



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:55 am GMT

PDB ID : 1LLW
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

<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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

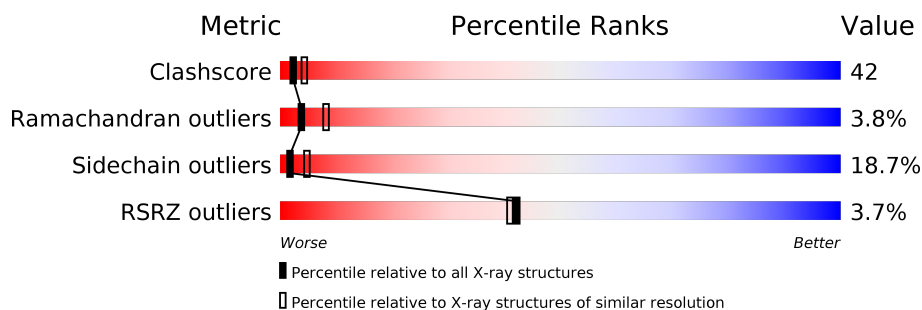
1 Overall quality at a glance

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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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 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.

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
2	FMN	A	2070	-	-	-	X
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.

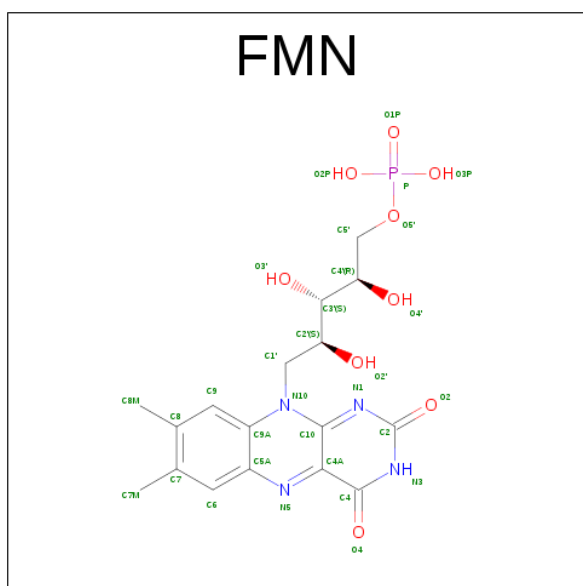
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

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:

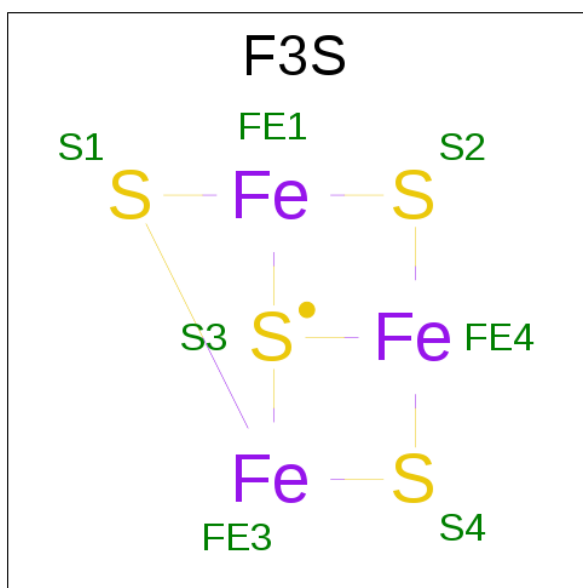
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	CONFLICT	UNP P55038
A	581	THR	ASP	CONFLICT	UNP P55038
A	1507	ASN	GLY	CONFLICT	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



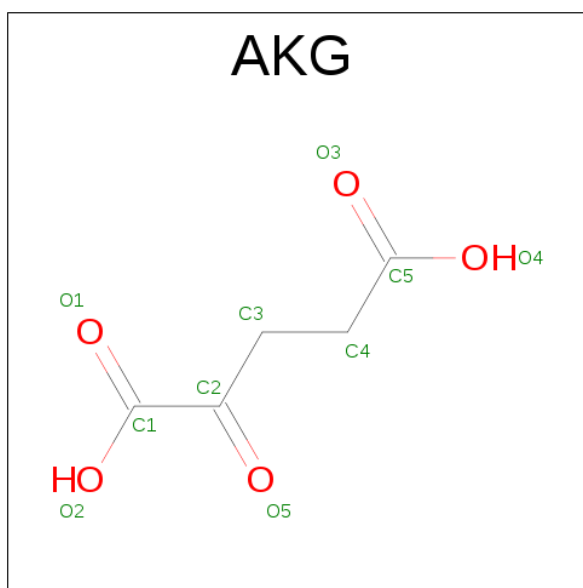
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: 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 (three-letter code: 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		

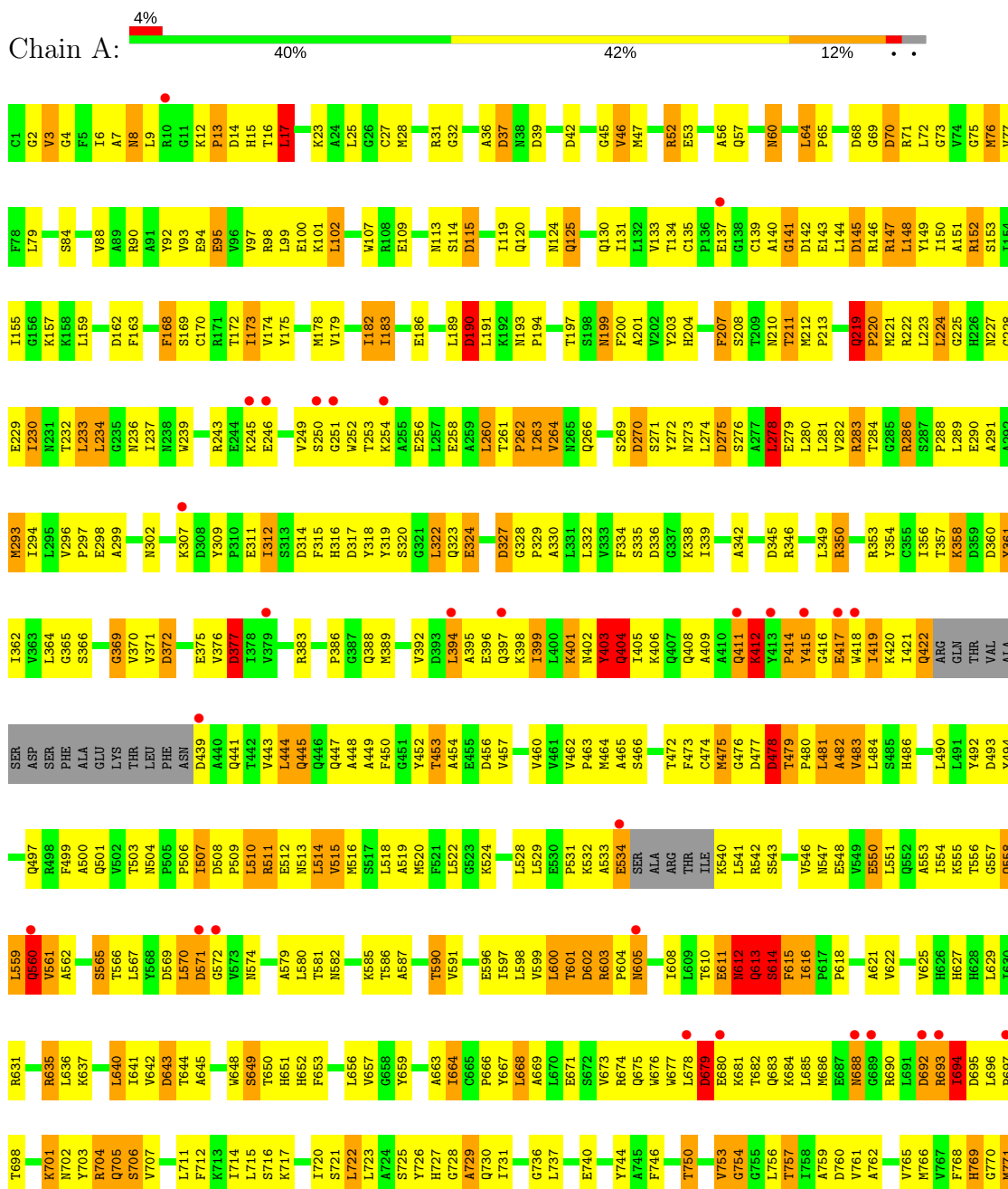
- Molecule 5 is water.

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

3 Residue-property plots

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

- Molecule 1: Ferredoxin-dependent glutamate synthase



I1480	I1481	W1484	S1485	D1486	Y1487	L1488	G1489	K1490	G1491	F1492	Q1493	A1494	P1497	S1498	P1503	E1504	M1507	ASP	VAL	SER	LEU	THR	GLY	GLU	LYS	THR	LEU	THR	SER	VAL																									
K1335	G1336	M1337	M1338	T1344	V1345	P1346	H1347	P1348	S1351	A1422	F1352	A1353	P1354	E1355	V1358	I1359	I1360	T1363	C1364	L1365	Y1366	T1369	G1370	G1371	M1372	L1373	Y1374	A1375	M1376	G1380	E1381	R1382	F1383	A1384	V1385	R1386	M1387	S1388	V1389	I1394	Q1395	D1399	H1400	C1401	E1402	E1403	E1404	M1405	T1406	V1409	I1410				
I1257	Q1258	A1259	I1261	N1262	H1263	Q1264	K1269	T1270	Y1271	R1272	L1273	V1274	N1275	T1276	D1277	R1278	T1279	V1280	G1281	T1282	R1283	I1288	Y1292	G1293	N1294	N1295	G1296	F1297	E1298	G1299	F1305	Q1306	G1307	A1308	A1309	G1310	Q1311	A1315	F1316	N1317	L1318	M1321	H1324	L1325	Q1326	G1327	E1328	A1329	Y1332						
L1185	L1188	G1189	Y1190	R1191	S1192	L1193	D1194	D1195	T1196	I1197	G1198	R1199	T1200	D1201	L1202	L1203	R1206	S1207	D1208	V1209	Q1210	L1211	S1212	K1213	T1214	Q1215	M1216	L1225	P1226	D1227	T1228	R1232	Q1233	W1234	L1235	E1238	P1239	V1240	H1241	S1242	P1245	V1246	L1247	D1248	D1249	D1250	I1251	L1252	A1253	D1254	D1256				
T1110	G1111	W1112	D1113	M1116	A1117	A1118	L1119	M1120	E1123	E1124	F1127	G1128	T1129	S1130	T1131	A1131	R1132	I1133	G1136	C1137	T1138	M1139	A1140	R1141	V1142	C1143	H1144	T1145	N1146	M1147	C1148	P1149	V1150	G1151	V1152	A1153	T1154	R1158	L1159	R1160	Q1161	Q1169	V1170	V1171	N1172	F1173	Y1175	F1176	I1177	E1180	V1181	R1182			
A1016	Q1017	L1018	D1021	L1022	A938	H1023	Q1024	I1025	Q1030	V1031	S1032	V1033	K1034	L1035	V952	T963	P954	E955	Y956	N958	K961	G962	L963	E964	N965	K966	H967	G970	A971	L1070	K972	P973	Q978	A891	M892	N893	R894	L895	K898	S899	N900	S901	G902	Y830	R831	Q832	Y833	L834	R910	K835	D836	Y911	L912	D916	T940
A772	F773	E774	E775	M776	A777	K778	L779	L780	F783	P790	G791	Y794	H795	M796	N797	S798	P799	M801	S802	L805	V809	A810	A811	Y812	LYS	VAL	GLY	GLY	ASN	ASN	ASN	GLY	GLU	ALA	Y824	D825	H826	Y827	E828	L829	Y830	R831	Q832	Y833	L834	R910	K835	D836	Y911	L912	D916	T940			
B843	D844	L845	L846	D847	F848	D851	R855	S856	L857	V860	E861	H863	V867	T872	G873	G874	M875	S876	L877	G878	S881	R882	E883	A884	H885	E886	T887	L888	A891	M892	N893	R894	L895	K898	S899	N900	S901	G902	Y830	R831	Q832	Y833	L834	R910	K835	D836	Y911	L912	D916	T940					
E920	P924	T937	A938	N939	S940	A941	T942	A946	R949	F950	G951	V952	T963	P954	E955	Y956	N958	K961	G962	L963	E964	N965	K966	H967	G970	A971	L1070	K972	P973	Q978	A891	M892	N893	R894	L895	K898	S899	N900	S901	G902	Y830	R831	Q832	Y833	L834	R910	K835	D836	Y911	L912	D916	T940			
A1016	Q1017	L1018	D1021	L1022	A938	H1023	Q1024	I1025	Q1030	V1031	S1032	V1033	K1034	L1035	V952	T963	P954	E955	Y956	N958	K961	G962	L963	E964	N965	K966	H967	G970	A971	L1070	K972	P973	Q978	A891	M892	N893	R894	L895	K898	S899	N900	S901	G902	Y830	R831	Q832	Y833	L834	R910	K835	D836	Y911	L912	D916	T940
T1110	G1111	W1112	D1113	M1116	A1117	A1118	L1119	M1120	E1123	E1124	F1127	G1128	T1129	S1130	T1131	A1131	R1132	I1133	G1136	C1137	T1138	M1139	A1140	R1141	V1142	C1143	H1144	T1145	N1146	M1147	C1148	P1149	V1150	G1151	V1152	A1153	T1154	R1158	L1159	R1160	Q1161	Q1169	V1170	V1171	N1172	F1173	Y1175	F1176	I1177	E1180	V1181	R1182			
L1185	L1188	G1189	Y1190	R1191	S1192	L1193	D1194	D1195	T1196	I1197	G1198	R1199	T1200	D1201	L1202	L1203	R1206	S1207	D1208	V1209	Q1210	L1211	S1212	K1213	T1214	Q1215	M1216	L1225	P1226	D1227	T1228	R1232	Q1233	W1234	L1235	E1238	P1239	V1240	H1241	S1242	P1245	V1246	L1247	D1248	D1249	D1250	I1251	L1252	A1253	D1254	D1256				
I1257	Q1258	A1260	I1261	N1262	H1263	Q1264	K1269	T1270	Y1271	R1272	L1273	V1274	N1275	T1276	D1277	R1278	T1279	V1280	G1281	T1282	R1283	I1288	Y1292	G1293	N1294	N1295	G1296	F1297	E1298	G1299	F1305	Q1306	G1307	A1308	A1309	G1310	Q1311	A1315	F1316	N1317	L1318	M1321	H1324	L1325	Q1326	G1327	E1328	A1329	Y1332						
K1335	G1336	M1337	M1338	T1344	V1345	P1346	H1347	P1348	S1351	A1422	F1352	A1353	P1354	E1355	V1358	I1359	I1360	T1363	C1364	L1365	Y1366	T1369	G1370	G1371	M1372	L1373	Y1374	A1375	M1376	G1380	E1381	R1382	F1383	A1384	V1385	R1386	M1387	S1388	V1389	I1394	Q1395	D1399	H1400	C1401	E1402	E1403	E1404	M1405	T1406	V1409	I1410				
W1411	V1412	L1413	G1414	P1415	V1416	G1417	R1418	M1419	K1420	G1421	A1422	F1423	M1424	T1425	L1428	A1429	Y1430	F1431	L1432	E1433	V1435	L1438	P1439	E1440	K1441	L1442	M1443	I1446	T1447	T1448	L1449	G1450	R1451	I1452	T1453	A1454	S1455	K1456	G1457	E1458	E1459	L1461	K1462	L1463	L1464	T1466	T1472	G1473	S1474	P1475	K1476				

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 11.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (12.00-2.70) 97.9 (11.99-2.70)	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 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.1	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	0.94	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: FMN, F3S, 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	0.89	5/11533 (0.0%)	1.15	62/15639 (0.4%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1433	ASP	CB-CG	7.41	1.67	1.51
1	A	952	VAL	CB-CG2	-6.62	1.39	1.52
1	A	796	MET	CG-SD	6.00	1.96	1.81
1	A	293	MET	SD-CE	5.52	2.08	1.77
1	A	692	ASP	CB-CG	5.27	1.62	1.51

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CG-OD2	9.22	126.60	118.30
1	A	31	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	478	ASP	CB-CG-OD2	8.13	125.61	118.30
1	A	877	LEU	CA-CB-CG	-8.01	96.87	115.30
1	A	1195	ASP	CB-CG-OD2	7.79	125.31	118.30

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	947	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	947	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 42.

The worst 5 of 947 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%)	4 8

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%)	976 (81%)	224 (19%)	2 5

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	613	GLN
1	A	771	MET
1	A	1406	THR
1	A	635	ARG
1	A	693	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	652	HIS
1	A	769	HIS
1	A	1419	ASN
1	A	675	GLN
1	A	730	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](#)

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	$\# Z > 2$
2	FMN	A	2070	-	31,33,33	1.39	3 (9%)	38,50,50	1.70	6 (15%)
3	F3S	A	2072	1	0,9,9	0.00	-	0,15,15	0.00	-
4	AKG	A	2073	-	3,9,9	3.58	1 (33%)	4,11,11	1.41	1 (25%)

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	FMN	A	2070	-	-	0/16/18/18	0/3/3/3
3	F3S	A	2072	1	-	0/0/24/24	0/0/3/3
4	AKG	A	2073	-	-	0/3/9/9	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2070	FMN	C10-N1	2.46	1.36	1.33
2	A	2070	FMN	C4A-N5	3.07	1.37	1.33
2	A	2070	FMN	C4-N3	3.55	1.39	1.33
4	A	2073	AKG	O5-C2	6.18	1.32	1.22

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2070	FMN	C4A-C4-N3	-3.07	119.11	123.48
2	A	2070	FMN	C1'-N10-C10	-2.98	115.44	118.50
4	A	2073	AKG	O5-C2-C3	2.12	124.09	120.32
2	A	2070	FMN	C4A-N5-C5A	2.35	119.25	116.76
2	A	2070	FMN	C4-C4A-N5	3.00	121.97	118.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2072	F3S	4	0
4	A	2073	AKG	2	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 [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%)	-0.26	54 (3%) 42 41	8, 42, 64, 100	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	776	MET	7.3
1	A	10	ARG	5.0
1	A	1507	ASN	4.9
1	A	605	ASN	4.8
1	A	1264	GLN	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	AKG	A	2073	10/10	0.96	0.23	8.59	81,85,87,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FMN	A	2070	31/31	0.97	0.17	2.03	80,85,88,88	0
3	F3S	A	2072	7/7	0.98	0.12	-0.31	85,91,94,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.