



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:58 am BST

PDB ID : 1EA0
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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

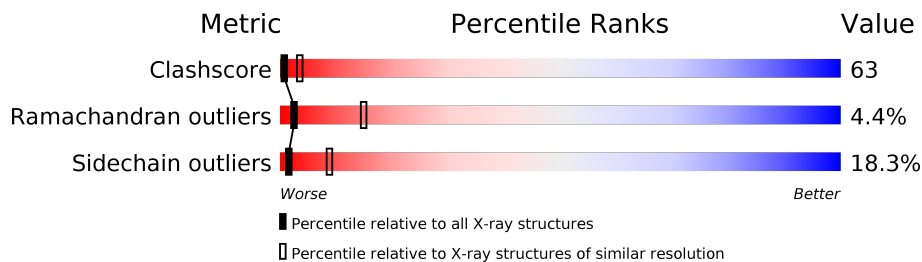
1 Overall quality at a glance

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 ≥ 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	-	-
5	F3S	A	2476	-	-	X	-
5	F3S	B	2476	-	-	X	-

2 Entry composition [i](#)

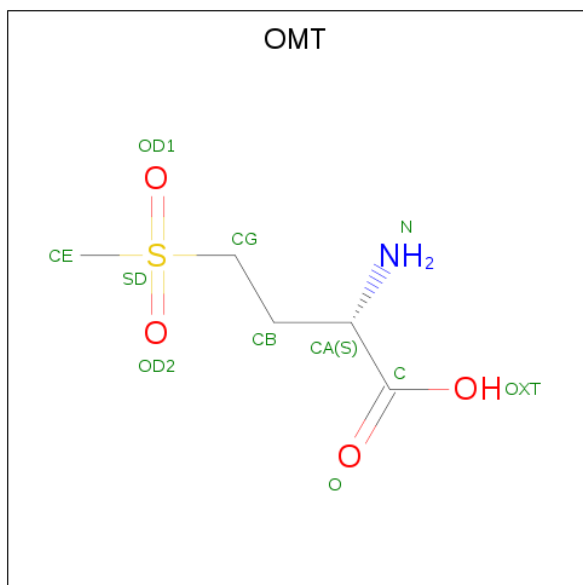
There are 5 unique types of molecules in this entry. The entry contains 22478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	11180	7018	2005	2098	59	0	0	0
1	B	1452	11180	7018	2005	2098	59	0	0	0

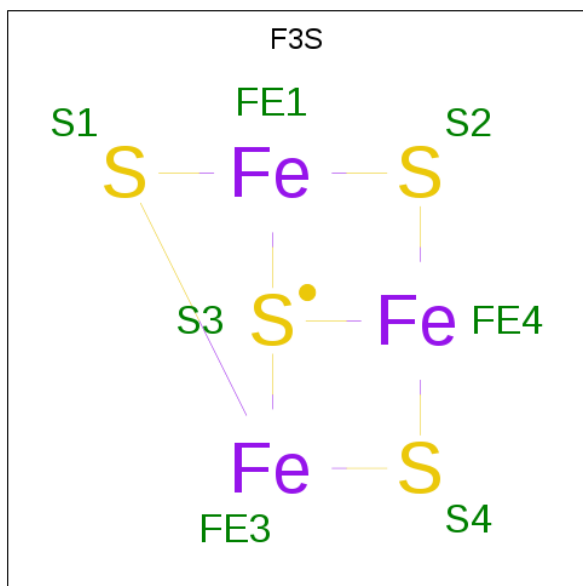
- Molecule 2 is S-DIOXYMETHIONINE (three-letter code: OMT) (formula: C₅H₁₁NO₄S).



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

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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		

S1157	F1090	A1018	A954	R820	K756	L689	H628	D564	Q501	P439	G366	V327	H230	V159
L1198	G1091	L1022	A955	F821	K757	E690	T629	T565	H502	S440	S367	L298	M251	L169
M1189	I1092	L1022	R956	F822	K758	E691	H630	T566	F503	D441	E368	G232	E162	E163
E1160	G1093	M1026	R957	R823	L759	G692	L631	E568	S504	M442	T369	E233	Q163	Q164
V1162	T1094	M1026	R958	O824	G760	M693	L632	I569	Q505	D443	I234	E234	M235	M165
G1163	A1095	M1026	S959	L825	E761	A694	R633	D570	M508	K444	I374	I235	M236	D166
L1164	S1096	T1030	T960	R826	H762	M695	S634	A571	P509	A445	D375	T236	V237	
L1164	L1097	G1031	R827	R827	A763	V696	M635	T572	P510	E446	E376	V237	V237	
R1165	C1102	A1032	L828	L828	T764	F697	L636	F573	P510	L447	T377	K238	K238	S171
L1166	S1033	M964	A765	A765	P574	K698	R637	R448	GLN	R448	Q378	G239	G239	L172
L1168	P1034	P1034	R830	R830	Y766	A699	T638	V575	D512	T308	V379	M240	M240	S173
L1169	F894	I966	I966	I966	N767	I700	F639	D576	S513	R450	I360	V241	V241	A174
Q1170	D897	R867	R867	R867	E768	D701	T640	G577	E381	Q451	E381	M242	M242	R175
V1171	R898	S833	S833	S833	E769	D702	S641	R515	R515	Q452	Q452	W243	W243	S176
S1172	R899	T834	T834	T834	V770	G703	L642	E580	R518	A453	K245	M244	M244	I177
S1173	R899	K635	K635	K635	L773	L704	M643	A581	R518	R313	K245	M244	M244	
S1174	R899	L704	L704	L704	L773	L704	M643	A581	R518	R313	K245	M244	M244	
S1175	R899	L705	L705	L705	L773	L705	M643	A581	R518	R313	K245	M244	M244	
S1176	R899	K706	K706	K706	L773	L706	M643	A581	R518	R313	K245	M244	M244	
S1177	R899	L707	L707	L707	L773	L707	M643	A581	R518	R313	K245	M244	M244	
S1178	R899	L707	L707	L707	L773	L707	M643	A581	R518	R313	K245	M244	M244	
S1179	R899	K710	K710	K710	L773	L710	M643	A581	R518	R313	K245	M244	M244	
S1180	R899	S714	S714	S714	L773	L714	M643	A581	R518	R313	K245	M244	M244	
S1181	R899	S717	S717	S717	L773	L717	M643	A581	R518	R313	K245	M244	M244	
S1182	R899	S718	S718	S718	L773	L718	M643	A581	R518	R313	K245	M244	M244	
S1183	R899	S719	S719	S719	L773	L719	M643	A581	R518	R313	K245	M244	M244	
S1184	R899	R720	R720	R720	L773	L720	M643	A581	R518	R313	K245	M244	M244	
S1185	R899	R721	R721	R721	L773	L721	M643	A581	R518	R313	K245	M244	M244	
S1186	R899	G722	G722	G722	L773	L722	M643	A581	R518	R313	K245	M244	M244	
S1187	R899	F725	F725	F725	L773	L725	M643	A581	R518	R313	K245	M244	M244	
S1188	R899	E726	E726	E726	L773	L726	M643	A581	R518	R313	K245	M244	M244	
S1189	R899	A727	A727	A727	L773	L727	M643	A581	R518	R313	K245	M244	M244	
S1190	R899	L730	L730	L730	L773	L730	M643	A581	R518	R313	K245	M244	M244	
S1191	R899	S731	S731	S731	L773	L731	M643	A581	R518	R313	K245	M244	M244	
S1192	R899	R732	R732	R732	L773	L732	M643	A581	R518	R313	K245	M244	M244	
S1193	R899	L733	L733	L733	L773	L733	M643	A581	R518	R313	K245	M244	M244	
S1194	R899	L734	L734	L734	L773	L734	M643	A581	R518	R313	K245	M244	M244	
S1195	R899	V735	V735	V735	L773	L735	M643	A581	R518	R313	K245	M244	M244	
S1196	R899	H738	H738	H738	L773	L738	M643	A581	R518	R313	K245	M244	M244	
S1197	R899	F739	F739	F739	L773	L739	M643	A581	R518	R313	K245	M244	M244	
S1198	R899	R694	R694	R694	L773	L694	M643	A581	R518	R313	K245	M244	M244	
S1199	R899	D805	D805	D805	L773	L805	M643	A581	R518	R313	K245	M244	M244	
S1200	R899	S806	S806	S806	L773	L806	M643	A581	R518	R313	K245	M244	M244	
S1201	R899	Y807	Y807	Y807	L773	L807	M643	A581	R518	R313	K245	M244	M244	
S1202	R899	T808	T808	T808	L773	L808	M643	A581	R518	R313	K245	M244	M244	
S1203	R899	T809	T809	T809	L773	L809	M643	A581	R518	R313	K245	M244	M244	
S1204	R899	F810	F810	F810	L773	L810	M643	A581	R518	R313	K245	M244	M244	
S1205	R899	R811	R811	R811	L773	L811	M643	A581	R518	R313	K245	M244	M244	
S1206	R899	R812	R812	R812	L773	L812	M643	A581	R518	R313	K245	M244	M244	
S1207	R899	Y813	Y813	Y813	L773	L813	M643	A581	R518	R313	K245	M244	M244	
S1208	R899	S814	S814	S814	L773	L814	M643	A581	R518	R313	K245	M244	M244	
S1209	R899	R815	R815	R815	L773	L815	M643	A581	R518	R313	K245	M244	M244	
S1210	R899	R816	R816	R816	L773	L816	M643	A581	R518	R313	K245	M244	M244	
S1211	R899	R817	R817	R817	L773	L817	M643	A581	R518	R313	K245	M244	M244	
S1212	R899	R818	R818	R818	L773	L818	M643	A581	R518	R313	K245	M244	M244	
S1213	R899	R819	R819	R819	L773	L819	M643	A581	R518	R313	K245	M244	M244	
S1214	R899	R820	R820	R820	L773	L820	M643	A581	R518	R313	K245	M244	M244	
S1215	R899	R821	R821	R821	L773	L821	M643	A581	R518	R313	K245	M244	M244	
S1216	R899	R822	R822	R822	L773	L822	M643	A581	R518	R313	K245	M244	M244	
S1217	R899	R823	R823	R823	L773	L823	M643	A581	R518	R313	K245	M244	M244	
S1218	R899	R824	R824	R824	L773	L824	M643	A581	R518	R313	K245	M244	M244	
S1219	R899	R825	R825	R825	L773	L825	M643	A581	R518	R313	K245	M244	M244	
S1220	R899	R826	R826	R826	L773	L826	M643	A581	R518	R313	K245	M244	M244	
S1221	R899	R827	R827	R827	L773	L827	M643	A581	R518	R313	K245	M244	M244	
S1222	R899	R828	R828	R828	L773	L828	M643	A581	R518	R313	K245	M244	M244	
S1223	R899	R829	R829	R829	L773	L829	M643	A581	R518	R313	K245	M244	M244	
S1224	R899	R830	R830	R830	L773	L830	M643	A581	R518	R313	K245	M244	M244	
S1225	R899	R831	R831	R831	L773	L831	M643	A581	R518	R313	K245	M244	M244	
S1226	R899	R832	R832	R832	L773	L832	M643	A581	R518	R313	K245	M244	M244	
S1227	R899	R833	R833	R833	L773	L833	M643	A581	R518	R313	K245	M244	M244	
S1228	R899	R834	R834	R834	L773	L834	M643	A581	R518	R313	K245	M244	M244	
S1229	R899	R835	R835	R835	L773	L835	M643	A581	R518	R313	K245	M244	M244	
S1230	R899	R836	R836	R836	L773	L836	M643	A581	R518	R313	K245	M244	M244	
S1231	R899	R837	R837	R837	L773	L837	M643	A581	R518	R313	K245	M244	M244	
S1232	R899	R838	R838	R838	L773	L838	M643	A581	R518	R313	K245	M244	M244	
S1233	R899	R839	R839	R839	L773	L839	M643	A581	R518	R313	K245	M244	M244	
S1234	R899	R840	R840	R840	L773	L840	M643	A581	R518	R313	K245	M244	M244	
S1235	R899	R841	R841	R841	L773	L841	M643	A581	R518	R313	K245	M244	M244	
S1236	R899	R842	R842	R842	L773	L842	M643	A581	R518	R313	K245	M244	M244	
S1237	R899	R843	R843	R843	L773	L843	M643	A581	R518	R313	K245	M244	M244	
S1238	R899	R844	R844	R844	L773	L844	M643	A581	R518	R313	K245	M244	M244	
S1239	R899	R845	R845	R845	L773	L845	M643	A581	R518	R313	K245	M244	M244	
S1240	R899	R846	R846	R846	L773	L846	M643	A581	R518	R313	K245	M244	M244	
S1241	R899	R847	R847	R847	L773	L847	M643	A581	R518	R313	K245	M244	M244	
S1242	R899	R848	R848	R848	L773	L848	M643	A581	R518	R313	K245	M244	M244	
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S1244	R899	R850	R850	R850	L773	L850	M643	A581	R518	R313	K245	M244	M244	
S1245	R899	R851	R851	R851	L773	L851	M643	A581	R518	R313	K245	M244	M244	
S1246	R899	R852	R852	R852	L773	L852	M643	A581	R518	R313	K245	M244	M244	
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S1255	R899	R861	R861	R861	L773	L861	M643	A581	R518	R313	K245	M244	M244	
S1256	R899	R862	R862	R862	L773	L862	M643	A581	R518	R313	K245	M244	M244	
S1257	R899	R863	R863	R863	L773	L863	M643</							

A1219	E1309	G1389	P1469
R1220	T1310	G1390	K1460
P1221	T1311	Y1393	E1461
L1222	E1316	Y1394	M1462
M1229	T1317	Y1395	L1463
Q1230	M1318	D1396	E1464
Y1233	L1397	L1397	R1466
R1236	I1322	D1398	L1466
M1237	I1323	D1399	L1466
T1238	G1324	S1400	V1468
Q1239	M1325	L1401	P1469
R1240	V1327	P1402	V1470
G1243	L1328	I1405	H1471
T1244	Y1329	M1406	L1472
R1245	K1335	D1407	PRO
L1246	L1336	E1408	LYS
S1247	F1337	S1409	ALA
S1248	A1338	V1410	ILE
M1249	A1339	I1411	SER
V1250	G1340	F1412	ALA
T1251	E1344	Q1413	GLU
R1252	R1345	R1414	
K1253	E1345	V1417	
M1256	F1346	G1418	
L1259	A1347	H1419	
Q1260	V1348	Y1420	
P1261	R1349	E1421	
I1264	T1354	S1422	
L1268	V1356	Q1423	
R1269	V1357	L1424	
Q1274	E1358	K1425	
A1278	G1359	H1426	
F1279	C1360	L1427	
A1280	E1366	I1428	
V1281	Y1367	E1429	
Q1282	M1368	E1430	
M1289	T1369	H1431	
G1290	G1370	V1432	
D1291	G1371	T1433	
A1292	G1372	E1434	
M1293	T1373	T1435	
D1294	A1374	Q1436	
K1298	V1375	S1437	
S1301	L1376	R1438	
G1302	I1375	F1439	
R1308	L1376	A1440	
	A1384	A1441	
	M1387	V1447	
	T1388	W1447	
		G1380	
		A1448	
		R1449	
		E1450	
		V1451	
		T1452	
		K1453	
		F1454	
		V1455	

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: FMN, F3S, AKG, 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	1.06	7/11383 (0.1%)	1.58	198/15390 (1.3%)
1	B	1.10	7/11383 (0.1%)	1.58	192/15390 (1.2%)
All	All	1.08	14/22766 (0.1%)	1.58	390/30780 (1.3%)

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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	838	VAL	CA-CB	-7.71	1.38	1.54
1	A	746	ILE	CA-CB	-7.47	1.37	1.54
1	A	848	ALA	CA-CB	-6.51	1.38	1.52
1	A	1065	VAL	CB-CG2	-6.15	1.40	1.52
1	A	3	VAL	CA-CB	-5.67	1.42	1.54

The worst 5 of 390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1062	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	A	608	ASP	CB-CG-OD2	12.18	129.26	118.30
1	A	141	ASP	CB-CG-OD2	11.98	129.08	118.30
1	B	888	GLY	N-CA-C	-11.68	83.89	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	ASP	CB-CG-OD1	11.31	128.48	118.30

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	1498	0
1	B	11180	0	11212	1318	0
2	A	11	0	10	2	0
2	B	11	0	10	1	0
3	A	31	0	19	4	0
3	B	31	0	19	6	0
4	A	10	0	4	0	0
4	B	10	0	4	2	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
All	All	22478	0	22488	2814	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 63.

The worst 5 of 2814 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:182:MET:HE3	1:A:217:PRO:CB	1.34	1.57
1:B:1449:ARG:CB	1:B:1449:ARG:HH11	0.97	1.56
1:B:182:MET:HE3	1:B:217:PRO:CB	1.09	1.54
1:A:182:MET:CE	1:A:217:PRO:HB2	1.45	1.47

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	14
1	B	1444/1479 (98%)	1170 (81%)	211 (15%)	63 (4%)	2	15
All	All	2888/2958 (98%)	2322 (80%)	438 (15%)	128 (4%)	2	15

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%)	970 (82%)	214 (18%)	1	9
1	B	1184/1206 (98%)	965 (82%)	219 (18%)	1	8
All	All	2368/2412 (98%)	1935 (82%)	433 (18%)	1	9

5 of 433 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1381	ASP
1	B	215	THR
1	B	1246	LEU
1	A	1413	GLN
1	B	40	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1320	ASN
1	B	113	ASN
1	B	1274	GLN
1	A	1363	ASN
1	B	30	HIS

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](#)

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	-	3,9,9	5.21	2 (66%)	4,11,11	4.04	2 (50%)
4	AKG	A	2475	-	3,9,9	4.84	2 (66%)	4,11,11	3.45	2 (50%)
5	F3S	B	2476	1	0,9,9	0.00	-	-	-	-
3	FMN	B	2474	-	31,33,33	1.49	3 (9%)	40,50,50	3.22	19 (47%)
2	OMT	A	2473	-	6,10,10	4.94	4 (66%)	6,14,14	5.93	5 (83%)
3	FMN	A	2474	-	31,33,33	1.56	6 (19%)	40,50,50	3.12	20 (50%)
5	F3S	A	2476	1	0,9,9	0.00	-	-	-	-
2	OMT	B	2473	-	6,10,10	4.89	4 (66%)	6,14,14	7.72	4 (66%)

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	-	-	1/3/9/9	-
4	AKG	A	2475	-	-	0/3/9/9	-
5	F3S	B	2476	1	-	-	0/3/3/3
3	FMN	B	2474	-	-	5/18/18/18	0/3/3/3
2	OMT	A	2473	-	-	5/6/10/10	-
3	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
5	F3S	A	2476	1	-	-	0/3/3/3
2	OMT	B	2473	-	-	5/6/10/10	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2475	AKG	O5-C2	8.69	1.36	1.22
4	A	2475	AKG	O5-C2	8.07	1.35	1.22
2	A	2473	OMT	CB-CG	-6.99	1.45	1.52
2	B	2473	OMT	CG-SD	-6.88	1.69	1.78
2	A	2473	OMT	CG-SD	-6.69	1.69	1.78

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	2473	OMT	OD2-SD-CG	-16.70	96.65	108.34
2	A	2473	OMT	OD2-SD-CE	-11.66	97.19	108.91
3	B	2474	FMN	C1'-N10-C10	8.14	125.70	118.41
3	A	2474	FMN	O5'-P-O1P	-7.87	84.41	106.47
3	B	2474	FMN	C1'-N10-C9A	-7.66	112.26	118.29

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

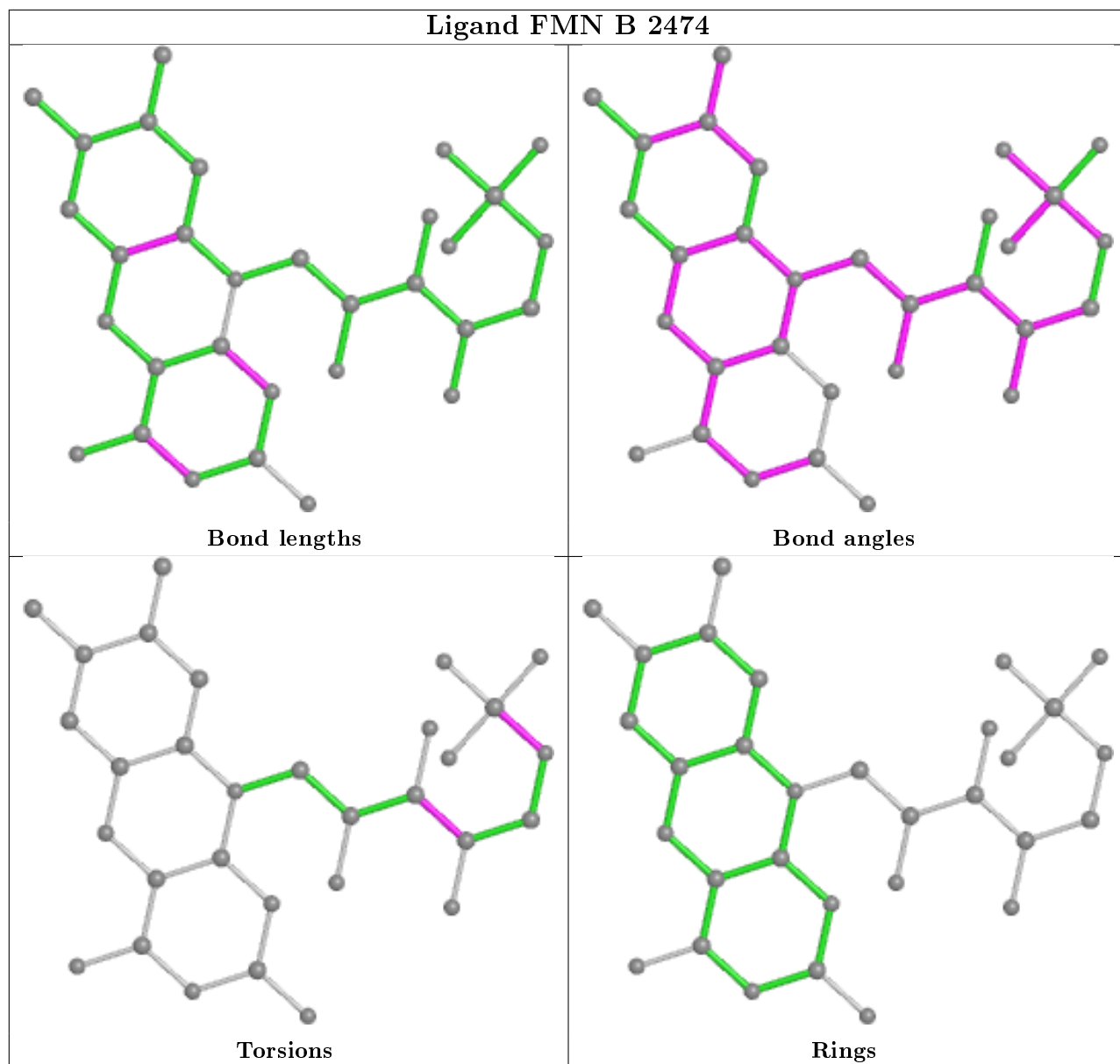
Mol	Chain	Res	Type	Atoms
3	B	2474	FMN	C2'-C3'-C4'-O4'
3	B	2474	FMN	O3'-C3'-C4'-O4'
2	A	2473	OMT	C-CA-CB-CG
2	A	2473	OMT	CB-CG-SD-OD1
2	A	2473	OMT	CB-CG-SD-OD2

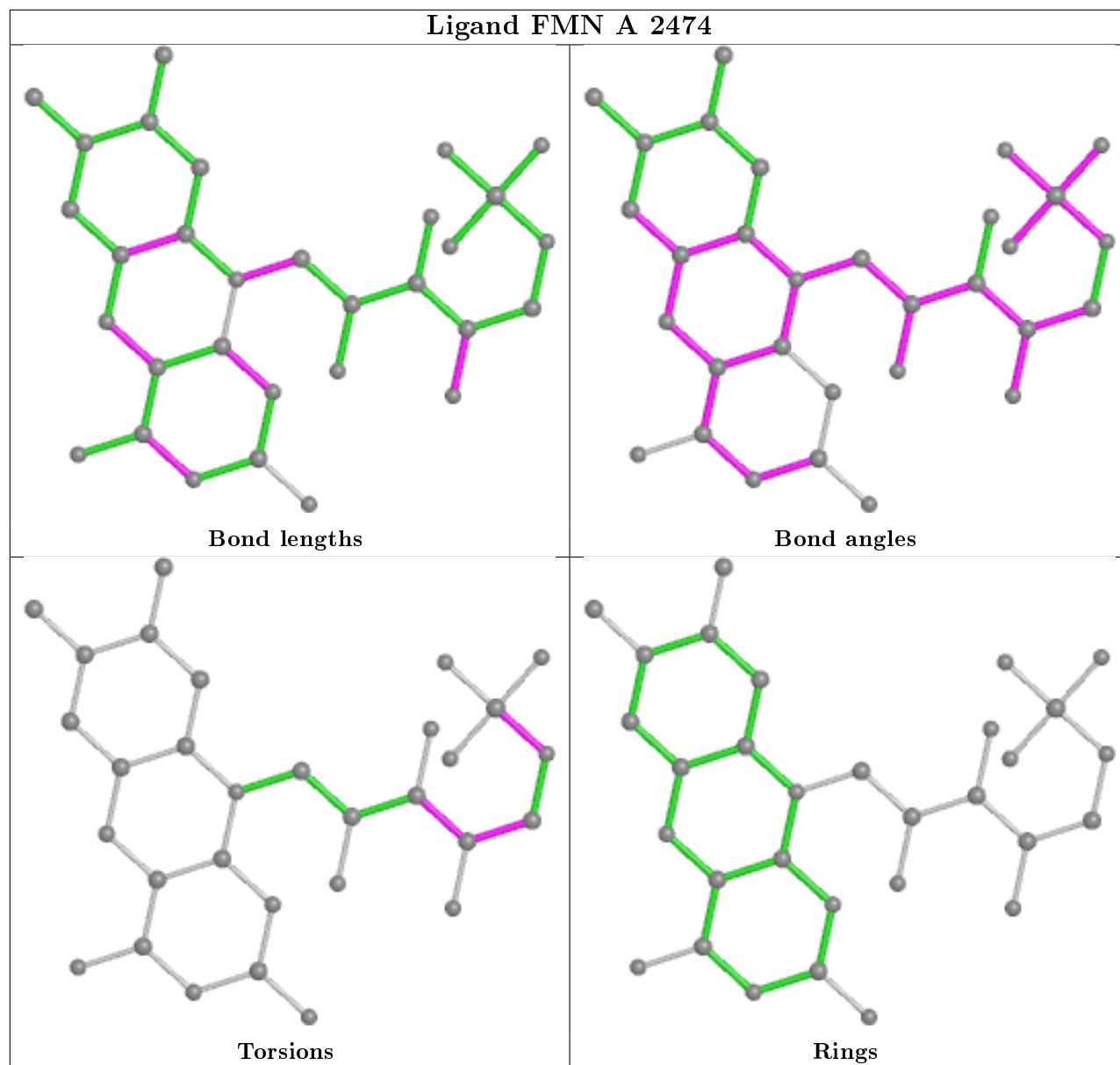
There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2475	AKG	2	0
5	B	2476	F3S	3	0
3	B	2474	FMN	6	0
2	A	2473	OMT	2	0
3	A	2474	FMN	4	0
5	A	2476	F3S	2	0
2	B	2473	OMT	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.





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.