



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 01:21 AM UTC

PDB ID : 1LLW / pdb_00001llw
Title : Structural studies on the synchronization of catalytic centers in glutamate synthase: complex with 2-oxoglutarate
Authors : van den Heuvel, R.H.; Ferrari, D.; Bossi, R.T.; Ravasio, S.; Curti, B.; Vanoni, M.A.; Florencio, F.J.; Mattevi, A.
Deposited on : 2002-04-30
Resolution : 2.70 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

<http://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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

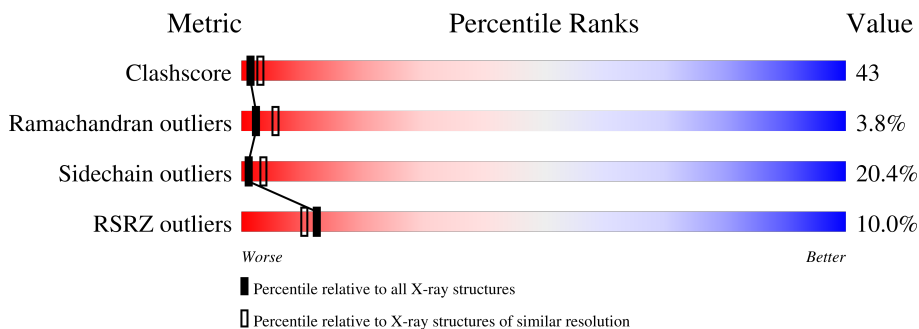
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	1520	

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	F3S	A	2072	-	-	X	-
4	AKG	A	2073	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11408 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.

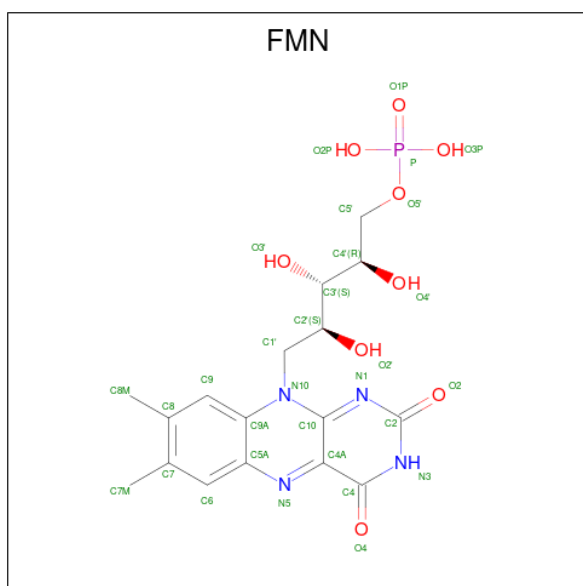
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1475	11311	7137	1970	2148	56	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

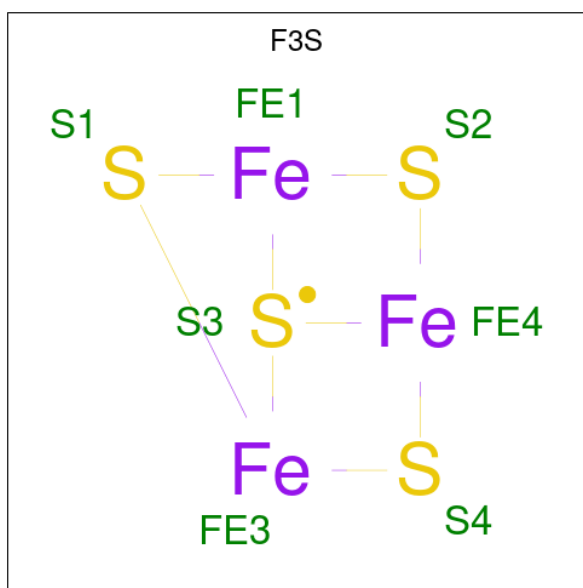
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



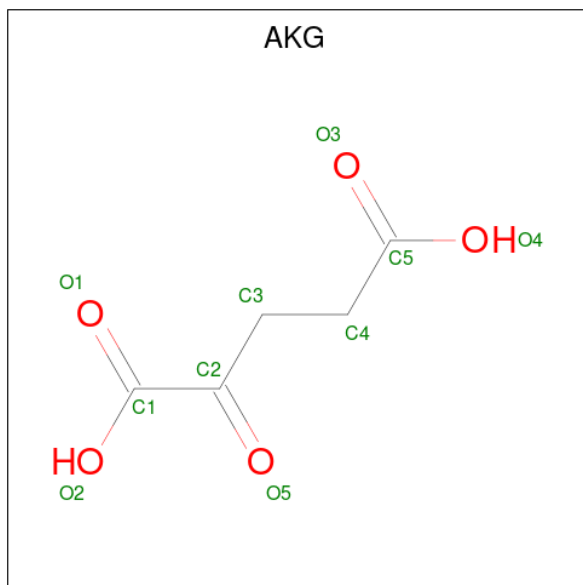
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $\text{C}_5\text{H}_6\text{O}_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		

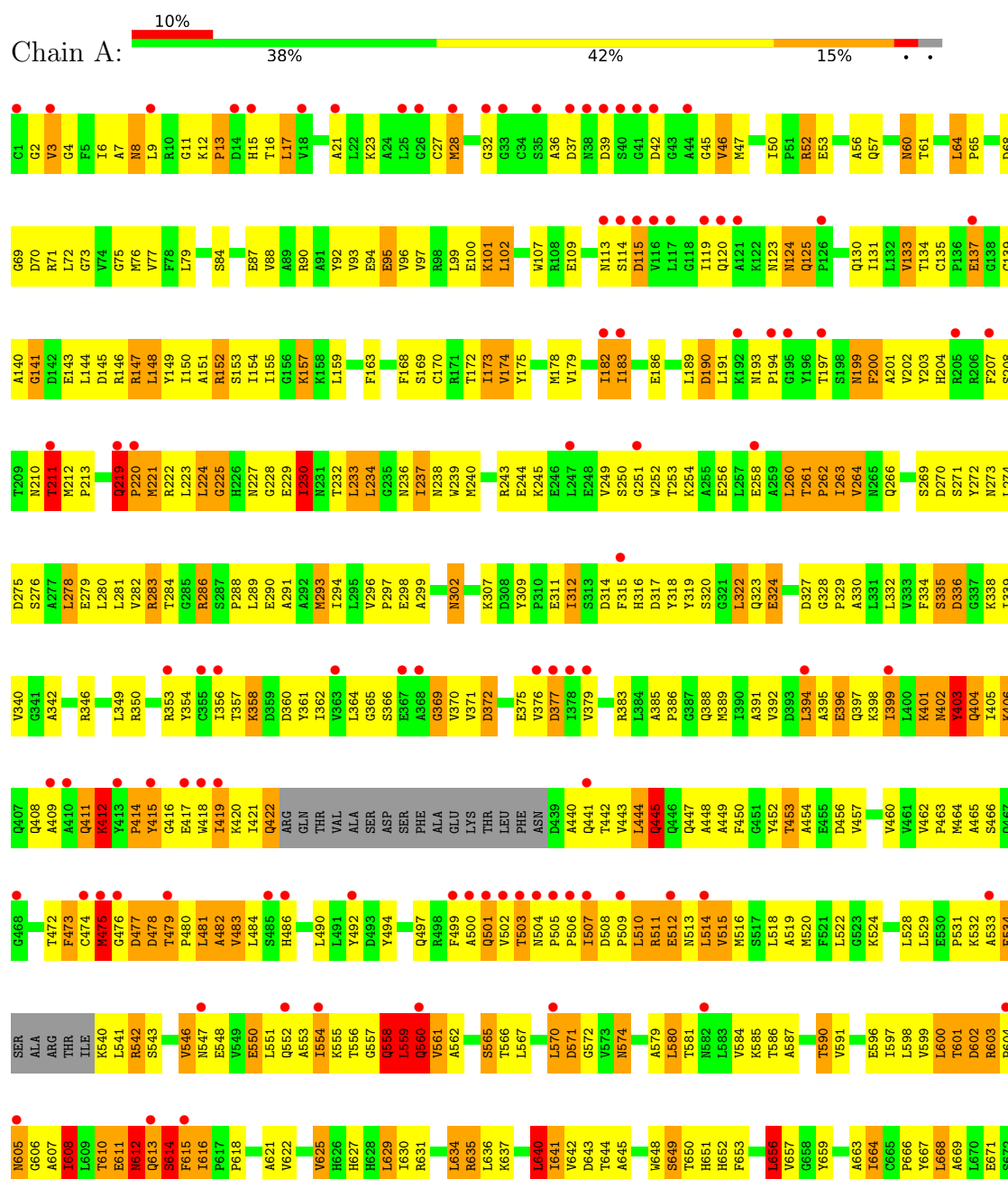
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		

3 Residue-property plots [i](#)

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 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: Ferredoxin-dependent glutamate synthase



G1489	K1490	F1491	W1492	Q1493	A1494	P1497	S1498	E1499	K1500	P1503	E1504	N1507	ASP	VAL	SER	LEU	THR	GLY	LYS	THR	LEU	THR	SER	VAL	G1421	A1422	G1423	M1424	T1425	L1428	A1429	Y1430	F1431	L1432	L1433	F1434	W1435	L1438	P1439	E1440	K1441	I1442	N1443	I1446	I1447	T1448	L1449	Q1450	L1451	I1452	T1453	A1454	S1455	K1456	E1457	E1458	E1459	Q1460	L1461	K1462	S1463	L1464	I1465	T1466	V1469	T1472	G1473	S1474	P1475	K1476	L1480	L1481	A1482	M1483	W1484	Y1487	L1488	F1352	A1353	P1354	E1355	D1356	N1357	V1358	I1359	I1360	G1361	N1362	T1363	C1364	L1365	Y1366	T1369	G1370	G1371	N1372	L1373	Y1374	A1375	N1376	G1380	E1381	R1382	F1383	A1384	V1385	R1386	N1387	S1388	V1389	I1394	E1395	D1399	H1400	C1401	C1402	E1403	Y1404	M1405	T1406	V1409	I1410	V1411	V1412	G1414	P1415	P1416	G1417	R1418	N1419	V1420	L1273	V1274	N1275	T1279	L1280	G1281	T1282	R1283	L1284	S1285	G1286	Q1287	I1288	Y1292	G1293	N1294	N1295	G1296	F1297	L1298	G1299	N1300	I1301	F1305	Q1306	G1307	A1308	A1309	G1310	Q1311	A1315	F1316	N1317	L1318	M1321	H1324	L1325	Q1326	G1327	E1328	A1329	K1335	G1336	M1337	N1338	T1344	V1345	P1346	H1347	P1348	S1351	R1199	T1200	L1203	D1208	V1209	Q1210	L1211	S1212	K1213	R1141	T1214	Q1215	N1216	L1225	P1226	T1227	T1228	K1229	R1232	Q1233	W1234	L1235	E1238	P1239	V1240	H1241	S1242	H1243	G1244	P1245	V1246	D1249	L1250	L1251	L1252	A1253	D1254	P1255	D1256	L1257	Q1258	E1259	A1260	L1261	N1262	H1263	T1265	L1266	A1267	T1268	K1269	T1270	L1271	R1272	L1130	A1131	M1132	I1133	G1136	C1137	I1138	M1139	A1140	R1141	C1142	P1143	H1144	T1145	N1146	C1147	G1148	P1149	V1150	V1151	A1152	A1153	T1154	R1158	L1159	R1160	Q1161	K1164	Q1169	V1170	N1171	N1172	F1173	F1174	Y1175	I1176	I1177	A1178	E1179	E1180	V1181	R1182	L1185	L1188	G1189	Y1190	L1191	S1192	L1193	D1194	P1195	L1196	I1197	G1198	N1052	A1053	I1055	H1061	D1062	T1065	G1066	A1067	S1068	L1070	S1071	G1077	W1080	E1081	E1085	E1086	V1087	H1088	R1089	M1092	E1093	N1094	Q1095	L1096	R1099	V1100	L1101	L1102	R1103	A1104	D1105	K1109	T1110	G1111	V1112	D1113	M1116	A1117	A1118	L1119	M1120	E1123	E1124	F1127	G1128	S1129	A988	P989	G970	A971	K972	P973	Q978	T988	L991	R992	R993	S994	N900	S901	P996	G997	V998	T999	L1000	P1004	P1005	H1006	H1007	D1008	I1012	S919	E1013	D1014	L1015	A1016	Q1017	L1018	D1021	L1022	H1023	Q1024	I1025	R949	F950	G951	V952	T953	L1035	V1036	E955	Y956	L957	M958	K961	Q962	L963	E964	P965	K966	N967	A884	H885	T886	L888	A891	M892	N893	R894	L895	K898	S899	N900	S901	P996	G997	V998	T999	L1000	P1004	P1005	H1006	H1007	D1008	I1012	S919	E1013	D1014	L1015	A1016	Q1017	L1018	D1021	L1022	H1023	Q1024	I1025	R949	F950	G951	V952	T953	L1035	V1036	E955	Y956	L957	M958	K961	Q962	L963	E964	P965	K966	N967	A810	A811	Y812	VAL	GLY	GLY	ASN	GLY	ASN	ASN	GLY	GLY	ALA	Y824	D825	N826	Y827	E828	L829	Y830	R831	Q832	Y833	L834	K835	D836	R837	P838	V839	Y840	R843	L846	D847	F848	T855	S856	L857	V860	E861	S862	V863	V867	T872	Q873	G874	N875	S876	L877	L878	Q878	S881	R882	K883	L737	E740	L744	Y745	F746	T749	S750	R751	Y752	W753	G754	L755	L756	T757	A759	D760	V761	A762	W765	W766	Y767	F768	H769	G770	W771	A772	F773	E775	A777	K778	Y779	L780	F783	G784	P790	G791	G792	E793	Y794	H795	W796	X797	S798	P799	E800	N801	S802	L805	V809	V673	R674	Q675	W676	W677	L678	D679	E680	K681	T682	Q683	K684	L685	M686	E687	N688	G689	R690	L691	D692	R693	I694	D695	L696	P697	T698	K701	W702	Y703	R704	Q705	S706	V707	L711	F712	F713	I714	L715	S716	K717	I720	S721	L722	L723	A724	S725	Y726	H727	G728	A729	Q730	L731	F732	E733	A734	G736
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.52Å 166.52Å 219.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 12.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (12.00-2.70) 96.6 (12.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.70Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.234 , 0.293 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, FMN, AKG

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	1.15	28/11533 (0.2%)	1.44	122/15639 (0.8%)

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	16

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	MET	SD-CE	11.69	2.08	1.79
1	A	221	MET	SD-CE	9.08	2.02	1.79
1	A	240	MET	SD-CE	7.64	1.98	1.79
1	A	237	ILE	CA-CB	7.57	1.64	1.54
1	A	1120	MET	SD-CE	-6.44	1.63	1.79

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	THR	N-CA-C	-10.19	100.25	111.36
1	A	219	GLN	N-CA-C	8.90	129.48	109.81
1	A	768	PHE	N-CA-C	8.69	123.61	112.92
1	A	402	ASN	N-CA-C	8.62	120.37	110.97
1	A	693	ARG	N-CA-C	-8.47	100.27	110.44

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	GLN	Peptide
1	A	260	LEU	Peptide
1	A	369	GLY	Peptide
1	A	403	TYR	Peptide
1	A	412	LYS	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	11311	0	11255	977	1
2	A	31	0	19	0	0
3	A	7	0	0	4	0
4	A	10	0	4	2	0
5	A	49	0	0	14	0
All	All	11408	0	11278	977	1

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 43.

The worst 5 of 977 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:383:ARG:NH1	1:A:1380:GLY:HA2	1.20	1.46
1:A:221:MET:SD	1:A:221:MET:CE	2.02	1.46
1:A:293:MET:SD	1:A:293:MET:CE	2.08	1.41
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.44	1.36
1:A:768:PHE:CE2	1:A:771:MET:HG2	1.68	1.28

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:ARG:CD	1:A:1324:HIS:CE1[4_475]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	1467/1520 (96%)	1215 (83%)	196 (13%)	56 (4%)	2 5

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	101	LYS
1	A	403	TYR
1	A	414	PRO
1	A	415	TYR

5.3.2 Protein sidechains

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	1200/1236 (97%)	955 (80%)	245 (20%)	1 3

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	656	LEU
1	A	1386	ARG
1	A	829	LEU
1	A	1381	GLU
1	A	1453	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1304	ASN
1	A	1372	ASN
1	A	1493	GLN
1	A	646	GLN
1	A	552	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](#)

3 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	A	2073	-	9,9,9	2.26	3 (33%)	11,11,11	1.60	4 (36%)
3	F3S	A	2072	1	0,9,9	-	-	-		
2	FMN	A	2070	-	33,33,33	1.21	4 (12%)	48,50,50	1.19	6 (12%)

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	A	2073	-	-	6/9/9/9	-
3	F3S	A	2072	1	-	-	0/3/3/3
2	FMN	A	2070	-	-	5/18/18/18	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2073	AKG	O5-C2	4.70	1.32	1.23
4	A	2073	AKG	O1-C1	3.86	1.32	1.22
2	A	2070	FMN	C4A-N5	3.23	1.37	1.30
4	A	2073	AKG	O3-C5	2.72	1.31	1.22
2	A	2070	FMN	C4A-C10	-2.21	1.37	1.44

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2070	FMN	C4A-C10-N10	3.13	120.96	116.48
2	A	2070	FMN	C4-C4A-N5	2.72	121.97	118.21
4	A	2073	AKG	O4-C5-O3	-2.71	116.36	123.33
2	A	2070	FMN	C4-N3-C2	-2.68	120.89	125.64
2	A	2070	FMN	C10-C4A-N5	-2.57	119.57	124.81

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2073	AKG	O2-C1-C2-C3
2	A	2070	FMN	O3'-C3'-C4'-O4'
2	A	2070	FMN	O3'-C3'-C4'-C5'
2	A	2070	FMN	C2'-C3'-C4'-C5'
2	A	2070	FMN	C2'-C3'-C4'-O4'

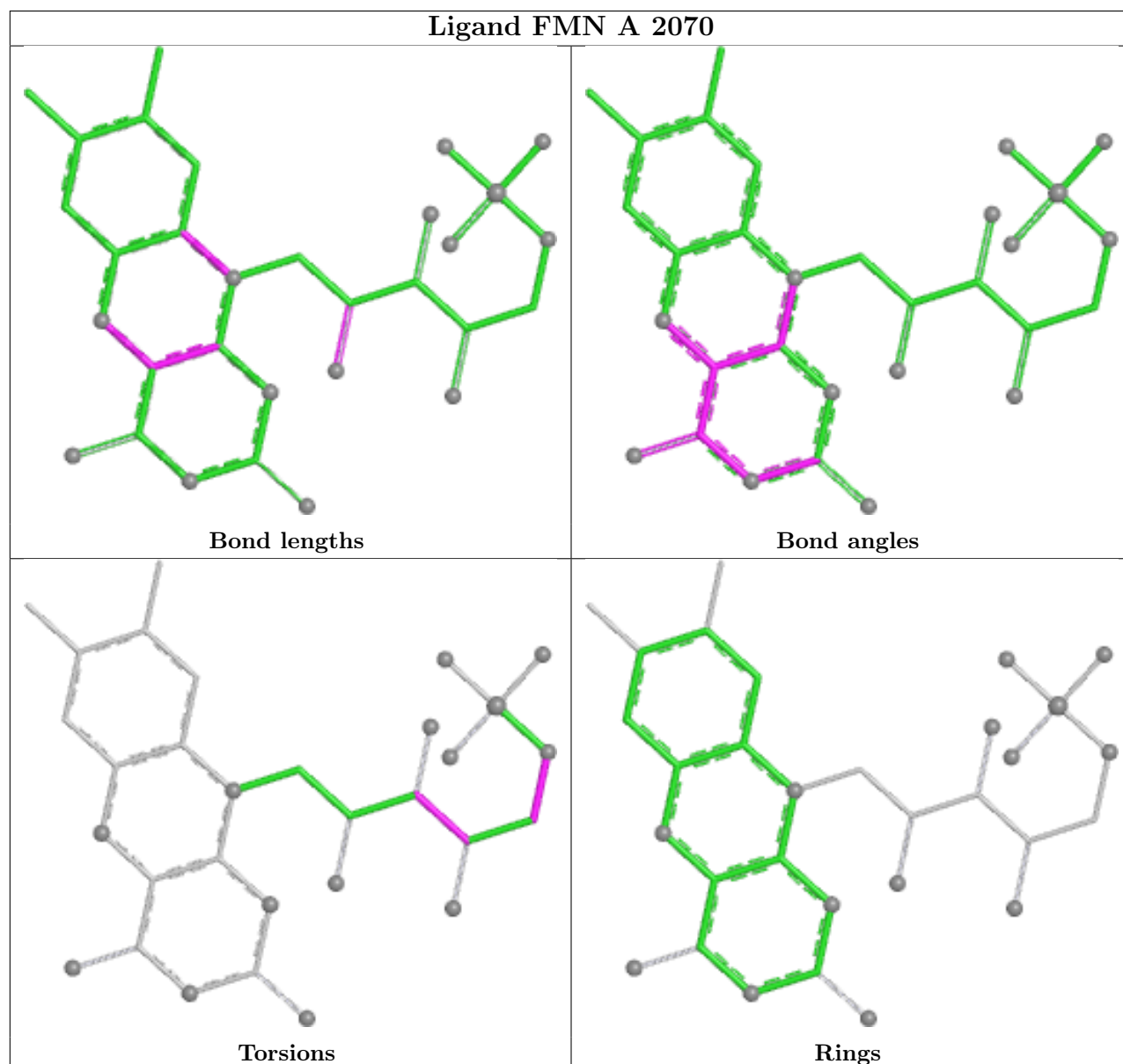
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2073	AKG	2	0
3	A	2072	F3S	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1475/1520 (97%)	0.61	147 (9%) 12 10	8, 42, 64, 100	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	TRP	6.7
1	A	376	VAL	6.3
1	A	500	ALA	5.2
1	A	41	GLY	5.2
1	A	1263	HIS	4.8

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](#)

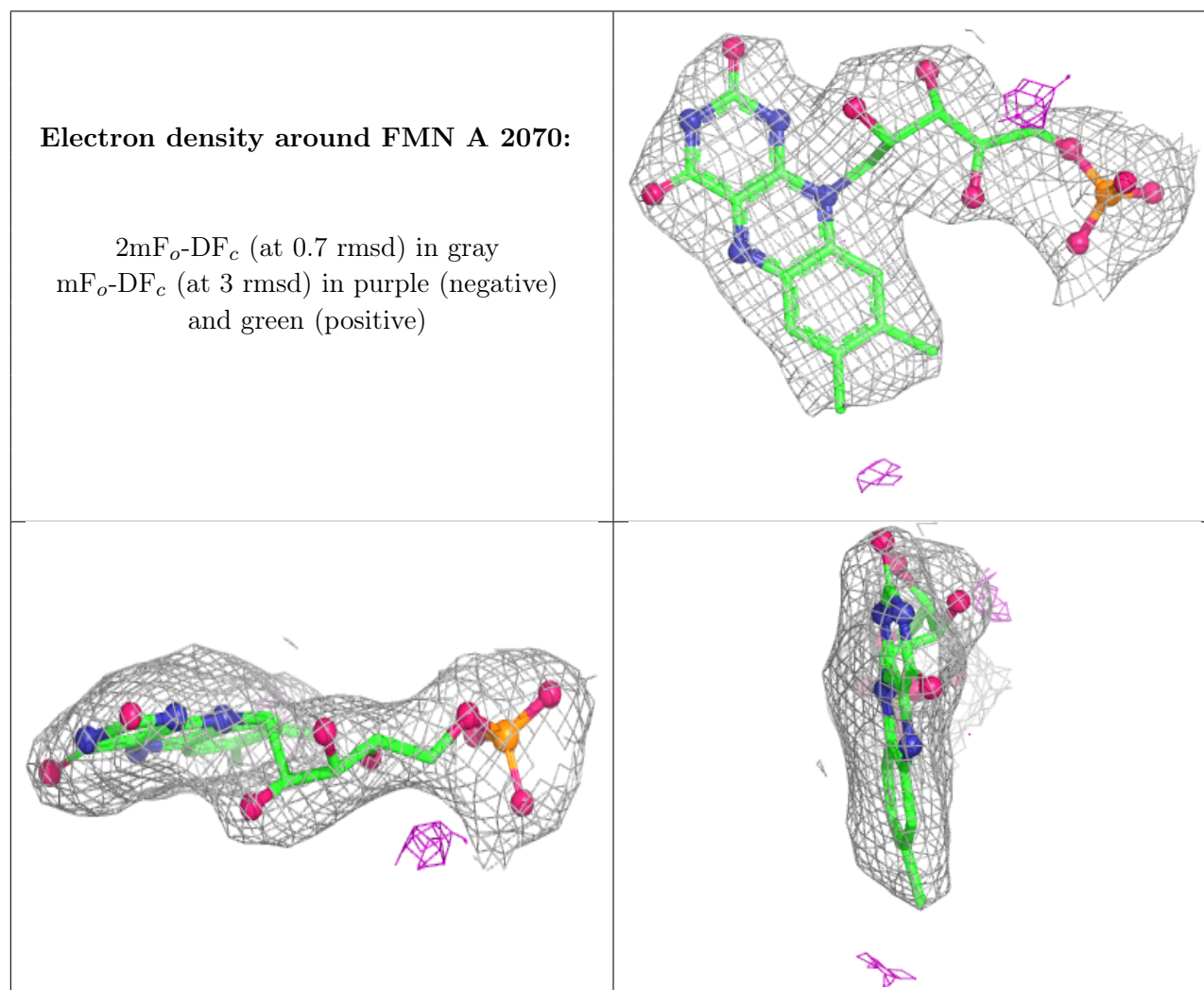
There are no oligosaccharides in this entry.

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, 95th 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(Å ²)	Q<0.9
4	AKG	A	2073	10/10	0.93	0.11	81,85,87,89	0
2	FMN	A	2070	31/31	0.96	0.10	80,85,88,88	0
3	F3S	A	2072	7/7	0.97	0.09	85,91,94,96	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.