



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:57 am GMT

PDB ID : 1LM1
Title : Structural studies on the synchronization of catalytic centers in glutamate synthase: native enzyme
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 : 2.80 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

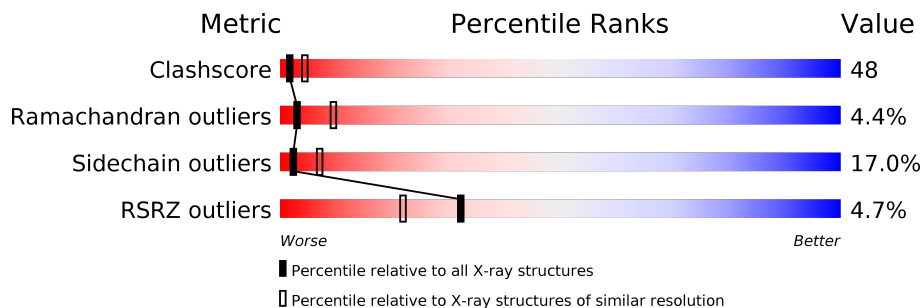
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	<div> <div>5%</div> <div>39%</div> <div>44%</div> <div>13%</div> <div>...</div> </div>

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	ACT	A	2074	-	-	X	X
2	ACT	A	2075	-	-	X	-
4	F3S	A	2072	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11395 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.

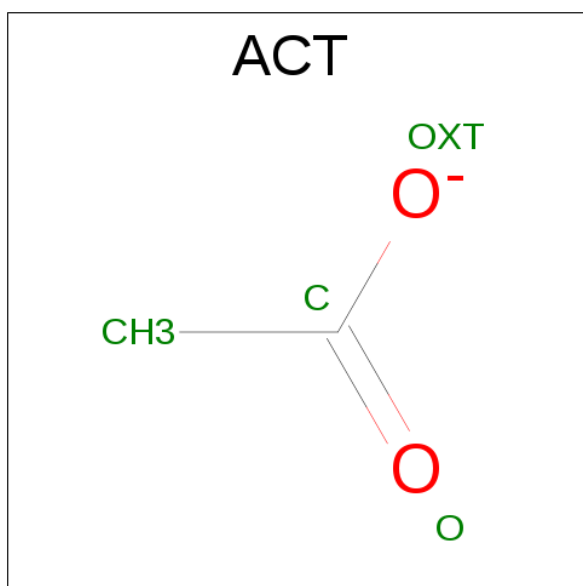
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

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 ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0

- # FMN
-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). The structure consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms) attached to a ribityl chain. The ribityl chain is a three-carbon chain with hydroxyl groups at the 2' and 3' positions. The 3' carbon is linked to a phosphate group, which is further linked to a ribose sugar (labeled C3'5') and a phosphate group (labeled O1P, O2P, O3P). The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The phosphate groups are labeled O1P, O2P, and O3P. The ribityl chain is labeled C1', C2', and C3'. The isoalloxazine ring system is labeled with atoms N1, N3, C2, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C

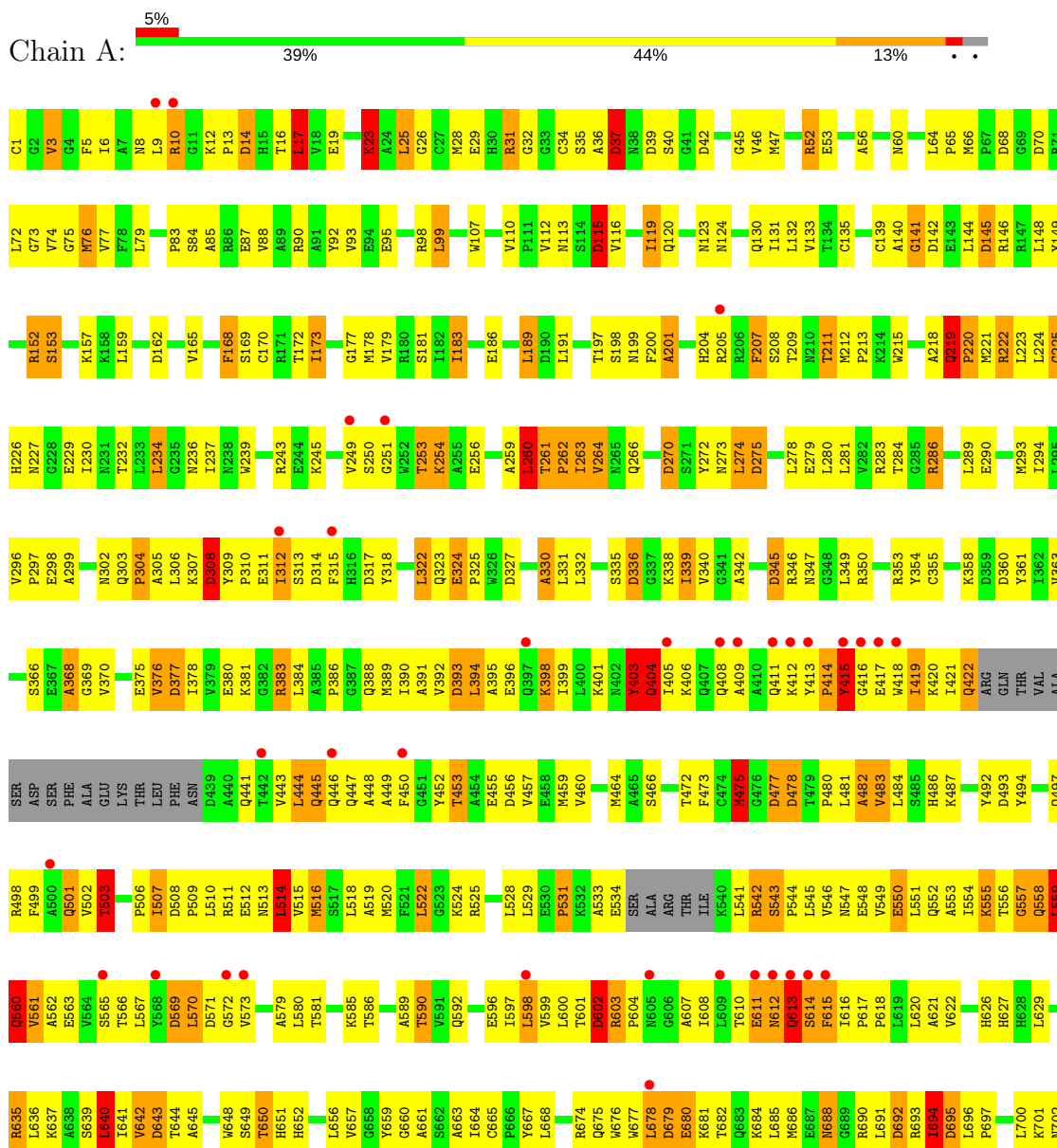


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0

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



LEU	E1440	K1441	N1376	L1303	K1229	Q1155	T1085	D1008	P924	D847	L780	V703
THR	K1442	G1377	F1382	N1304	Q1230	Q1156	E1086	I1009	H930	F848	E781	R704
GLY	N1443	R1378	F1383	Q1306	M1231	L1159	R1089	E1013	G931	D851	N782	Q705
LYS	P1444	G1379	A1384	G1307	Q1233	Q1160	M1092	L1014	L932	Q852	F783	S706
THR	E1445	G1380	A1385	A1308	W1234	Q1161	M1093	L1015	Q933	L855	G710	L711
LEU	I1446	E1381	F1382	Q1311	L1235	V1166	M1094	Q1017	N834	S856	L712	F712
THR	I1447	R1382	F1383	A1315	E1238	V1167	Q1095	L1018	T937	L857	Y788	
SER	T1448	A1384	F1384	A1316	P1239	Q1169	Q1096	L1021	A938	G791	L716	L715
VAL	Q1450	V1385	V1386	F1316	V1240	V1170	R1097	H1022	N939	E858	S716	K717
	R1451	R1386	R1387	N1317	H1241	V1171	D1098	H1023	S940	Y794	H795	
	L1452	L1387	L1318	N1318	V1246	F1173	H1024	Q1024	K943	V883	K796	L722
	T1453	S1388	D1319	D1320	L1247	F1174	L1101	I1025	A946	V867	N797	L723
	A1454	G1389	M1321	L1248	D1249	F1175	L1102	E1028	R949	T872	E800	A724
	K1456	A1391	T1322	D1250	I1177	F1176	L1103	Q1030	T953	M875	N801	Y726
		V1392	H1324	I1251	A1178	A1178	D1105	V1036	P954	L880	S802	H727
	E1459	V1393	H1325	D1254	V1181	L1188	G1107	E1038	Y955	L881	L805	G728
	Q1460	I1394	E1328	P1255	S1182	L1189	L1108	L1035	E955	S876	A729	
	L1461	E1395	A1329	D1256	S1183	G1189	K1109	L1036	Y956	L877	Q730	Y744
	K1462	G1396	E1332	I1257	L1184	L1190	T1110	V1037	L957	G878	GLY	F746
	S1463	A1397	V1332	Q1258	L1188	L1191	G1111	A1037	M958	L879	GLY	A747
	L1464	G1398	V1333	E1259	L1189	L1192	T1112	E1038	P954	T887	ASN	T750
	I1465	T1399	G1334	E1263	G1189	L1193	W1113	E1038	P954	L888	ASN	S751
	T1472	C1402	G1335	H1263	Y1190	S1192	D1113	L1039	K972	A891	ASN	R752
	G1473	E1403	K1336	Q1264	Y1191	S1193	E1124	G1040	P973	M892	GLY	V753
	L1474	Y1404	G1337	T1265	L1196	S1194	E1125	L1041	M973	N893	GLU	G754
	P1475	M1405	M1337	T1266	L1197	L1195	E1126	G1042	G976	L895	ALA	G755
	K1476	T1406	N1338	L1267	R1272	D1194	L1119	T1043	Q977	L895	L756	L756
	G1477	V1409	I1344	A1267	L1270	D1195	M1120	E1053	Q978	S899	D825	L757
		I1410	V1345	T1268	L1201	D1196	L1132	A1054	L979	N900	H826	I758
	I1480	V1411	P1346	K1269	L1202	L1197	E1127	I1055	L979	E827	A759	A759
	W1484	V1412	H1347	Y1271	L1203	L1198	E1128	I1058	V964	E828	D760	D760
	S1485	G1416	P1348	L1272	L1204	G1199	E1129	S1059	S901	L829	V761	V761
	D1486	G1417	A1350	L1273	D1205	T1200	S1130	G1060	G902	Y830	A762	A762
	T1487	R1418	S1351	V1274	L1206	D1201	E1131	H1061	E903	R831	V765	V765
	L1488	N1419	F1352	M1275	L1207	L1202	E1132	D1062	D907	Q832	M766	M766
	G1489	V1420	A1353	T1276	L1208	L1203	E1133	T1065	V908	L833	L834	L834
	K1490	G1421	P1354	D1277	D1208	L1204	E1134	G1066	N909	K835	K835	K835
	F1491	A1422	E1355	R1278	L1209	Q1215	A1135	A1067	R992	R836	F768	F768
	Q1493	G1423	D1356	T1279	L1210	L1216	E1136	S1068	S994	R837	H769	H769
	A1494	M1424	V1358	T1282	L1211	L1217	C1137	S1071	K995	P838	M771	M771
	P1497	T1425	I1359	R1283	L1212	L1218	E1138	G1075	P996	L914	A772	A772
	L1428	L1429	I1360	T1284	Q1213	L1219	E1139	A1076	G997	D915	T840	T840
	E1499	Y1430	T1363	T1285	L1214	L1220	E1140	H1075	S997	D916	P773	P773
	K1500	F1431	C1364	A1289	Q1215	D1220	A1140	A1076	L991	V917	P774	P774
	D1501	L1432	L1365	A1290	L1216	L1221	R1141	E1081	R993	L842	E775	E775
	S1502	D1433	V1366	N1295	L1217	L1222	E1142	P1003	S994	D918	H776	H776
	P1503	E1434	G1367	G1296	L1218	L1223	E1143	F1004	K995	S919	D844	D844
	E1504	V1435	A1368	F1297	L1219	L1224	E1144	P1005	K996	L845	K778	K778
	W1507	G1436	T1369	E1298	L1220	L1225	E1145	H1006	G997	S923	L846	L846
	ASP	D1437	N1372	E1299	L1221	L1226	E1146					
	VAL	L1438	L1373	T1302	L1222	L1227	N1147					
	SER	P1439			L1223	L1228	C1148					

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.08Å 166.08Å 219.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.80 61.52 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (129.10-2.80) 99.4 (61.52-2.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.236 , 0.287 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11395	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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

5.1 Standard geometry

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

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	0.95	13/11533 (0.1%)	1.18	88/15639 (0.6%)

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	0	11

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1433	ASP	CB-CG	6.96	1.66	1.51
1	A	615	PHE	CE1-CZ	6.10	1.49	1.37
1	A	911	TYR	CD2-CE2	5.83	1.48	1.39
1	A	1008	ASP	CB-CG	-5.70	1.39	1.51
1	A	272	TYR	CE1-CZ	5.67	1.46	1.38

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CB-CG-OD2	11.88	129.00	118.30
1	A	498	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	A	220	PRO	N-CD-CG	-8.50	90.45	103.20
1	A	1399	ASP	CB-CG-OD2	8.50	125.95	118.30
1	A	949	ARG	NE-CZ-NH2	-8.19	116.20	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASN	Peptide
1	A	219	GLN	Peptide
1	A	403	TYR	Peptide
1	A	445	GLN	Peptide
1	A	99	LEU	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	11256	1070	0
2	A	8	0	6	6	0
3	A	31	0	19	4	0
4	A	7	0	0	3	0
5	A	38	0	0	7	0
All	All	11395	0	11281	1077	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 48.

The worst 5 of 1077 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:293:MET:SD	1:A:293:MET:CE	2.03	1.46
1:A:875:MET:CE	1:A:875:MET:SD	2.04	1.45
1:A:768:PHE:CE2	1:A:771:MET:HG2	1.55	1.42
1:A:686:MET:CE	1:A:692:ASP:HA	1.61	1.31
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.32	1.25

There are no symmetry-related clashes.

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%)	1232 (84%)	171 (12%)	64 (4%)	3 9

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	395	ALA
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%)	996 (83%)	204 (17%)	2 7

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	641	ILE
1	A	834	LEU
1	A	1425	THR
1	A	650	THR
1	A	750	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	730	GLN
1	A	978	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1419	ASN
1	A	885	HIS
1	A	486	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](#)

4 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	$\# Z > 2$
3	FMN	A	2070	-	31,33,33	1.39	4 (12%)	38,50,50	1.70	8 (21%)
4	F3S	A	2072	1	0,9,9	0.00	-	0,15,15	0.00	-
2	ACT	A	2074	-	1,3,3	0.85	0	0,3,3	0.00	-
2	ACT	A	2075	-	1,3,3	1.73	0	0,3,3	0.00	-

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
3	FMN	A	2070	-	-	0/16/18/18	0/3/3/3
4	F3S	A	2072	1	-	0/0/24/24	0/0/3/3
2	ACT	A	2074	-	-	0/0/0/0	0/0/0/0
2	ACT	A	2075	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2070	FMN	C4A-C10	-2.90	1.35	1.41
3	A	2070	FMN	C6-C5A	-2.17	1.38	1.41
3	A	2070	FMN	C4A-N5	2.21	1.36	1.33
3	A	2070	FMN	C4-N3	3.45	1.39	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2070	FMN	C8M-C8-C7	-3.58	113.21	120.72
3	A	2070	FMN	C4A-C4-N3	-3.44	118.59	123.48
3	A	2070	FMN	C7M-C7-C8	-2.03	116.46	120.72
3	A	2070	FMN	O4'-C4'-C3'	2.16	114.46	109.09
3	A	2070	FMN	O3P-P-O5'	2.18	112.53	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2070	FMN	4	0
4	A	2072	F3S	3	0
2	A	2074	ACT	6	0
2	A	2075	ACT	5	0

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%)	0.12	69 (4%)	32 22	24, 34, 41, 85	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	TYR	5.9
1	A	415	TYR	5.6
1	A	613	GLN	5.3
1	A	1487	TYR	5.0
1	A	411	GLN	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 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
2	ACT	A	2074	4/4	0.84	0.39	5.70	61,62,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ACT	A	2075	4/4	0.93	0.25	1.23	59,60,62,62	0
3	FMN	A	2070	31/31	0.98	0.22	1.21	53,57,60,62	0
4	F3S	A	2072	7/7	1.00	0.15	-1.01	60,63,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.