



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 09:52 am GMT

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

<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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

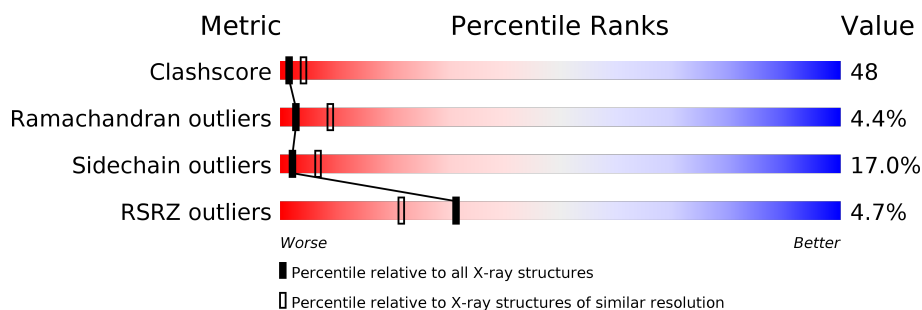
1 Overall quality at a glance

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	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (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	

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	-
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.

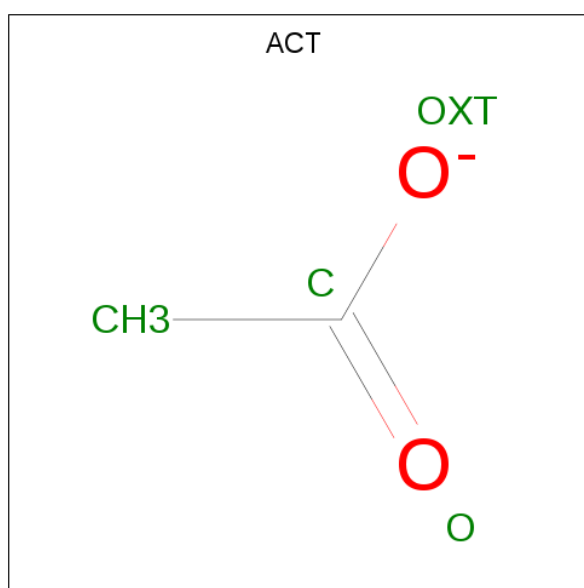
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

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:

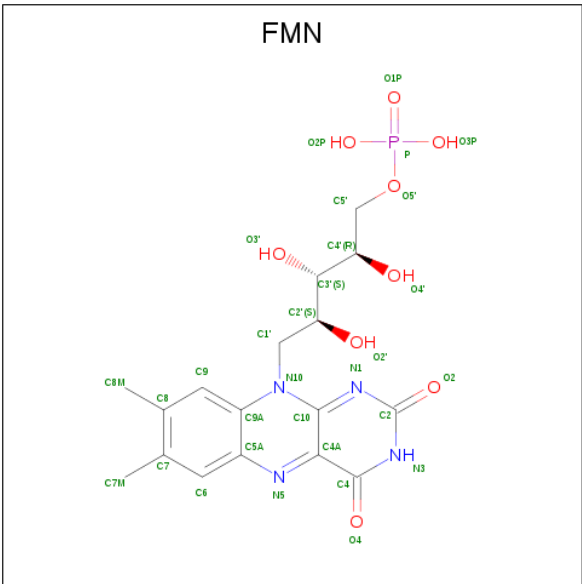
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	CONFLICT	UNP P55038
A	581	THR	ASP	CONFLICT	UNP P55038
A	1507	ASN	GLY	CONFLICT	UNP P55038

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



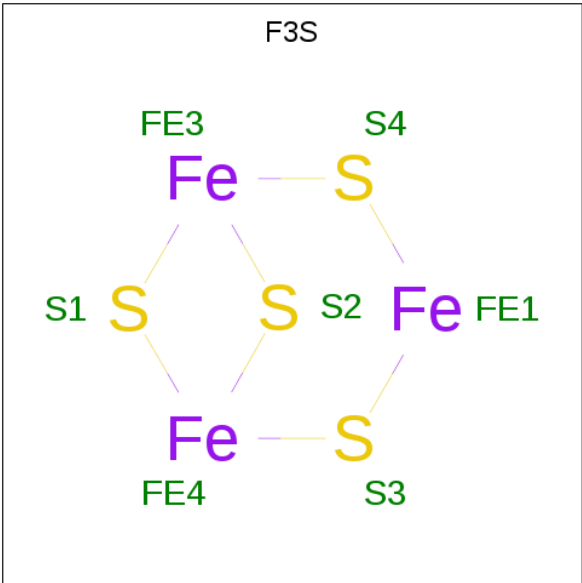
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



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

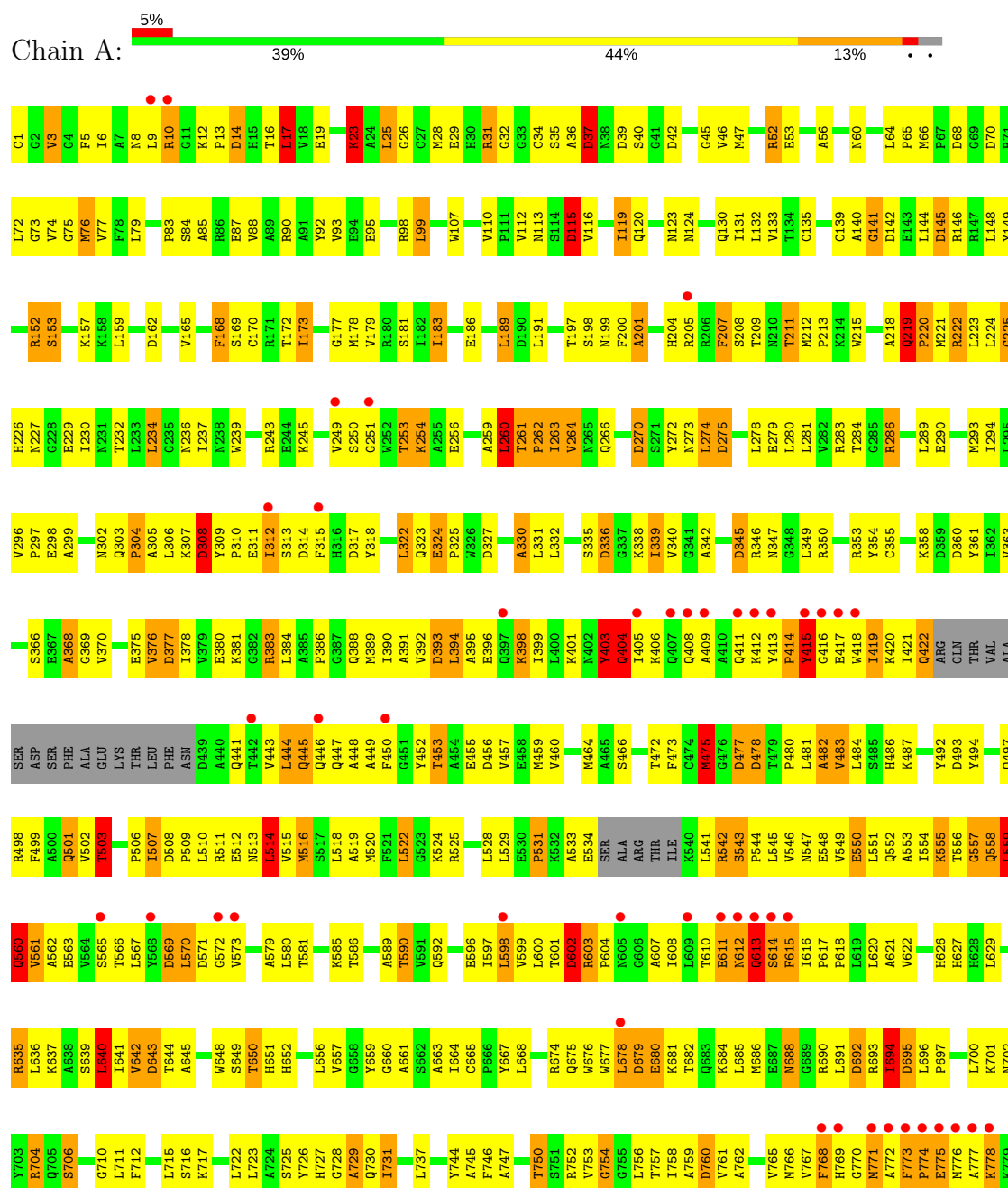
- Molecule 5 is water.

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	M1376	L1303	K1229	Q1155	T1085	D1008	P924	D847	L780
THR	K1441	G1377	M1304	Q1230	Q1156	E1086	I1009	H930	F846	E781
GLY	I1442	R1377	F1305	M1231	L1159	R1089	E1013	G931	D851	N782
GLU	N1443	Q1306	Q1306	R1232	L1161	R1095	D1014	G932	Q852	F783
LYS	P1444	A1379	G1307	Q1233	Q1161	M1092	L1015	G933	G784	G784
THR	E1445	G1380	A1308	W1234	V1166	E1093	L1016	H934	F785	F785
LEU	I1446	E1381	Q1311	L1235	V1166	M1094	Q1017	I855	Y788	Y788
THR	I1447	R1382	G1311	E1238	Q1169	Q1095	L1018	L857	G791	G791
SER	T1448	F1383	A1315	P1239	Q1169	R1097	D1021	A938	E858	E858
VAL	L1449	V1385	F1316	V1240	W1170	R1097	H1022	N939	E859	E859
	Q1450	R1386	N1317	H1241	W1171	R1098	Q1024	S940	V860	Y794
	R1451	R1387	L1318	V1246	F1173	R1099	H1025	K943	V863	Y795
	I1452	S1388	D1319	L1247	F1174	V1100	Q1024	V867	N797	H796
	T1453	V1389	G1320	L1248	W1175	L1101	I1025			
	A1454	K1391	M1321	D1248	F1176	L1102				
	S1455	E1392	L1323	D1250	A1177	R1103	A1028			
	K1456	A1393	H1324	I1251	A1178	R1104	A1029			
		V1394	L1325			D1105	Q1030			
	E1459	I1394	L1325	D1254	V1181	G1106	V1031			
	Q1460	E1395		P1255	R1182	G1107	S1032			
	K1462	G1396	E1328	D1256	R1183	K1109	L1035			
	S1463	A1397	A1329	I1257	L1184	T1110	V1036			
	L1464	G1398	Y1332	Q1258	L1188	G1111	A1037			
	I1465	D1399	V1333	E1259	L1188	W1112	E1038			
			G1394	H1263	G1189	D1113	I1039			
	T1472	E1402	K1336	Q1264	V1190	M1116	G1040			
	G1473	E1403	G1336	T1265	R1191	A1117	L1041			
	S1474	Y1404	M1337	T1266	S1192	G1042	I945			
	P1475	M1405	N1338	T1267	L1193	T1043	A968			
	K1476	T1406		A1267	D1194		Q969			
	G1477			T1268	D1195					
		V1409	T1344	K1269	T1196		K972			
	I1480	I1410	V1345	T1270	I1197		P973			
	W1484	V1411	P1346	Y1271	G1198		N892			
	S1485	V1412	H1347	R1272	R1199		N893			
	D1486		P1348	L1273	T1200		G976			
	T1487	V1416	Q1349	L1274	D1201		G977			
	L1488	G1417	A1350	N1275	L1202		Q978			
	G1489	R1418	S1351	T1276	L1203		L979			
	K1490	N1419	F1352	D1277						
		V1420	A1353	D1278						
	F1491	G1421	P1354	R1278	D1208		I1058			
	W1492	A1422	E1355	T1279			S1059			
	Q1493	G1423	D1356		L1211		G1060			
	A1494	M1424	V1358	T1282	S1212		H1061			
		T1425	I1359	R1283	T1214		D1062			
	P1497	L1428	I1360	I1288	Q1215		T1065			
	S1498	A1429	T1363	A1289	N1216		A1067			
	E1499	Y1430	C1364	Y1292	L1217		S1068			
	K1500	F1431	G1366	G1293	D1220		S1071			
	D1501	L1432	Y1366	N1294	L1223		P996			
	P1503	D1433	G1367	N1295	C1148		G997			
	E1504	E1434	A1368	G1296	T1224		H1075			
		V1435	T1369	F1297	L1225		A1076			
		G1436		E1298	P1226		E1081			
	N1507	D1437	N1372	T1302	T1227		V1084			
ASP										
VAL										
SER										

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.	wwPDB-VP
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 [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	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 [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	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

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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	1.42	4 (12%)	39,50,50	1.72	8 (20%)
4	F3S	A	2072	1	0,8,8	0.00	-	0,11,11	0.00	-
2	ACT	A	2074	-	1,3,3	0.87	0	0,3,3	0.00	-
2	ACT	A	2075	-	1,3,3	1.74	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	-	0/0/14/14	1/1/2/2
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	-3.17	1.35	1.41
3	A	2070	FMN	C6-C5A	-2.07	1.38	1.41
3	A	2070	FMN	C4A-N5	2.18	1.36	1.33
3	A	2070	FMN	C4-N3	3.49	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	-3.59	113.21	120.72
3	A	2070	FMN	C4A-C4-N3	-3.43	118.59	123.47
3	A	2070	FMN	C7M-C7-C8	-2.04	116.46	120.72
3	A	2070	FMN	O4'-C4'-C3'	2.17	114.46	109.10
3	A	2070	FMN	O3P-P-O5'	2.18	112.53	106.73

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2072	F3S	FE3-FE4-S1-S2

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	70 (4%)	31 21	24, 34, 41, 85	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	TYR	5.8
1	A	415	TYR	5.6
1	A	613	GLN	5.4
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. 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
2	ACT	A	2074	4/4	0.84	0.39	61,62,63,63	0
2	ACT	A	2075	4/4	0.93	0.25	59,60,62,62	0

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

6.5 Other polymers [i](#)

There are no such residues in this entry.