



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 3, 2017 – 08:36 PM EDT

PDB ID : 2V10
Title : Crystal Structure of Renin with Inhibitor 9
Authors : Rahuel, J.; Rasetti, V.; Maibaum, J.; Rueger, H.; Goschke, R.; Cohen, N.C.;
Stutz, S.; Cumin, F.; Fuhrer, W.; Wood, J.M.; Grutter, M.G.
Deposited on : unknown
Resolution : 3.10 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

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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

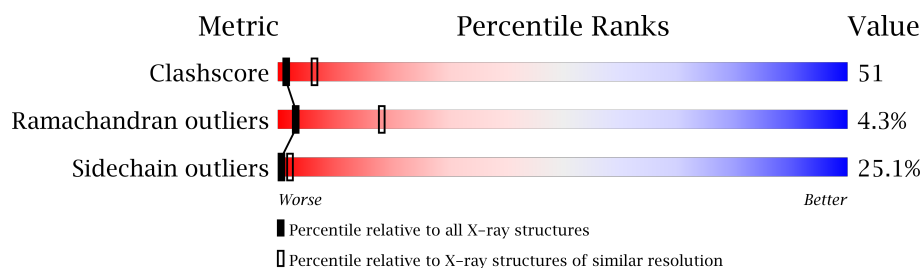
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	
1	O	340	

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
2	C61	C	1341	-	-	X	-

2 Entry composition [i](#)

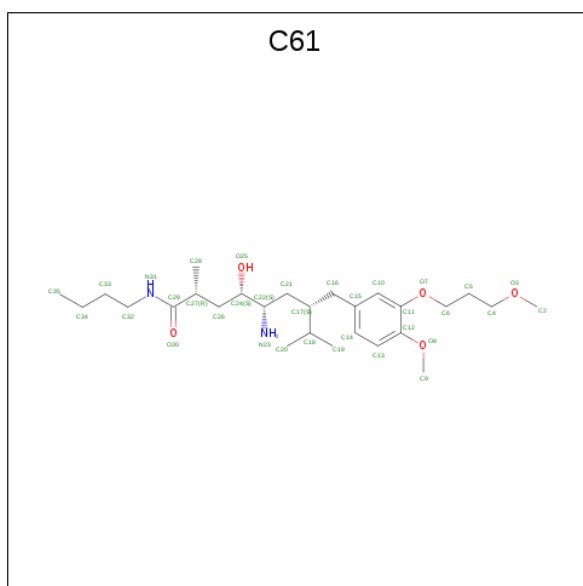
There are 2 unique types of molecules in this entry. The entry contains 5192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is (2R,4S,5S,7S)-5-AMINO-N-BUTYL-4-HYDROXY-7-[4-METHOXY-3-(3-METHOXYPROPOXY)BENZYL]-2,8-DIMETHYLNONANAMIDE (three-letter code: C61) (formula: C₂₇H₄₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			34	27	2	5		
2	O	1	Total	C	N	O	0	0
			34	27	2	5		

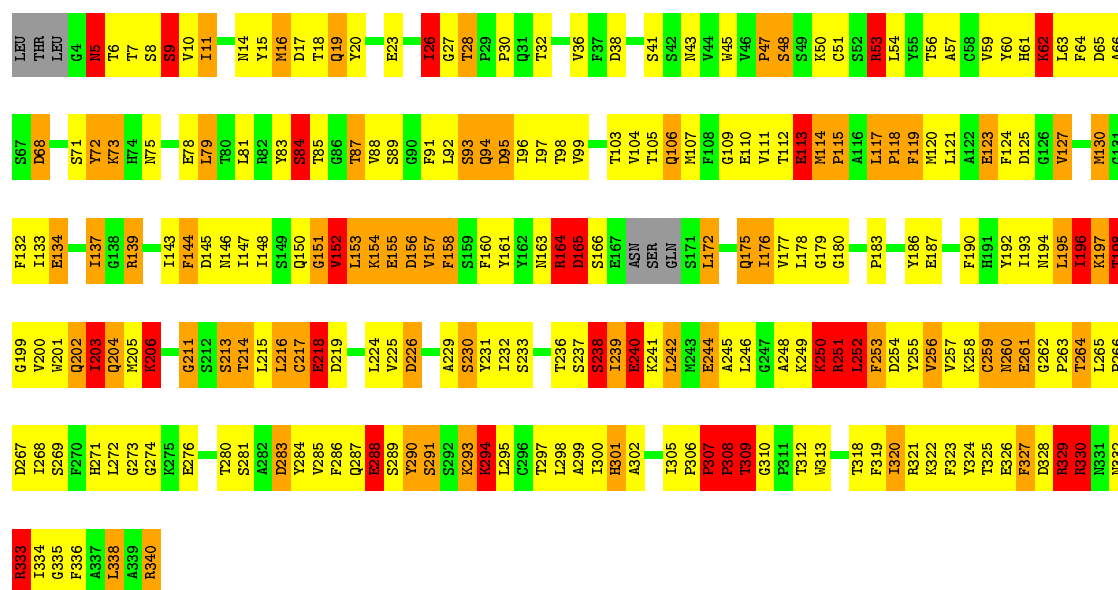
3 Residue-property plots

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.

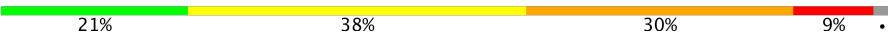
Note EDS was not executed.

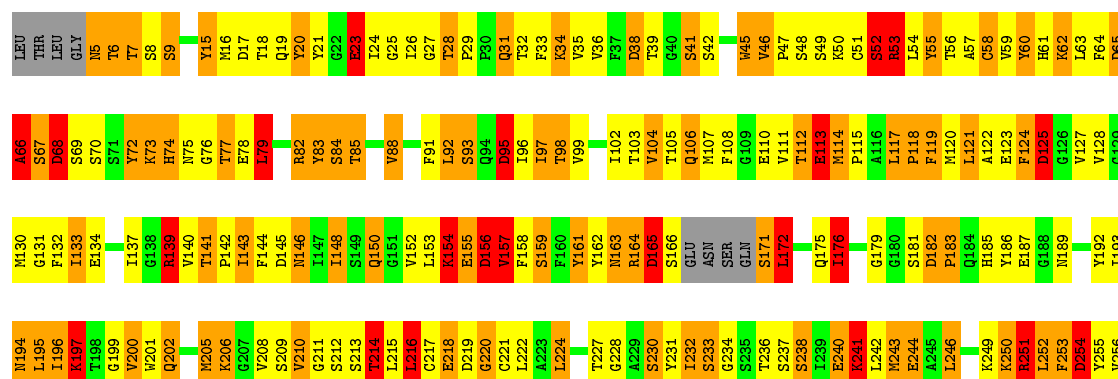
• Molecule 1: RENIN

Chain C: 



• Molecule 1: RENIN

Chain O: 



T318	T319	T320	T321	T322	T323	T324	T325	T326	T327	T328	T329	T330	T331	T332	T333	T334	T335	T336	T337	T338	T339	T340	T341	T342	T343	T344	T345	T346	T347	T348	T349	T350	T351	T352	T353	T354	T355	T356	T357	T358	T359	T360	T361	T362	T363	T364	T365	T366	T367	T368	T369	T370	T371	T372	T373	T374	T375	T376	T377	T378	T379	T380	T381	T382	T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	143.00 Å 143.00 Å 143.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5192	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C61

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	C	1.62	31/2626 (1.2%)	2.25	133/3560 (3.7%)
1	O	1.59	24/2616 (0.9%)	2.41	169/3547 (4.8%)
All	All	1.60	55/5242 (1.0%)	2.33	302/7107 (4.2%)

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	C	5	0
1	O	3	0
All	All	8	0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	251	ARG	NE-CZ	11.26	1.47	1.33
1	C	244	GLU	CD-OE2	11.00	1.37	1.25
1	O	288	GLU	CD-OE2	10.50	1.37	1.25
1	O	78	GLU	CD-OE2	9.96	1.36	1.25
1	C	218	GLU	CD-OE2	9.77	1.36	1.25

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	330	ARG	NE-CZ-NH1	14.47	127.54	120.30
1	O	164	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	C	15	TYR	CB-CG-CD2	12.78	128.66	121.00
1	C	15	TYR	CB-CG-CD1	-12.76	113.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	PHE	CB-CG-CD1	12.10	129.27	120.80

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	56	THR	CA
1	C	75	ASN	CA
1	C	203	ILE	CB
1	C	206	LYS	CA
1	C	259	CYS	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2498	241	0
1	O	2557	0	2489	282	0
2	C	34	0	48	22	0
2	O	34	0	48	9	0
All	All	5192	0	5083	524	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 51.

The worst 5 of 524 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:C:260:ASN:HD22	1:C:261:GLU:N	1.41	1.16
1:C:216:LEU:HD12	1:C:238:SER:HB3	1.28	1.11
1:O:196:ILE:HG22	1:O:197:LYS:HG2	1.14	1.09
1:C:127:VAL:HG21	2:C:1341:C61:C19	1.83	1.09
1:C:96:ILE:HG22	1:C:105:THR:HG22	1.41	1.03

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	C	330/340 (97%)	288 (87%)	31 (9%)	11 (3%)	4	25
1	O	328/340 (96%)	281 (86%)	30 (9%)	17 (5%)	2	14
All	All	658/680 (97%)	569 (86%)	61 (9%)	28 (4%)	3	18

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	196	ILE
1	C	218	GLU
1	C	251	ARG
1	C	252	LEU
1	O	66	ALA

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	C	283/290 (98%)	222 (78%)	61 (22%)	1	5
1	O	282/290 (97%)	201 (71%)	81 (29%)	0	1
All	All	565/580 (97%)	423 (75%)	142 (25%)	0	2

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	9	SER

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Mol	Chain	Res	Type
1	O	70	SER
1	O	288	GLU
1	O	23	GLU
1	O	41	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	332	ASN
1	O	61	HIS
1	O	202	GLN
1	C	301	HIS
1	O	287	GLN

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C61	C	1341	-	34,34,34	1.44	4 (11%)	37,43,43	1.84	8 (21%)
2	C61	O	1341	-	34,34,34	1.13	3 (8%)	37,43,43	2.18	8 (21%)

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	C61	C	1341	-	-	0/37/37/37	0/1/1/1
2	C61	O	1341	-	-	0/37/37/37	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1341	C61	C19-C18	-4.13	1.37	1.52
2	O	1341	C61	C14-C13	2.24	1.42	1.38
2	C	1341	C61	C28-C27	2.48	1.61	1.52
2	O	1341	C61	O7-C11	3.26	1.44	1.37
2	C	1341	C61	O7-C11	3.35	1.44	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1341	C61	C27-C26-C24	-5.72	106.81	114.32
2	O	1341	C61	C27-C26-C24	-5.29	107.38	114.32
2	O	1341	C61	C6-O7-C11	-3.91	108.17	117.70
2	C	1341	C61	C15-C16-C17	-3.59	107.66	113.77
2	C	1341	C61	C6-O7-C11	-3.29	109.69	117.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1341	C61	22	0
2	O	1341	C61	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.