



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2020 – 06:18 pm BST

PDB ID : 2Z87  
Title : Crystal structure of chondroitin polymerase from Escherichia coli strain K4 (K4CP) complexed with UDP-GalNAc and UDP  
Authors : Osawa, T.; Sugiura, N.; Shimada, H.; Hirooka, R.; Tsuji, A.; Kimura, M.; Kimata, K.; Kakuta, Y.  
Deposited on : 2007-09-03  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

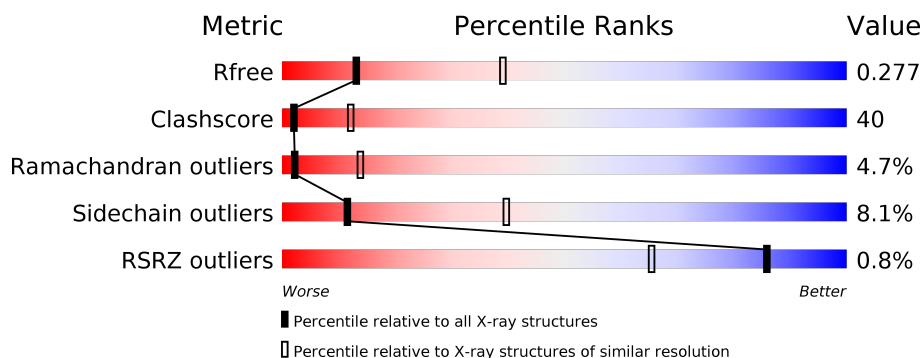
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	624	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>46%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	624	<div> <div>%</div> <div> <div></div> <div>36%</div> <div>50%</div> <div>8%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UDP	A	684	-	-	X	-

## 2 Entry composition [i](#)

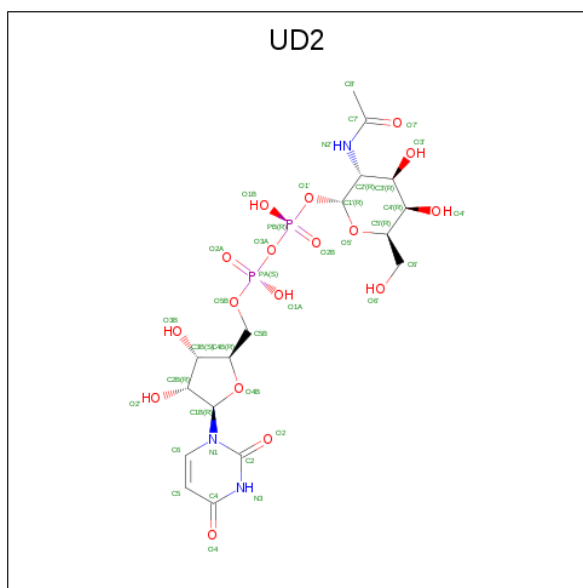
There are 5 unique types of molecules in this entry. The entry contains 9983 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chondroitin synthase.

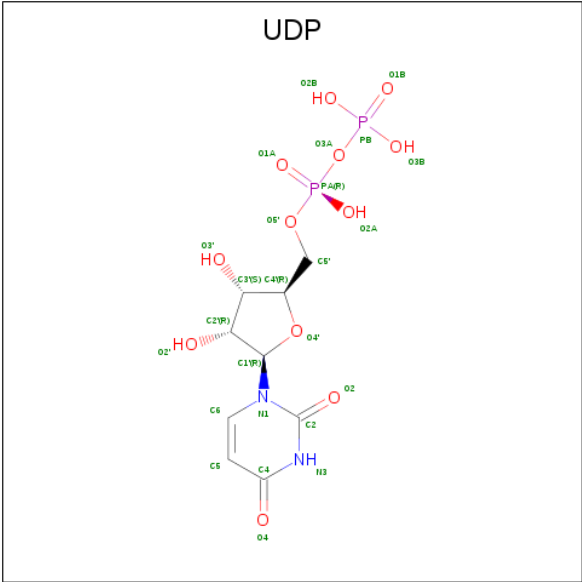
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	25	0	0
			4894	3119	835	916	24			
1	B	591	Total	C	N	O	S	25	0	0
			4816	3071	822	899	24			

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYL GALACTOSAMINE (three-letter code: UD2) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mn	0	0
			2	2		
4	A	2	Total	Mn	0	0
			2	2		

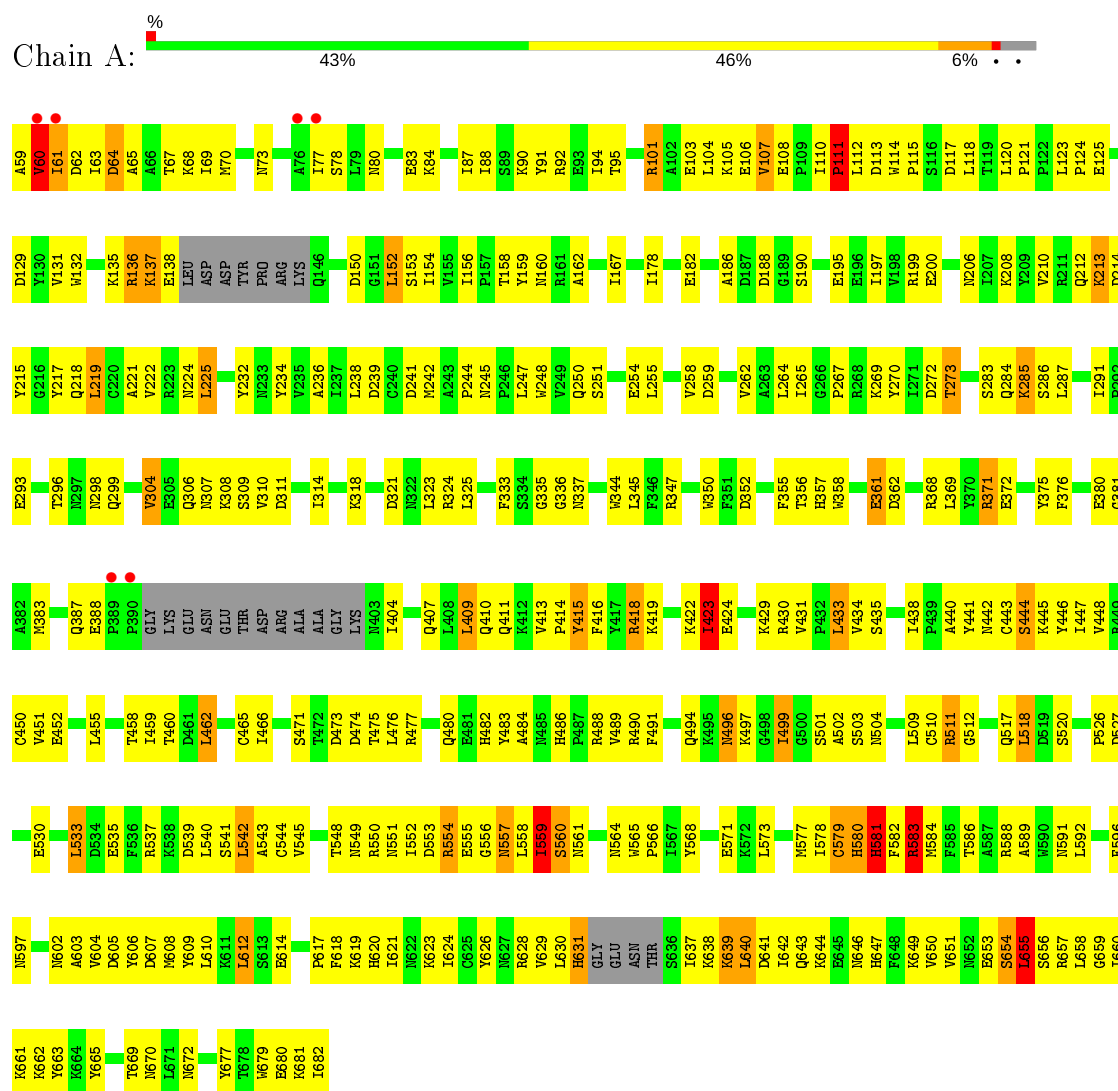
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	63	Total	O	0	0
			63	63		

### 3 Residue-property plots

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

#### • Molecule 1: Chondroitin synthase



#### • Molecule 1: Chondroitin synthase



Q643	RG44	BE45	RG46	HE47	FE48	RG49	VS50	VS51	HE52	BE53	SE54	SE55	SE56	RG57	LE58	GE59	IG60	VE61	RG62	RG63	RG64	YG65		
S569	RG70	SE71	SE72	TE73	SE74	SE75	AS76	ME77	SE78	SE79	HE80	HE81	FE82	RG83	TE86	SE87	SE88	IG89	VE90	VE91	VE92	VE93	VE94	
S503	RS04	TE05		RS08	LS09	CE10	RS11	RS12	RS13	RS14	RS17	LS18	RS19		D522	FE23	FE24	FE25	FE26	FE27	AS28	VS29	VS30	VS31
R430	VS32	VS33	VS34	VS35	VS36	VS37	VS38	VS39	VS40	VS41	VS42	VS43	VS44	VS45	VS46	VS47	VS48	VS49	VS50	VS51	VS52	VS53	VS54	VS55
R431	VS56	VS57	VS58	VS59	VS60	VS61	VS62	VS63	VS64	VS65	VS66	VS67	VS68	VS69	VS70	VS71	VS72	VS73	VS74	VS75	VS76	VS77	VS78	VS79
R432	VS80	VS81	VS82	VS83	VS84	VS85	VS86	VS87	VS88	VS89	VS90	VS91	VS92	VS93	VS94	VS95	VS96	VS97	VS98	VS99	VS100	VS101	VS102	VS103
R433	VS104	VS105	VS106	VS107	VS108	VS109	VS110	VS111	VS112	VS113	VS114	VS115	VS116	VS117	VS118	VS119	VS120	VS121	VS122	VS123	VS124	VS125	VS126	VS127
R434	VS128	VS129	VS130	VS131	VS132	VS133	VS134	VS135	VS136	VS137	VS138	VS139	VS140	VS141	VS142	VS143	VS144	VS145	VS146	VS147	VS148	VS149	VS150	VS151
R435	VS152	VS153	VS154	VS155	VS156	VS157	VS158	VS159	VS160	VS161	VS162	VS163	VS164	VS165	VS166	VS167	VS168	VS169	VS170	VS171	VS172	VS173	VS174	VS175
R436	VS176	VS177	VS178	VS179	VS180	VS181	VS182	VS183	VS184	VS185	VS186	VS187	VS188	VS189	VS190	VS191	VS192	VS193	VS194	VS195	VS196	VS197	VS198	VS199
R437	VS200	VS201	VS202	VS203	VS204	VS205	VS206	VS207	VS208	VS209	VS210	VS211	VS212	VS213	VS214	VS215	VS216	VS217	VS218	VS219	VS220	VS221	VS222	VS223
R438	VS224	VS225	VS226	VS227	VS228	VS229	VS230	VS231	VS232	VS233	VS234	VS235	VS236	VS237	VS238	VS239	VS240	VS241	VS242	VS243	VS244	VS245	VS246	VS247
R439	VS248	VS249	VS250	VS251	VS252	VS253	VS254	VS255	VS256	VS257	VS258	VS259	VS260	VS261	VS262	VS263	VS264	VS265	VS266	VS267	VS268	VS269	VS270	VS271
R440	VS272	VS273	VS274	VS275	VS276	VS277	VS278	VS279	VS280	VS281	VS282	VS283	VS284	VS285	VS286	VS287	VS288	VS289	VS290	VS291	VS292	VS293	VS294	VS295
R441	VS296	VS297	VS298	VS299	VS300	VS301	VS302	VS303	VS304	VS305	VS306	VS307	VS308	VS309	VS310	VS311	VS312	VS313	VS314	VS315	VS316	VS317	VS318	VS319
R442	VS320	VS321	VS322	VS323	VS324	VS325	VS326	VS327	VS328	VS329	VS330	VS331	VS332	VS333	VS334	VS335	VS336	VS337	VS338	VS339	VS340	VS341	VS342	VS343
R443	VS344	VS345	VS346	VS347	VS348	VS349	VS350	VS351	VS352	VS353	VS354	VS355	VS356	VS357	VS358	VS359	VS360	VS361	VS362	VS363	VS364	VS365	VS366	VS367
R444	VS368	VS369	VS370	VS371	VS372	VS373	VS374	VS375	VS376	VS377	VS378	VS379	VS380	VS381	VS382	VS383	VS384	VS385	VS386	VS387	VS388	VS389	VS390	VS391
R445	VS392	VS393	VS394	VS395	VS396	VS397	VS398	VS399	VS400	VS401	VS402	VS403	VS404	VS405	VS406	VS407	VS408	VS409	VS410	VS411	VS412	VS413	VS414	VS415
R446	VS416	VS417	VS418	VS419	VS420	VS421	VS422	VS423	VS424	VS425	VS426	VS427	VS428	VS429	VS430	VS431	VS432	VS433	VS434	VS435	VS436	VS437	VS438	VS439
R447	VS440	VS441	VS442	VS443	VS444	VS445	VS446	VS447	VS448	VS449	VS450	VS451	VS452	VS453	VS454	VS455	VS456	VS457	VS458	VS459	VS460	VS461	VS462	VS463
R448	VS464	VS465	VS466	VS467	VS468	VS469	VS470	VS471	VS472	VS473	VS474	VS475	VS476	VS477	VS478	VS479	VS480	VS481	VS482	VS483	VS484	VS485	VS486	VS487
R449	VS488	VS489	VS490	VS491	VS492	VS493	VS494	VS495	VS496	VS497	VS498	VS499	VS500	VS501	VS502	VS503	VS504	VS505	VS506	VS507	VS508	VS509	VS510	VS511
R450	VS512	VS513	VS514	VS515	VS516	VS517	VS518	VS519	VS520	VS521	VS522	VS523	VS524	VS525	VS526	VS527	VS528	VS529	VS530	VS531	VS532	VS533	VS534	VS535
R451	VS536	VS537	VS538	VS539	VS540	VS541	VS542	VS543	VS544	VS545	VS546	VS547	VS548	VS549	VS550	VS551	VS552	VS553	VS554	VS555	VS556	VS557	VS558	VS559
R452	VS560	VS561	VS562	VS563	VS564	VS565	VS566	VS567	VS568	VS569	VS570	VS571	VS572	VS573	VS574	VS575	VS576	VS577	VS578	VS579	VS580	VS581	VS582	VS583
R453	VS584	VS585	VS586	VS587	VS588	VS589	VS590	VS591	VS592	VS593	VS594	VS595	VS596	VS597	VS598	VS599	VS600	VS601	VS602	VS603	VS604	VS605	VS606	VS607
R454	VS608	VS609	VS610	VS611	VS612	VS613	VS614	VS615	VS616	VS617	VS618	VS619	VS620	VS621	VS622	VS623	VS624	VS625	VS626	VS627	VS628	VS629	VS630	VS631
R455	VS632	VS633	VS634	VS635	VS636	VS637	VS638	VS639	VS640	VS641	VS642	VS643	VS644	VS645	VS646	VS647	VS648	VS649	VS650	VS651	VS652	VS653	VS654	VS655
R456	VS656	VS657	VS658	VS659	VS660	VS661	VS662	VS663	VS664	VS665	VS666	VS667	VS668	VS669	VS670	VS671	VS672	VS673	VS674	VS675	VS676	VS677	VS678	VS679
R457	VS680	VS681	VS682	VS683	VS684	VS685	VS686	VS687	VS688	VS689	VS690	VS691	VS692	VS693	VS694	VS695	VS696	VS697	VS698	VS699	VS700	VS701	VS702	VS703
R458	VS704	VS705	VS706	VS707	VS708	VS709	VS710	VS711	VS712	VS713	VS714	VS715	VS716	VS717	VS718	VS719	VS720	VS721	VS722	VS723	VS724	VS725	VS726	VS727
R459	VS728	VS729	VS730	VS731	VS732	VS733	VS734	VS735	VS736	VS737	VS738	VS739	VS740	VS741	VS742	VS743	VS744	VS745	VS746	VS747	VS748	VS749	VS750	VS751
R460	VS752	VS753	VS754	VS755	VS756	VS757	VS758	VS759	VS760	VS761	VS762	VS763	VS764	VS765	VS766	VS767	VS768	VS769	VS770	VS771	VS772	VS773	VS774	VS775
R461	VS776	VS777	VS778	VS779	VS780	VS781	VS782	VS783	VS784	VS785	VS786	VS787	VS788	VS789	VS790	VS791	VS792	VS793	VS794	VS795	VS796	VS797	VS798	VS799
R462	VS800	VS801	VS802	VS803	VS804	VS805	VS806	VS807	VS808	VS809	VS810	VS811	VS812	VS813	VS814	VS815	VS816	VS817	VS818	VS819	VS820	VS821	VS822	VS823
R463	VS824	VS825	VS826	VS827	VS828	VS829	VS830	VS831	VS832	VS833	VS834	VS835	VS836	VS837	VS838	VS839	VS840	VS841	VS842	VS843	VS844	VS845	VS846	VS847
R464	VS848	VS849	VS850	VS851	VS852	VS853	VS854	VS855	VS856	VS857	VS858	VS859	VS860	VS861	VS862	VS863	VS864	VS865	VS866	VS867	VS868	VS869	VS870	VS871
R465	VS872	VS873	VS874	VS875	VS876	VS877	VS878	VS879	VS880	VS881	VS882	VS883	VS884	VS885	VS886	VS887	VS888	VS889	VS890	VS891	VS892	VS893	VS894	VS895
R466	VS896	VS897	VS898	VS899	VS900	VS901	VS902	VS903	VS904	VS905	VS906	VS907	VS908	VS909	VS910	VS911	VS912	VS913	VS914	VS915	VS916	VS917	VS918	VS919
R467	VS920	VS921	VS922	VS923	VS924	VS925	VS926	VS927	VS928	VS929	VS930	VS931	VS932	VS933	VS934	VS935	VS936	VS937	VS938	VS939	VS940	VS941	VS942	VS943
R468	VS944	VS945	VS946	VS947	VS948	VS949	VS950	VS951	VS952	VS953	VS954	VS955	VS956	VS957	VS958	VS959	VS960	VS961	VS962	VS963	VS964	VS965	VS966	VS967
R469	VS968	VS969	VS970	VS971	VS972	VS973	VS974	VS975	VS976	VS977	VS978	VS979	VS980	VS981	VS982	VS983	VS984	VS985	VS986	VS987	VS988	VS989	VS990	VS991
R470	VS992	VS993	VS994	VS995	VS996	VS997	VS998	VS999	VS1000	VS1001	VS1002	VS1003	VS1004	VS1005	VS1006	VS1007	VS1008	VS1009	VS1010	VS1011	VS1012	VS1013	VS1014	VS1015
R471	VS1016	VS1017	VS1018	VS1019	VS1020	VS1021	VS1022	VS1023	VS1024	VS1025	VS1026	VS1027	VS1028	VS1029	VS1030	VS1031	VS1032	VS1033	VS1034	VS1035	VS1036	VS1037	VS1038	VS1039
R472	VS1040	VS1041	VS1042	VS1043	VS1044	VS1045	VS1046	VS1047	VS1048	VS1049	VS1050	VS1051	VS1052	VS1053	VS1054	VS1055	VS1056	VS1057	VS1058	VS1059	VS1060	VS1061	VS1062	VS1063
R473	VS1064	VS1065	VS1066	VS1067	VS1068	VS1069	VS1070	VS1071	VS1072	VS1073	VS1074	VS1075	VS1076	VS1077	VS1078	VS1079	VS1080	VS1081	VS1082	VS1083	VS1084	VS1085	VS1086	VS1087
R474	VS1088	VS1089	VS1090	VS1091	VS1092	VS1093	VS1094	VS1095	VS1096	VS1097	VS1098	VS1099	VS1100	VS1101	VS1102	VS1103	VS1104	VS1105	VS1106	VS1107	VS1108	VS1109	VS1110	VS1111
R475	VS1112	VS1113	VS1114	VS1115	VS1116	VS1117	VS1118	VS1119	VS1120	VS1121	VS1122	VS1123	VS1124	VS1125	VS1126	VS1127	VS1128	VS1129	VS1130	VS1131	VS1132	VS1133	VS1134	VS1135
R476	VS1136	VS1137	VS1138	VS1139	VS1140	VS1141	VS1142	VS1143	VS1144	VS1145	VS1146	VS1147	VS1148	VS1149	VS1150	VS1151	VS1152	VS1153	VS1154	VS1155	VS1156	VS1157	VS1158	VS1159
R477	VS1160	VS1161	VS1162	VS1163	VS1164	VS1165	VS1166	VS1167	VS1168	VS1169	VS1170	VS1171	VS1172	VS1173	VS1174	VS1175	VS1176	VS1177	VS1178	VS1179	VS1180	VS1181	VS1182	VS1183
R478	VS1184	VS1185	VS1186	VS1187	VS1188	VS1189	VS1190	VS1191	VS1192	VS1193	VS1194	VS1195	VS1196	VS1197	VS1198	VS1199	VS1200	VS1201	VS1202	VS1203	VS1204	VS1205	VS1206	VS1207
R479	VS1208	VS1209	VS1210	VS1211	VS1212	VS1213	VS1214	VS1215	VS1216	VS1217	VS1218	VS1219	VS1220	VS1221	VS1222	VS1223	VS1224	VS1225	VS1226	VS1227	VS1228	VS1229	VS1230	VS12

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.37Å 109.28Å 85.58Å 90.00° 103.47° 90.00°	Depositor
Resolution (Å)	19.96 – 3.00 46.94 – 2.76	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.96-3.00) 80.8 (46.94-2.76)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.199 , 0.283 0.198 , 0.277	Depositor DCC
$R_{free}$ test set	1440 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UD2, UDP, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.74	15/4998 (0.3%)	0.73	5/6761 (0.1%)
1	B	0.72	15/4919 (0.3%)	0.69	4/6651 (0.1%)
All	All	0.73	30/9917 (0.3%)	0.71	9/13412 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	PHE	CE1-CZ	-15.79	1.07	1.37
1	A	583	ARG	CZ-NH1	-14.93	1.13	1.33
1	A	582	PHE	CE1-CZ	-14.83	1.09	1.37
1	A	582	PHE	CE2-CZ	-14.67	1.09	1.37
1	B	582	PHE	CE2-CZ	-14.01	1.10	1.37

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	ARG	NE-CZ-NH2	15.13	127.86	120.30
1	A	583	ARG	NE-CZ-NH1	-9.31	115.64	120.30
1	B	583	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	582	PHE	N-CA-C	-5.64	95.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	581	HIS	CA-C-N	5.42	129.11	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	581	HIS	Peptide
1	B	581	HIS	Peptide
1	B	582	PHE	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	4894	0	4853	361	0
1	B	4816	0	4775	422	0
2	A	39	0	25	0	0
2	B	39	0	25	1	0
3	A	25	0	11	8	0
3	B	25	0	11	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	78	0	0	47	0
5	B	63	0	0	26	0
All	All	9983	0	9700	782	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

The worst 5 of 782 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:A:539:ASP:HB3	1:A:542:LEU:HD22	1.20	1.18
1:A:273:THR:HG21	1:A:387:GLN:HE21	0.99	1.07
3:A:684:UDP:H5'1	3:A:684:UDP:O1B	1.54	1.05

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*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ILE:HD12	1:B:423:ILE:H	1.20	1.04
1:B:466:ILE:HA	5:B:709:HOH:O	1.59	1.01

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/624 (95%)	507 (86%)	63 (11%)	23 (4%)	3	17
1	B	581/624 (93%)	472 (81%)	77 (13%)	32 (6%)	2	10
All	All	1174/1248 (94%)	979 (83%)	140 (12%)	55 (5%)	2	14

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	136	ARG
1	A	137	LYS
1	A	337	ASN
1	A	410	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/557 (97%)	489 (91%)	50 (9%)	9	33
1	B	530/557 (95%)	493 (93%)	37 (7%)	15	47
All	All	1069/1114 (96%)	982 (92%)	87 (8%)	11	40

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	ASN
1	A	655	LEU
1	B	628	ARG
1	A	559	ILE
1	A	612	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	ASN
1	B	174	ASN
1	B	631	HIS
1	A	631	HIS
1	A	647	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UD2	A	683	4	34,41,41	1.08	3 (8%)	45,62,62	1.49	7 (15%)
3	UDP	A	684	-	20,26,26	1.67	3 (15%)	25,40,40	2.18	7 (28%)
2	UD2	B	683	4	34,41,41	0.86	1 (2%)	45,62,62	1.57	9 (20%)
3	UDP	B	1	4	20,26,26	1.69	4 (20%)	25,40,40	1.97	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UD2	A	683	4	-	8/24/63/63	0/3/3/3
3	UDP	A	684	-	-	4/14/32/32	0/2/2/2
2	UD2	B	683	4	-	11/24/63/63	0/3/3/3
3	UDP	B	1	4	-	5/14/32/32	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	UDP	C6-N1	-4.11	1.30	1.35
3	A	684	UDP	C6-N1	-3.67	1.31	1.35
2	A	683	UD2	C6-N1	3.40	1.40	1.35
3	B	1	UDP	C2-N3	-3.02	1.32	1.38
3	A	684	UDP	C2'-C1'	-2.97	1.49	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	684	UDP	PA-O3A-PB	-6.71	109.81	132.83
3	B	1	UDP	PA-O3A-PB	-5.99	112.26	132.83
2	B	683	UD2	C3'-C2'-N2'	-4.19	102.71	110.62
3	A	684	UDP	O3'-C3'-C2'	-3.91	99.17	111.82
2	B	683	UD2	O3A-PB-O1'	-3.66	95.11	102.48

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	683	UD2	C2B-C1B-N1-C6
2	A	683	UD2	O4B-C1B-N1-C6
2	A	683	UD2	C5B-O5B-PA-O1A
2	A	683	UD2	C5B-O5B-PA-O3A
2	B	683	UD2	C1'-C2'-N2'-C7'

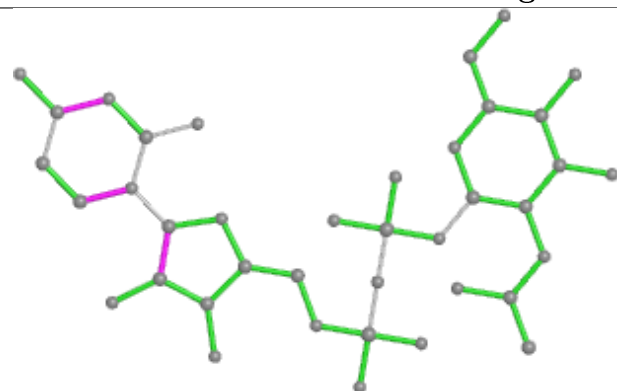
There are no ring outliers.

3 monomers are involved in 10 short contacts:

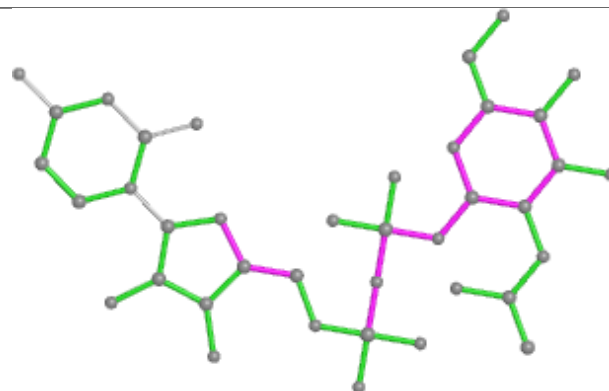
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	684	UDP	8	0
2	B	683	UD2	1	0
3	B	1	UDP	1	0

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

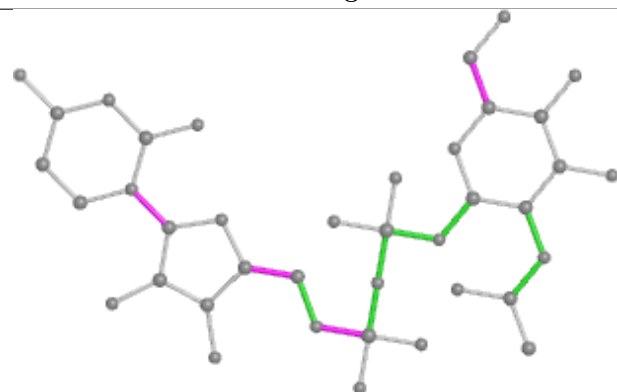
## Ligand UD2 A 683



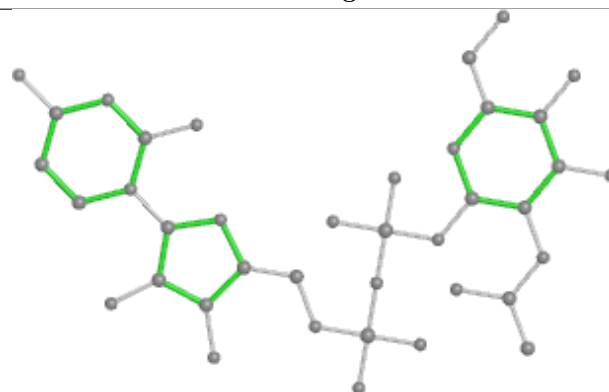
Bond lengths



Bond angles

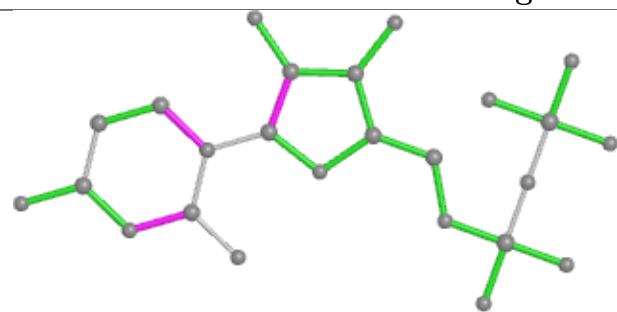


Torsions

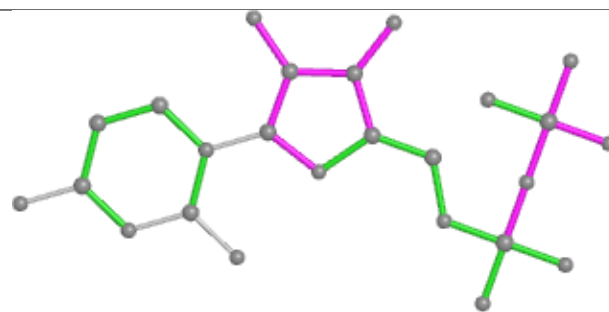


Rings

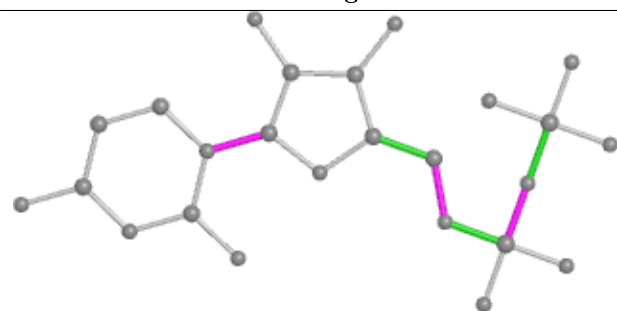
## Ligand UDP A 684



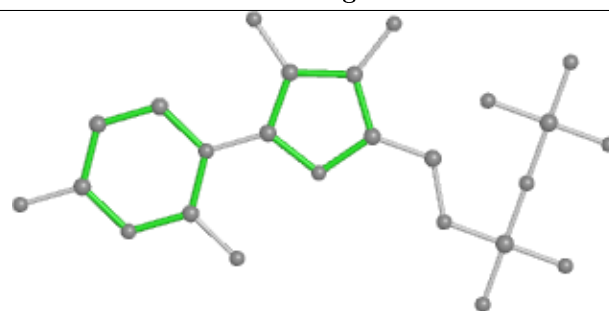
Bond lengths



Bond angles

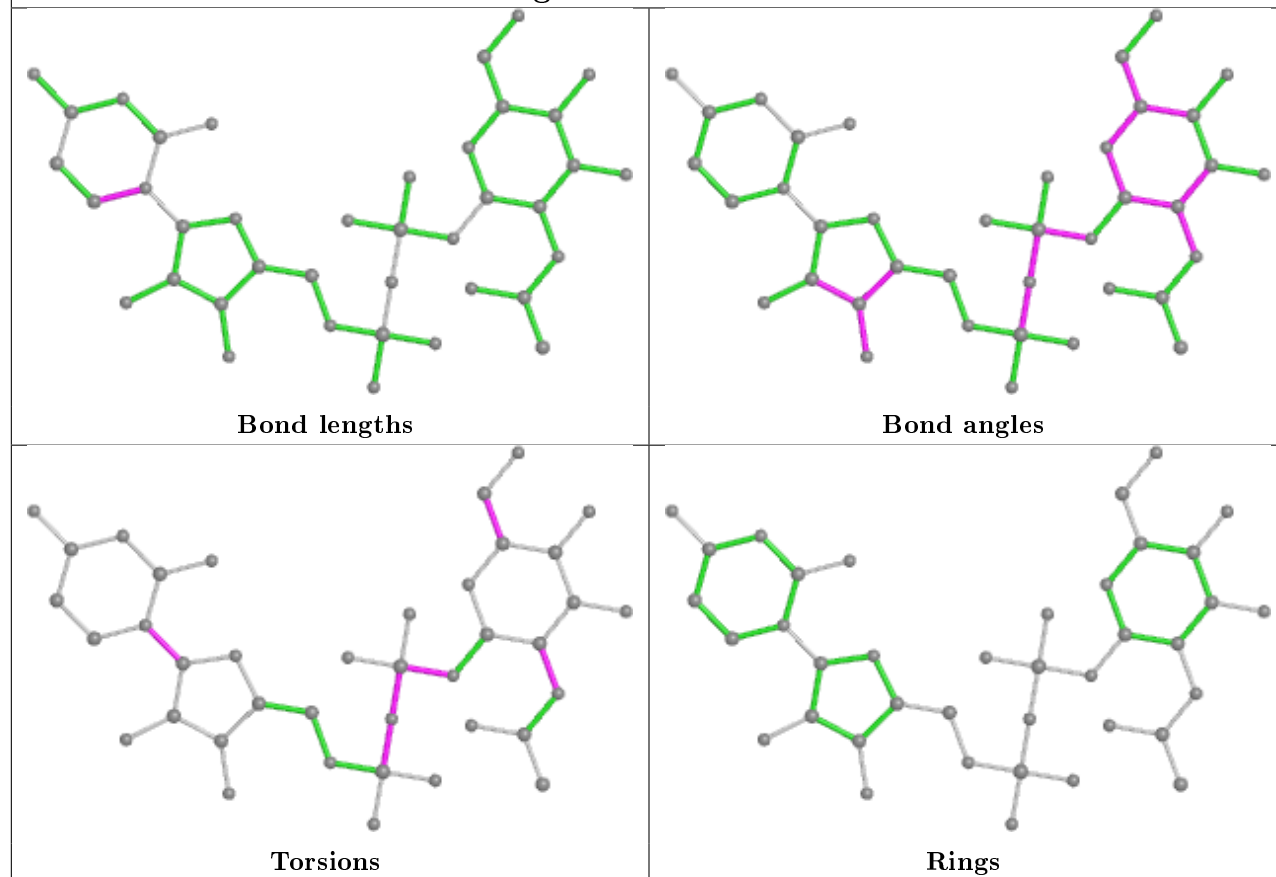


Torsions

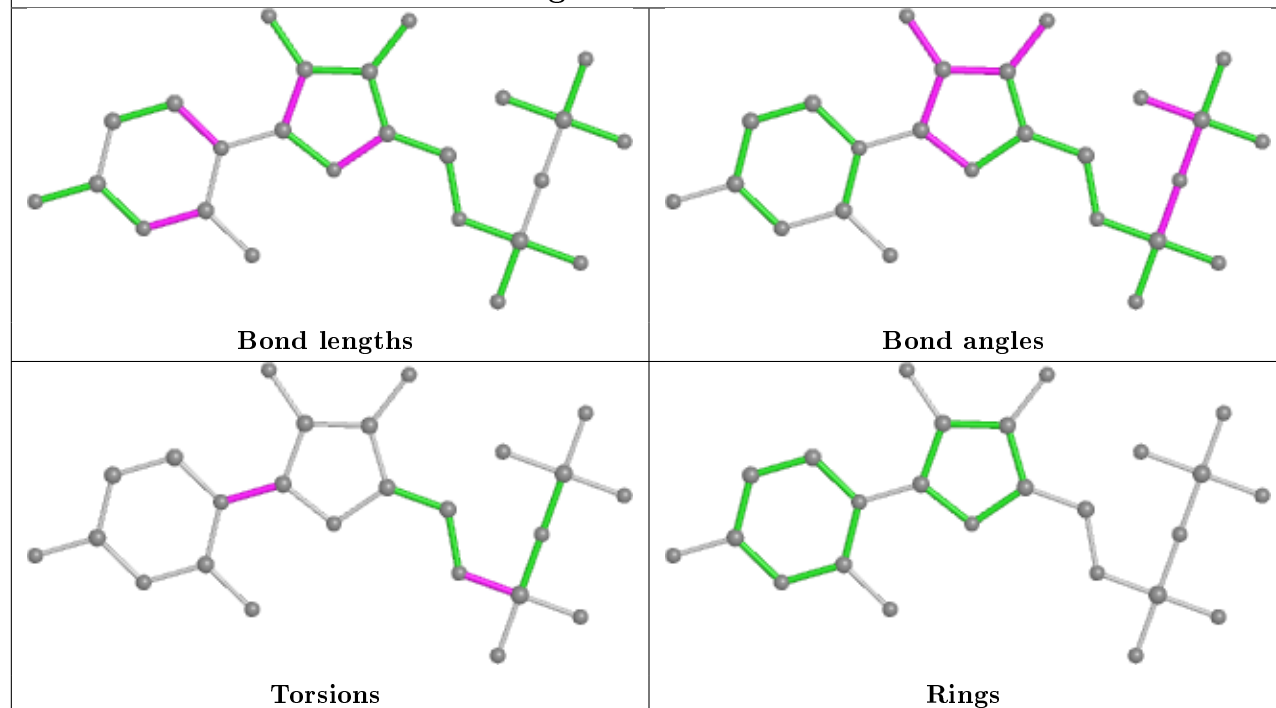


Rings

## Ligand UD2 B 683



## Ligand UDP B 1



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	601/624 (96%)	-0.46	6 (0%) 82 59	23, 49, 87, 122	22 (3%)
1	B	591/624 (94%)	-0.39	4 (0%) 87 69	23, 52, 95, 119	21 (3%)
All	All	1192/1248 (95%)	-0.43	10 (0%) 86 65	23, 50, 90, 122	43 (3%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ALA	4.6
1	A	77	ILE	3.3
1	A	60	VAL	2.9
1	B	77	ILE	2.8
1	A	61	ILE	2.8

### 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](#)

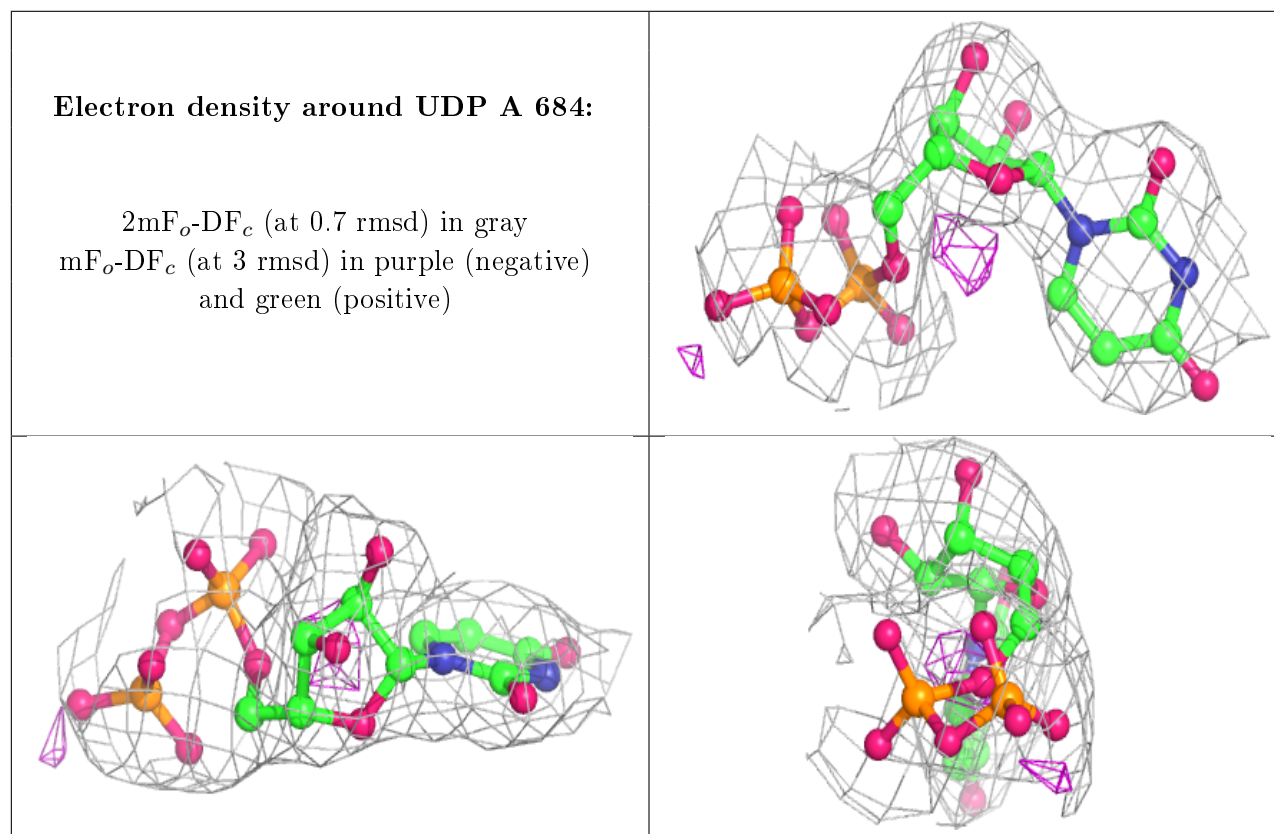
There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

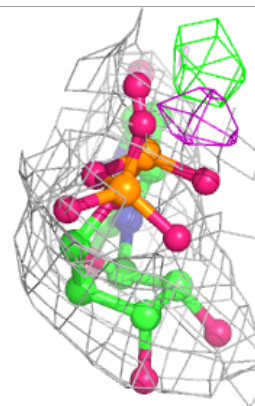
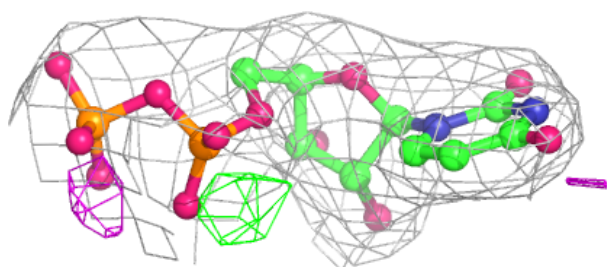
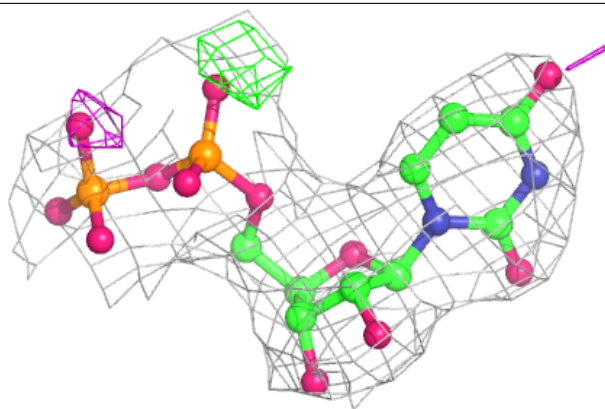
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MN	B	4	1/1	0.91	0.10	65,65,65,65	0
3	UDP	A	684	25/25	0.91	0.19	52,80,106,110	0
3	UDP	B	1	25/25	0.93	0.18	51,66,124,131	0
4	MN	A	2	1/1	0.96	0.10	62,62,62,62	0
2	UD2	A	683	39/39	0.96	0.18	29,55,99,102	0
2	UD2	B	683	39/39	0.97	0.17	29,55,72,79	0
4	MN	B	3	1/1	0.97	0.13	48,48,48,48	0
4	MN	A	1	1/1	0.99	0.13	47,47,47,47	0

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

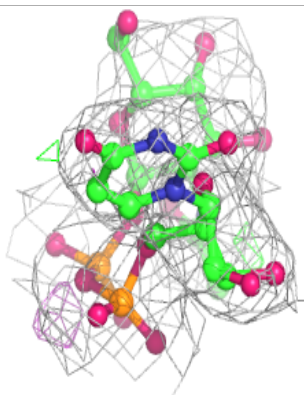
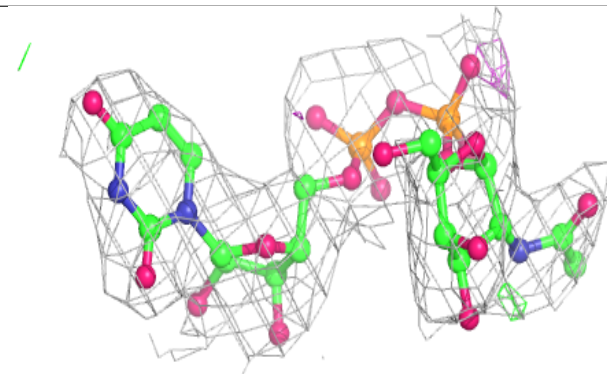
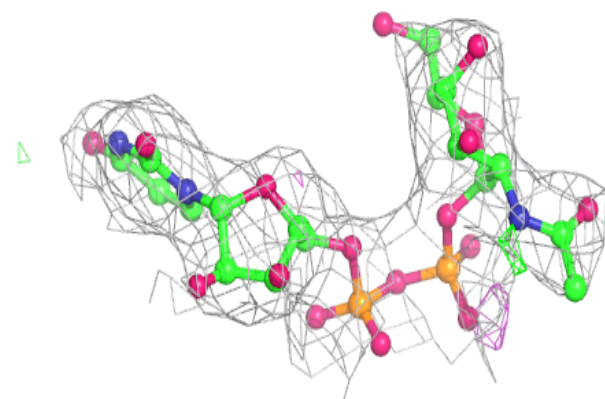


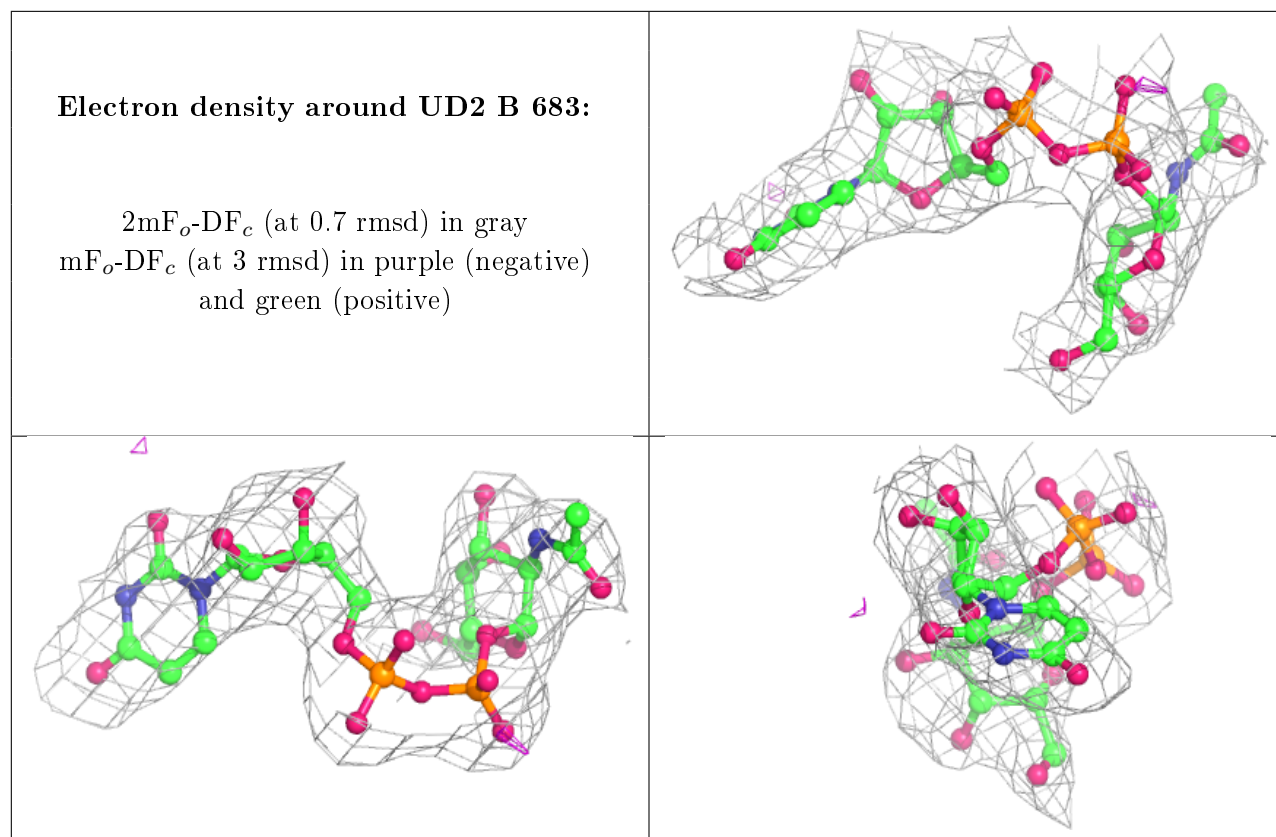
**Electron density around UDP B 1:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around UD2 A 683:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.