNK:O	1:P:318:UNK:C	2.68	0.41
1:P:514:UNK:O	1:P:517:UNK:CB	2.68	0.41
1:T:2221:UNK:C	1:T:2223:UNK:N	2.80	0.41
1:X:908:UNK:C	1:X:910:UNK:N	2.83	0.41
1:C:909:UNK:O	1:C:911:UNK:N	2.53	0.41
1:D:706:UNK:C	1:D:708:UNK:N	2.83	0.41
1:P:1412:UNK:HA	1:P:1415:UNK:N	2.36	0.41
1:S:313:UNK:O	1:S:315:UNK:N	2.54	0.41
1:T:1518:UNK:O	1:T:1522:UNK:N	2.54	0.41
1:T:3414:UNK:O	1:T:3415:UNK:C	2.64	0.41
1:T:817:UNK:O	1:T:818:UNK:C	2.68	0.41
1:X:1062:UNK:C	1:X:1064:UNK:N	2.82	0.41
1:A:1310:UNK:O	1:A:1312:UNK:N	2.53	0.41
1:B:909:UNK:O	1:B:910:UNK:C	2.66	0.41
1:C:113:UNK:O	1:C:116:UNK:N	2.54	0.41
1:C:1214:UNK:O	1:C:1216:UNK:N	2.53	0.41
1:C:1309:UNK:O	1:C:1311:UNK:N	2.54	0.41
1:D:315:UNK:C	1:D:318:UNK:N	2.84	0.41
1:F:1412:UNK:O	1:F:1415:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:2208:UNK:O	1:Q:2210:UNK:N	2.42	0.41
1:R:307:UNK:C	1:R:309:UNK:N	2.81	0.41
1:T:2319:UNK:O	1:T:2321:UNK:C	2.69	0.41
1:F:1517:UNK:O	1:F:1518:UNK:C	2.68	0.41
1:F:1518:UNK:O	1:F:1522:UNK:N	2.54	0.41
1:F:2319:UNK:O	1:F:2321:UNK:C	2.69	0.41
1:P:1015:UNK:O	1:P:1016:UNK:C	2.68	0.41
1:P:909:UNK:O	1:P:910:UNK:C	2.66	0.41
1:T:1412:UNK:O	1:T:1415:UNK:N	2.54	0.41
1:B:1412:UNK:HA	1:B:1415:UNK:N	2.36	0.41
1:C:1115:UNK:O	1:C:1117:UNK:N	2.54	0.41
1:F:209:UNK:O	1:F:211:UNK:N	2.54	0.41
1:F:410:UNK:HA	1:F:413:UNK:CB	2.51	0.41
1:Q:1309:UNK:O	1:Q:1311:UNK:N	2.54	0.41
1:B:911:UNK:O	1:B:913:UNK:N	2.54	0.41
1:D:307:UNK:C	1:D:309:UNK:N	2.80	0.41
1:F:410:UNK:O	1:F:413:UNK:N	2.53	0.41
1:Q:113:UNK:O	1:Q:116:UNK:N	2.54	0.41
1:Q:507:UNK:O	1:Q:509:UNK:N	2.54	0.41
1:T:410:UNK:HA	1:T:413:UNK:CB	2.51	0.41
1:T:705:UNK:C	1:T:707:UNK:N	2.84	0.41
1:B:1715:UNK:O	1:B:1716:UNK:O	2.38	0.41
1:E:313:UNK:O	1:E:315:UNK:N	2.54	0.41
1:O:1312:UNK:O	1:O:1315:UNK:N	2.54	0.41
1:Q:1819:UNK:HA	1:Q:1822:UNK:CB	2.51	0.41
1:R:1112:UNK:C	1:R:1114:UNK:N	2.84	0.41
1:R:210:UNK:O	1:R:211:UNK:C	2.69	0.41
1:D:1112:UNK:C	1:D:1114:UNK:N	2.84	0.40
1:F:1018:UNK:C	1:F:1020:UNK:N	2.84	0.40
1:T:1417:UNK:O	1:T:1419:UNK:N	2.54	0.40
1:T:305:UNK:O	1:T:306:UNK:O	2.40	0.40
1:A:2307:UNK:O	1:A:2308:UNK:C	2.69	0.40
1:D:605:UNK:C	1:D:606:UNK:O	2.66	0.40
1:P:911:UNK:O	1:P:913:UNK:N	2.54	0.40
1:R:315:UNK:C	1:R:318:UNK:N	2.84	0.40
1:X:1033:UNK:O	1:X:1037:UNK:N	2.54	0.40
1:Y:1062:UNK:C	1:Y:1064:UNK:N	2.82	0.40
1:A:1509:UNK:C	1:A:1511:UNK:N	2.71	0.40
1:B:811:UNK:C	1:B:813:UNK:N	2.82	0.40
1:C:1407:UNK:O	1:C:1411:UNK:N	2.55	0.40
1:C:2216:UNK:O	1:C:2218:UNK:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:UNK:O	1:D:213:UNK:O	2.38	0.40
1:D:715:UNK:O	1:D:718:UNK:N	2.55	0.40
1:E:112:UNK:C	1:E:114:UNK:N	2.76	0.40
1:O:1521:UNK:C	1:O:1523:UNK:N	2.83	0.40
1:T:1018:UNK:C	1:T:1020:UNK:N	2.84	0.40
1:T:810:UNK:C	1:T:812:UNK:N	2.82	0.40
1:C:1511:UNK:O	1:C:1513:UNK:N	2.55	0.40
1:C:2612:UNK:C	1:C:2614:UNK:N	2.83	0.40
1:D:1008:UNK:O	1:D:1012:UNK:N	2.54	0.40
1:F:3420:UNK:O	1:F:3423:UNK:C	2.70	0.40
1:O:1312:UNK:O	1:O:1313:UNK:C	2.70	0.40
1:O:2307:UNK:O	1:O:2308:UNK:C	2.69	0.40
1:Q:1407:UNK:O	1:Q:1408:UNK:C	2.68	0.40
1:Q:1814:UNK:O	1:Q:1815:UNK:O	2.39	0.40
1:R:715:UNK:O	1:R:718:UNK:N	2.55	0.40
1:Y:906:UNK:O	1:Y:908:UNK:N	2.54	0.40
1:A:1811:UNK:O	1:A:1815:UNK:N	2.55	0.40
1:A:2315:UNK:C	1:A:2317:UNK:N	2.79	0.40
1:F:2107:UNK:O	1:F:2108:UNK:C	2.69	0.40
1:Q:1511:UNK:O	1:Q:1513:UNK:N	2.55	0.40
1:R:1008:UNK:O	1:R:1012:UNK:N	2.54	0.40

All (48) 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)
1:O:619:UNK:C	1:T:2418:UNK:O[1_545]	0.56	1.64
1:O:620:UNK:C	1:T:2419:UNK:CA[1_545]	0.57	1.63
1:O:622:UNK:N	1:T:2418:UNK:N[1_545]	0.67	1.53
1:O:622:UNK:C	1:T:2417:UNK:O[1_545]	0.68	1.52
1:O:621:UNK:O	1:T:2417:UNK:CA[1_545]	0.91	1.29
1:O:621:UNK:O	1:T:2417:UNK:N[1_545]	0.91	1.29
1:O:619:UNK:O	1:T:2418:UNK:O[1_545]	0.97	1.23
1:O:620:UNK:CA	1:T:2419:UNK:CA[1_545]	1.05	1.15
1:O:622:UNK:CA	1:T:2418:UNK:N[1_545]	1.06	1.14
1:O:622:UNK:O	1:T:2417:UNK:O[1_545]	1.14	1.06
1:O:620:UNK:C	1:T:2419:UNK:CB[1_545]	1.18	1.02
1:O:622:UNK:CA	1:T:2417:UNK:C[1_545]	1.26	0.94
1:O:619:UNK:O	1:T:2418:UNK:C[1_545]	1.28	0.92
1:O:622:UNK:CB	1:T:2418:UNK:CA[1_545]	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:621:UNK:N	1:T:2419:UNK:N[1_545]	1.34	0.86
1:O:620:UNK:C	1:T:2419:UNK:N[1_545]	1.35	0.85
1:O:622:UNK:N	1:T:2417:UNK:C[1_545]	1.48	0.72
1:O:620:UNK:O	1:T:2420:UNK:N[1_545]	1.48	0.72
1:O:622:UNK:N	1:T:2418:UNK:CA[1_545]	1.50	0.70
1:O:620:UNK:O	1:T:2419:UNK:CA[1_545]	1.51	0.69
1:O:620:UNK:O	1:T:2419:UNK:CB[1_545]	1.52	0.68
1:O:622:UNK:CA	1:T:2418:UNK:CA[1_545]	1.54	0.66
1:O:619:UNK:CA	1:T:2418:UNK:O[1_545]	1.55	0.65
1:O:622:UNK:CA	1:T:2417:UNK:O[1_545]	1.59	0.61
1:O:622:UNK:CB	1:T:2418:UNK:CB[1_545]	1.61	0.59
1:O:620:UNK:O	1:T:2419:UNK:C[1_545]	1.62	0.58
1:O:621:UNK:O	1:T:2417:UNK:C[1_545]	1.63	0.57
1:O:619:UNK:C	1:T:2418:UNK:C[1_545]	1.63	0.57
1:O:621:UNK:C	1:T:2417:UNK:C[1_545]	1.65	0.55
1:O:622:UNK:C	1:T:2417:UNK:C[1_545]	1.67	0.53
1:O:621:UNK:N	1:T:2419:UNK:CA[1_545]	1.69	0.51
1:O:621:UNK:C	1:T:2418:UNK:N[1_545]	1.74	0.46
1:O:621:UNK:C	1:T:2417:UNK:CA[1_545]	1.77	0.43
1:O:620:UNK:N	1:T:2418:UNK:O[1_545]	1.81	0.39
1:O:620:UNK:C	1:T:2419:UNK:C[1_545]	1.84	0.36
1:O:621:UNK:N	1:T:2419:UNK:CB[1_545]	1.86	0.34
1:O:621:UNK:C	1:T:2417:UNK:N[1_545]	1.86	0.34
1:O:621:UNK:O	1:T:2416:UNK:C[1_545]	1.90	0.30
1:O:620:UNK:CA	1:T:2419:UNK:C[1_545]	1.92	0.28
1:O:620:UNK:N	1:T:2419:UNK:CA[1_545]	2.01	0.19
1:O:619:UNK:O	1:T:2419:UNK:O[1_545]	2.03	0.17
1:O:620:UNK:O	1:T:2419:UNK:N[1_545]	2.04	0.16
1:O:620:UNK:CA	1:T:2419:UNK:CB[1_545]	2.06	0.14
1:O:622:UNK:CB	1:T:2418:UNK:N[1_545]	2.07	0.13
1:O:622:UNK:N	1:T:2419:UNK:N[1_545]	2.09	0.11
1:O:622:UNK:N	1:T:2418:UNK:C[1_545]	2.10	0.10
1:O:621:UNK:O	1:T:2417:UNK:CB[1_545]	2.16	0.04
1:O:619:UNK:O	1:T:2419:UNK:N[1_545]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	0/4128	-	-	-	-
1	B	0/4128	-	-	-	-
1	C	0/4128	-	-	-	-
1	D	0/4128	-	-	-	-
1	E	0/4128	-	-	-	-
1	F	0/4128	-	-	-	-
1	O	0/4128	-	-	-	-
1	P	0/4128	-	-	-	-
1	Q	0/4128	-	-	-	-
1	R	0/4128	-	-	-	-
1	S	0/4128	-	-	-	-
1	T	0/4128	-	-	-	-
1	X	0/4128	-	-	-	-
1	Y	0/4128	-	-	-	-
All	All	0/57792	-	-	-	-

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.