



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 1EA0 / pdb_00001ea0
Title : Alpha subunit of A. brasilense glutamate synthase
Authors : Binda, C.; Bossi, R.T.; Vanoni, M.A.; Mattevi, A.
Deposited on : 2000-11-02
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

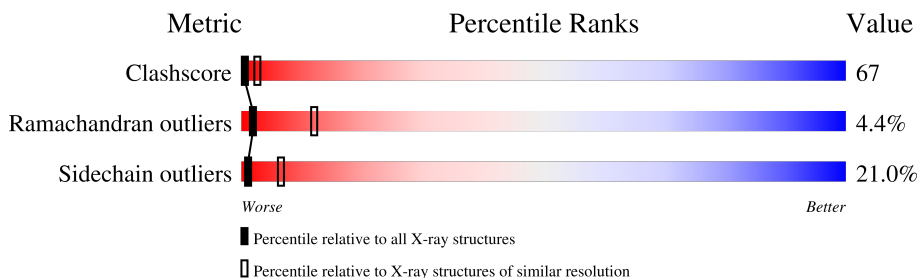
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1479	
1	B	1479	

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	OMT	A	2473	-	X	-	-
2	OMT	B	2473	-	X	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition [i](#)

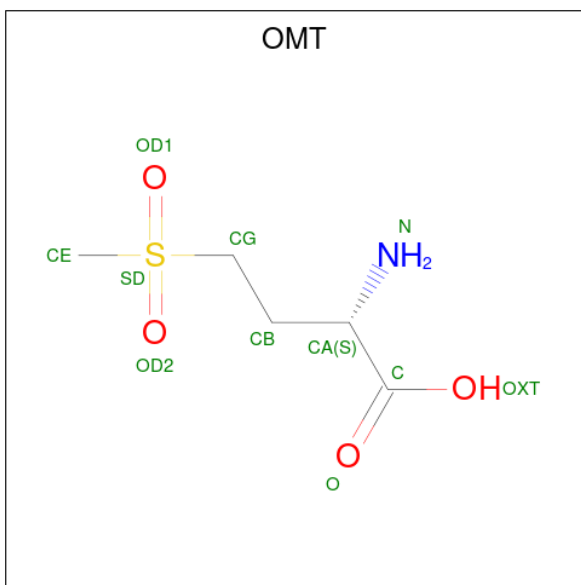
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1452	Total 11180	C 7018	N 2005	O 2098	S 59	0	0	0
1	B	1452	Total 11180	C 7018	N 2005	O 2098	S 59	0	0	0

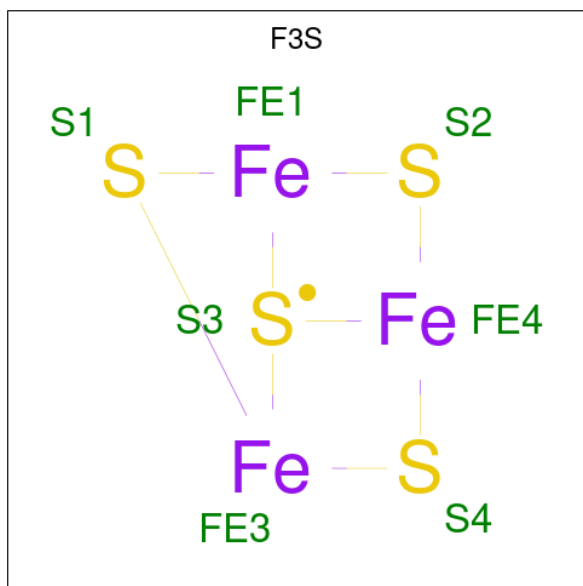
- Molecule 2 is S-DIOXYMETHIONINE (CCD ID: OMT) (formula: C₅H₁₁NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 11	C 5	N 1	O 4	S 1	0	0
2	B	1	Total 11	C 5	N 1	O 4	S 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



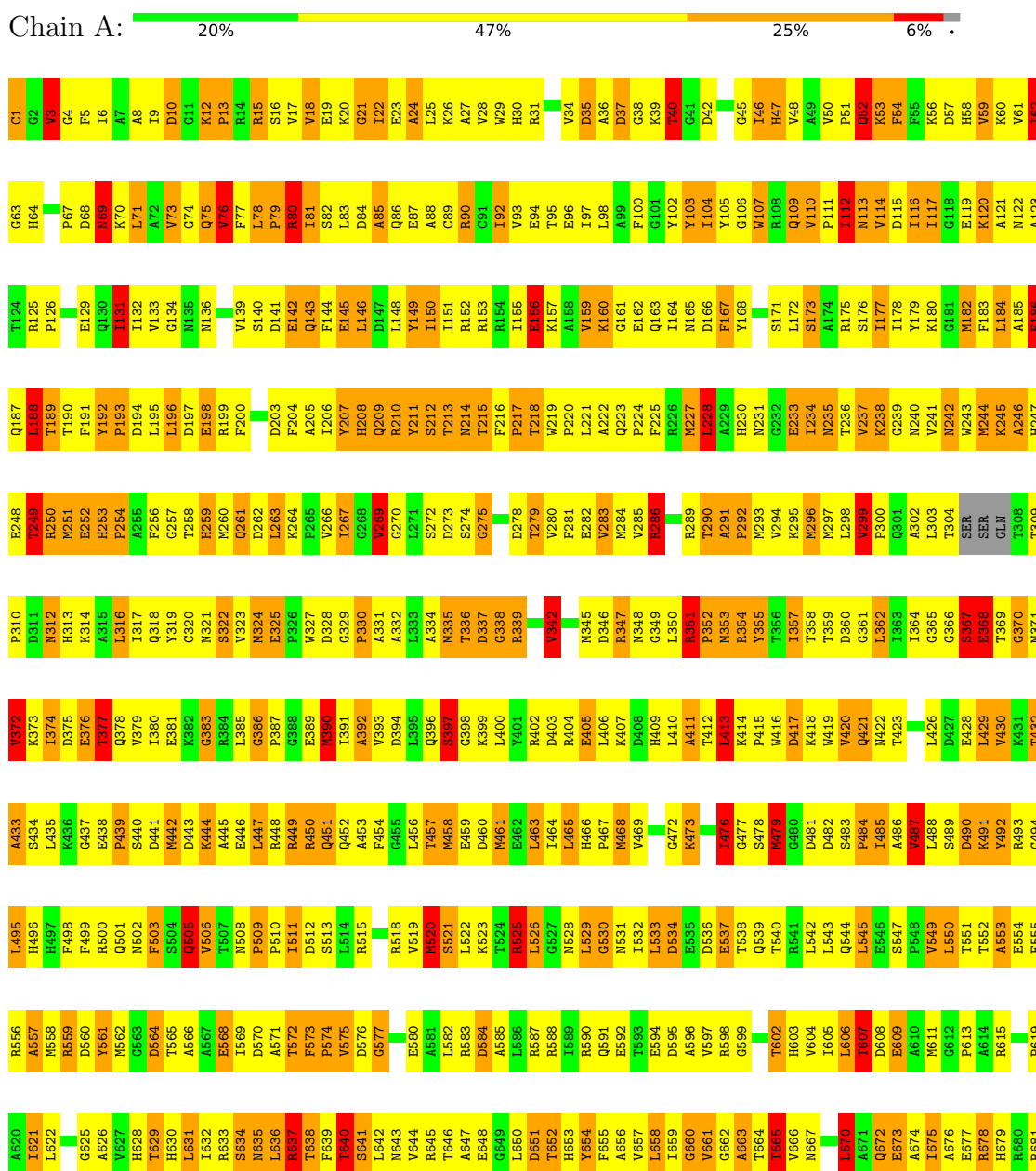
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		
5	B	1	Total	Fe	S	0	0
			7	3	4		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN



P1034	P1035	P1036	P1037	P1038	P1039	P1040	P1041	P1042	P1043	P1044	P1045	P1046	P1047	P1048	P1049	P1050	P1051	P1052	P1053	P1054	P1055	P1056	P1057	P1058	P1059	P1060	P1061	P1062	P1063	P1064	P1065	P1066	P1067	P1068	P1069	P1070	P1071	P1072	P1073	P1074	P1075	P1076	P1077	P1078	P1079	P1080	P1081	P1082	P1083	P1084	P1085	P1086	P1087	P1088	P1089	P1090	P1091	P1092	P1093	P1094	P1095																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	P1000	P1001	P1002	P1003	P1004	P1005	P1006	P1007	P1008	P1009	P1010	P1011	P1012	P1013	P1014	P1015	P1016	P1017	P1018	P1019	P1020	P1021	P1022	P1023	P1024	P1025	P1026	P1027	P1028	P1029	P1030	P1031	P1032	P1033																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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P776	P777	P778	P779	P780	P781	P782	P783	P784	P785	P786	P787	P788	P789	P790	P791	P792	P793	P794	P795	P796	P797	P798	P799	P800	P801	P802	P803	P804	P805	P806	P807	P808	P809	P810	P811	P812	P813	P814	P815	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760	P761	P762	P763	P764	P765	P766	P767	P768	P769	P770	P771	P772	P773	P774	P775																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
H466	P467	M468	V469	G470	D471	L472	E473	F474	G475	H476	I477	L478	M479	N480	O481	P482	Q483	R484	S485	T486	U487	V488	W489	X490	Y491	Z492	A493	B494	C495	D496	E497	F498	G499	H500	I501	J502	K503	L504	M505	N506	O507	P508	Q509	R510	S511	T512	U513	V514	W515	X516	Y517	Z518	A519	B520	C521	D522	E523	F524	G525	H526	I527	J528	K529	L530	M531	N532	O533	P534	Q535	R536	S537	T538	U539	V540	W541	X542	Y543	Z544	A545	B546	C547	D548	E549	F550	G551	H552	I553	J554	K555	L556	M557	N558	O559	P560	Q561	R562	S563	T564	U565	V566	W567	X568	Y569	Z570	A571	B572	C573	D574	E575	F576	G577	H578	I579	J580	K581	L582	M583	N584	O585	P586	Q587	R588	S589	T590	U591	V592	W593	X594	Y595	Z596	A597	B598	C599	D600	E601	F602	G603	H604	I605	J606	K607	L608	M609	N610	O611	P612	Q613	R614	S615	T616	U617	V618	W619	X620	Y621	Z622	A623	B624	C625	D626	E627	F628	G629	H630	I631	J632	K633	L634	M635	N636	O637	P638	Q639	R640	S641	T642	U643	V644	W645	X646	Y647	Z648	A649	B650	C651	D652	E653	F654	G655	H656	I657	J658	K659	L660	M661	N662	O663	P664	Q665	R666	S667	T668	U669	V670	W671	X672	Y673	Z674	A675	B676	C677	D678	E679	F680	G681	H682	I683	J684	K685	L686	M687	N688	O689	P690	Q691	R692	S693	T694	U695	V696	W697	X698	Y699	Z700	A701	B702	C703	D704	E705	F706	G707	H708	I709	J710	K711	L712	M713	N714	O715	P716	Q717	R718	S719	T720	U721	V722	W723	X724	Y725	Z726	A727	B728	C729	D730	E731	F732	G733	H734	I735	J736	K737	L738	M739	N740	O741	P742	Q743	R744	S745	T746	U747	V748	W749	X750	Y751	Z752	A753	B754	C755	D756	E757	F758	G759	H760	I761	J762	K763	L764	M765	N766	O767	P768	Q769	R770	S771	T772	U773	V774	W775	X776	Y777	Z778	A779	B780	C781	D782	E783	F784	G785	H786	I787	J788	K789	L790	M791	N792	O793	P794	Q795	R796	S797	T798	U799	V800	W801	X802	Y803	Z804	A805	B806	C807	D808	E809	F810	G811	H812	I813	J814	K815	L816	M817	N818	O819	P820	Q821	R822	S823	T824	U825	V826	W827	X828	Y829	Z830	A831	B832	C833	D834	E835	F836	G837	H838	I839	J840	K841	L842	M843	N844	O845	P846	Q847	R848	S849	T850	U851	V852	W853	X854	Y855	Z856	A857	B858	C859	D860	E861	F862	G863	H864	I865	J866	K867	L868	M869	N870	O871	P872	Q873	R874	S875	T876	U877	V878	W879	X880	Y881	Z882	A883	B884	C885	D886	E887	F888	G889	H890	I891	J892	K893	L894	M895	N896	O897	P898	Q899	R900	S901	T902	U903	V904	W905	X906	Y907	Z908	A909	B910	C911	D912	E913	F914	G915	H916	I917	J918	K919	L920	M921	N922	O923	P924	Q925	R926	S927	T928	U929	V930	W931	X932	Y933	Z934	A935	B936	C937	D938	E939	F940	G941	H942	I943	J944	K945	L946	M947	N948	O949	P950	Q951	R952	S953	T954	U955	V956	W957	X958	Y959	Z960	A961	B962	C963	D964	E965	F966	G967	H968	I969	J970	K971	L972	M973	N974	O975	P976	Q977	R978	S979	T980	U981	V982	W983	X984	Y985	Z986	A987	B988	C989	D990	E991	F992	G993	H994	I995	J996	K997	L998	M999	N1000	O1001	P1002	Q1003	R1004	S1005	T1006	U1007	V1008	W1009	X1010	Y1011	Z1012	A1013	B1014	C1015	D1016	E1017	F1018	G1019	H1020	I1021	J1022	K1023	L1024	M1025	N1026	O1027	P1028	Q1029	R1030	S1031	T1032	U1033	V1034	W1035	X1036	Y1037	Z1038	A1039	B1040	C1041	D1042	E1043	F1044	G1045	H1046	I1047	J1048	K1049	L1050	M1051	N1052	O1053	P1054	Q1055	R1056	S1057	T1058	U1059	V1060	W1061	X1062	Y1063	Z1064	A1065	B1066	C1067	D1068	E1069	F1070	G1071	H1072	I1073	J1074	K1075	L1076	M1077	N1078	O1079	P1080	Q1081	R1082	S1083	T1084	U1085	V1086	W1087	X1088	Y1089	Z1090	A1091	B1092	C1093	D1094	E1095	F1096	G1097	H1098	I1099	J1100	K1101	L1102	M1103	N1104	O1105	P1106	Q1107	R1108	S1109	T1110	U1111	V1112	W1113	X1114	Y1115	Z1116	A1117	B1118	C1119	D1120	E1121	F1122	G1123	H1124	I1125	J1126	K1127	L1128	M1129	N1130	O1131	P1132	Q1133	R1134	S1135	T1136	U1137	V1138	W1139	X1140	Y1141	Z1142	A1143	B1144	C1145	D1146	E1147	F1148	G1149	H1150	I1151	J1152	K1153	L1154	M1155	N1156	O1157	P1158	Q1159	R1160	S1161	T1162	U1163	V1164	W1165	X1166	Y1167	Z1168	A1169	B1170	C1171	D1172	E1173	F1174	G1175	H1176	I1177	J1178	K1179	L1180	M1181	N1182	O1183	P1184	Q1185	R1186	S1187	T1188	U1189	V1190	W1191	X1192	Y1193	Z1194	A1195	B1196	C1197	D1198	E1199	F1200	G1201	H1202	I1203	J1204	K1205	L1206	M1207	N1208	O1209	P1210	Q1211	R1212	S1213	T1214	U1215	V1216	W1217	X1218	Y1219	Z1220	A1221	B1222	C1223	D1224	E1225	F1226	G1227	H1228	I1229	J1230	K1231	L1232	M1233	N1234	O1235	P1236	Q1237	R1238	S1239	T1240	U1241	V1242	W1243	X1244	Y1245	Z1246	A1247	B1248	C1249	D1250	E1251	F1252	G1253	H1254	I1255	J1256	K1257	L1258	M1259	N1260	O1261	P1262	Q1263	R1264	S1265	T1266	U1267	V1268	W1269	X1270	Y1271	Z1272	A1273	B1274	C1275	D1276	E1277	F1278	G1279	H1280	I1281	J1282	K1283	L1284	M1285	N1286	O1287	P1288	Q1289	R1290	S1291	T1292	U1293	V1294	W1295	X1296	Y1297	Z1298	A1299	B1300	C1301	D1302	E1303	F1304	G1305	H1306	I1307	J1308	K1309	L1310	M1311	N1312	O1313	P1314	Q1315	R1316	S1317	T1318	U1319	V1320	W1321	X1322	Y1323	Z1324	A1325	B1326	C1327	D1328	E1329	F1330	G1331	H1332	I1333	J1334	K1335	L1336	M1337	N1338	O1339	P1340	Q1341	R1342	S1343	T1344	U1345	V1346	W1347	X1348	Y1349	Z1350	A1351	B1352	C

D1446	W1447	A1448	R1449	E1450	V1451	T1452	K1453	F1454	W1455	P1459	K1460	E1461	M1462	L1463	N1464	R1465	L1466	E1467	V1468	P1469	V1470	H1471	L1472	PRO	LYS	ALA	ILE	SER	ALA	GLU																												
V1379	G1380	D1381	M1382	F1383	A1384	A1385	G1386	M1387	T1388	G1389	G1390	Y1393	V1394	Y1395	D1396	L1397	D1398	D1399	S1400	L1401	P1402	I1405	M1406	D1407	E1408	A1409	V1410	I1411	F1412	Q1413	R1414	V1417	G1418	H1419	Y1420	E1421	S1422	Q1423	L1424	K1425	H1426	L1427	I1428	E1429	E1430	H1431	V1432	T1433	E1434	T1435	Q1436	S1437	R1438	F1439	I1440	A1441		
S1301	G1302	R1308	F1309	T1310	T1311	E1316	T1317	M1318	I1322	I1323	G1324	M1325	T1326	V1327	L1328	Y1329	G1334	K1335	L1336	F1337	A1338	A1339	G1340	Q1341	A1342	G1343	E1344	F1345	F1346	A1347	V1348	R1349	M1350	T1354	V1355	V1356	V1357	E1358	G1359	C1360	E1366	Y1367	M1368	T1369	G1370	G1371	T1372	A1373	V1374	I1375	L1376	K1298						
D1218	A1219	R1220	P1221	L1222	R1229	Y1233	R1236	N1237	T1238	Q1239	R1240	G1243	T1244	R1245	L1246	S1247	S1248	M1249	V1250	T1251	R1252	K1253	M1256	F1257	G1258	L1259	Q1260	P1261	I1264	T1265	L1268	R1269	G1270	T1271	Q1274	G1277	A1278	F1279	A1280	V1281	Q1282	M1289	D1291	A1292	N1293	D1294	K1298											
S1096	L1097	I1098	A1099	M1100	G1101	C1102	I1103	M1104	V1105	R1106	Q1107	C1108	H1109	S1110	M1111	C1112	C1113	P1114	V1115	G1116	V1117	C1118	V1119	Q1120	D1121	D1122	M1123	L1124	R1125	Q1126	K1127	F1128	V1129	G1130	T1131	P1132	E1133	K1134	V1135	V1136	M1137	L1138	F1139	T1140	F1141	L1142	A1143	E1144	E1145	V1146	R1147	E1148	A1151	G1152	L1153	G1154	F1155	R1156
S1157	L1158	M1159	A1160	V1161	I1162	G1163	R1164	T1165	D1166	L1167	L1168	H1169	Q1170	V1171	SER	ARG	GLY	ALA	GLU	HIS	LEU	ASP	D1180	L1181	D1182	L1183	M1184	P1185	R1186	L1187	V1190	F1191	P1192	G1193	GLU	ASN	ALA	ARG	TYR	CYS	THR	LEU	GLN	G1203	R1204	N1205	E1206	V1207	P1208	D1209	T1210	L1211	D1212	A1213	R1214	I1215	V1216	A1217

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.61Å 233.61Å 305.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.6 (20.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.256 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22478	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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: AKG, FMN, F3S, OMT

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	1.44	81/11383 (0.7%)	2.01	407/15390 (2.6%)
1	B	1.49	93/11383 (0.8%)	1.99	404/15390 (2.6%)
All	All	1.47	174/22766 (0.8%)	2.00	811/30780 (2.6%)

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	1	2
1	B	0	2
All	All	1	4

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-18.76	1.38	1.55
1	A	746	ILE	CA-CB	-12.96	1.37	1.54
1	A	848	ALA	CA-CB	-9.35	1.38	1.53
1	A	849	ILE	CA-CB	-9.22	1.43	1.54
1	B	1289	MET	SD-CE	9.03	2.02	1.79

The worst 5 of 811 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	888	GLY	N-CA-C	-18.23	83.89	110.88
1	B	671	ALA	N-CA-C	-15.81	96.60	114.62
1	A	672	GLN	N-CA-C	-15.18	94.81	111.36
1	B	337	ASP	N-CA-C	-14.54	88.66	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	GLN	CA-C-N	-14.14	104.75	121.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

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	A	11180	0	11210	1601	0
1	B	11180	0	11212	1396	0
2	A	11	0	10	3	0
2	B	11	0	10	2	0
3	A	31	0	19	5	0
3	B	31	0	19	7	0
4	A	10	0	4	0	0
4	B	10	0	4	3	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
All	All	22478	0	22488	2997	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 67.

The worst 5 of 2997 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:182:MET:CE	1:B:217:PRO:HB2	1.30	1.59
1:A:875:MET:HE1	1:A:1139:PHE:CE2	1.35	1.58
1:B:1449:ARG:HH11	1:B:1449:ARG:CB	0.97	1.56
1:A:182:MET:HE3	1:A:217:PRO:CB	1.18	1.54
1:B:182:MET:HE3	1:B:217:PRO:CB	1.01	1.49

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	1444/1479 (98%)	1152 (80%)	227 (16%)	65 (4%)	2	12
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2	12
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2	12

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY

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	1184/1206 (98%)	933 (79%)	251 (21%)	1	6
1	B	1184/1206 (98%)	938 (79%)	246 (21%)	1	7
All	All	2368/2412 (98%)	1871 (79%)	497 (21%)	1	6

5 of 497 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1388	THR
1	B	1145	GLU
1	B	249	THR
1	B	1122	ASP
1	B	1349	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	452	GLN
1	B	1035	GLN
1	B	505	GLN
1	B	762	HIS
1	B	1274	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
4	AKG	B	2475	-	9,9,9	3.58	4 (44%)	11,11,11	2.77	4 (36%)
2	OMT	B	2473	-	9,10,10	4.56	5 (55%)	9,14,14	6.31	5 (55%)
3	FMN	B	2474	-	33,33,33	1.38	4 (12%)	48,50,50	2.69	20 (41%)
3	FMN	A	2474	-	33,33,33	1.49	5 (15%)	48,50,50	2.80	18 (37%)
2	OMT	A	2473	-	9,10,10	4.70	5 (55%)	9,14,14	5.25	6 (66%)
4	AKG	A	2475	-	9,9,9	3.16	4 (44%)	11,11,11	2.99	4 (36%)
5	F3S	B	2476	1	0,9,9	-	-	-	-	-
5	F3S	A	2476	1	0,9,9	-	-	-	-	-

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
4	AKG	B	2475	-	-	1/9/9/9	-
2	OMT	B	2473	-	-	5/10/10/10	-
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
3	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
2	OMT	A	2473	-	-	4/10/10/10	-
4	AKG	A	2475	-	-	2/9/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2473	OMT	CB-CG	-7.95	1.45	1.52
2	B	2473	OMT	CG-SD	-7.13	1.69	1.78
2	A	2473	OMT	CG-SD	-6.93	1.69	1.78
2	B	2473	OMT	CB-CG	-6.84	1.46	1.52
2	B	2473	OMT	OD1-SD	6.68	1.57	1.44

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2473	OMT	OD2-SD-CG	-16.19	96.65	108.33
2	A	2473	OMT	OD2-SD-CE	-12.57	97.19	108.87
3	B	2474	FMN	C4'-C3'-C2'	-8.97	98.65	113.57
3	A	2474	FMN	O5'-P-O1P	-8.15	84.41	106.44
4	B	2475	AKG	C4-C3-C2	-7.61	98.63	112.91

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

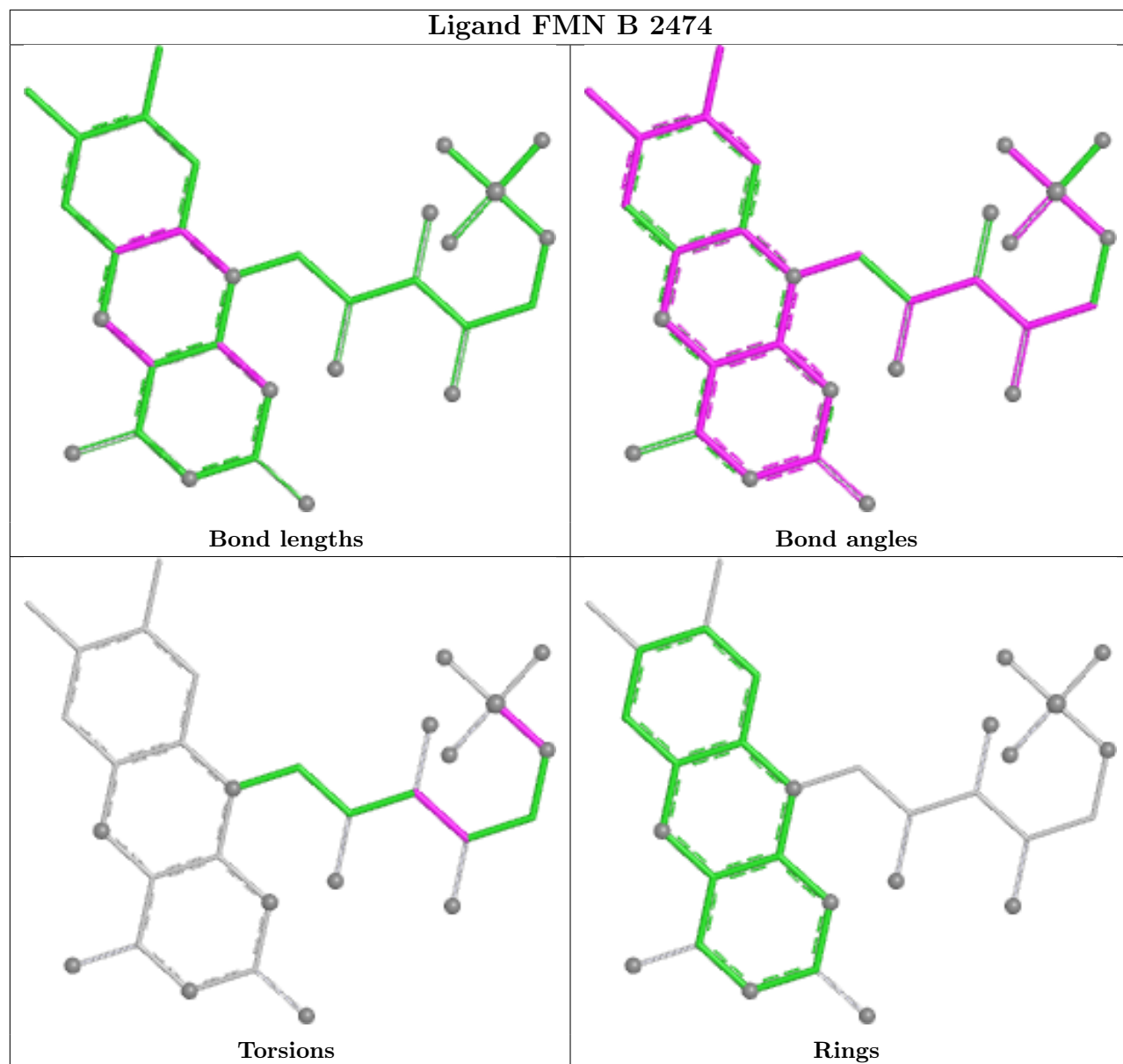
Mol	Chain	Res	Type	Atoms
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2
2	B	2473	OMT	N-CA-CB-CG
2	B	2473	OMT	C-CA-CB-CG

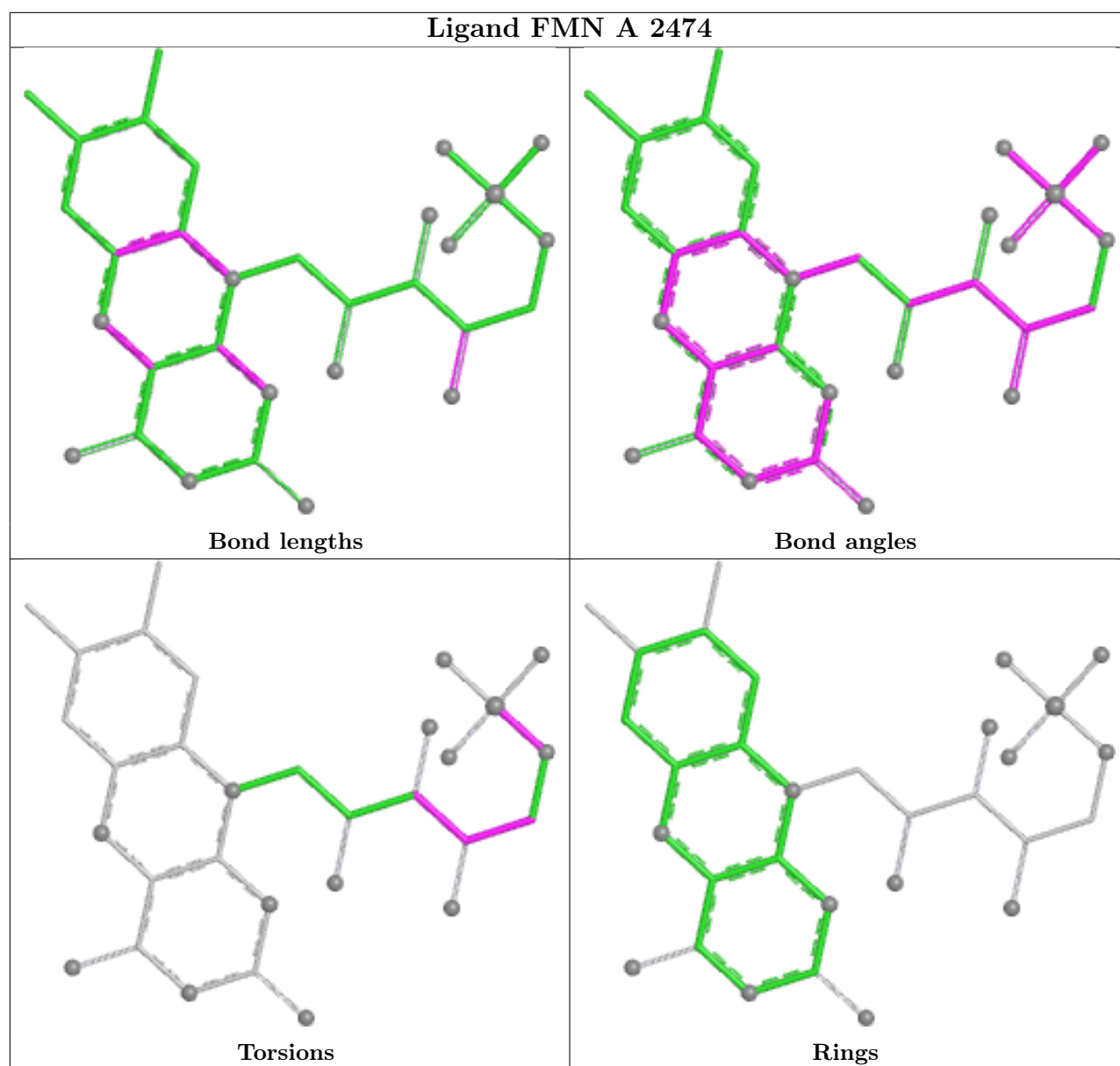
There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2475	AKG	3	0
2	B	2473	OMT	2	0
3	B	2474	FMN	7	0
3	A	2474	FMN	5	0
2	A	2473	OMT	3	0
5	B	2476	F3S	3	0
5	A	2476	F3S	2	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.





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.