



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:46 PM BST

PDB ID : 4V59  
Title : Crystal structure of fatty acid synthase complexed with nadp+ from thermomyces lanuginosus at 3.1 angstrom resolution.  
Authors : JENNI, S.; LEIBUNDGUT, M.; BOEHRINGER, D.; FRICK, C.; MIKOLASEK, B.; BAN, N.  
Deposited on : 2007-03-09  
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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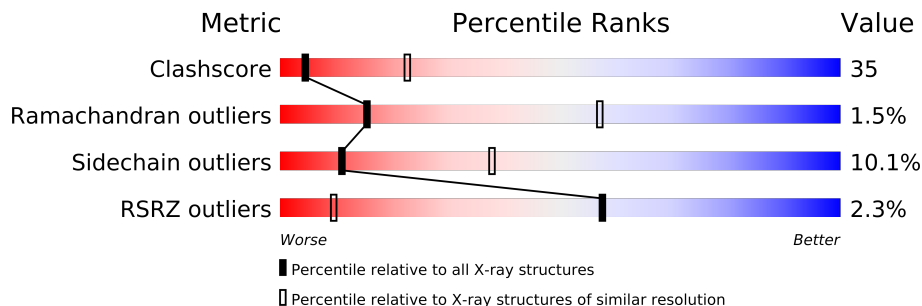
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1878	
1	B	1878	
1	C	1878	
1	D	1878	
1	E	1878	
1	F	1878	
2	G	2060	
2	H	2060	
2	I	2060	
2	J	2060	
2	K	2060	
2	L	2060	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 167247 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FATTY ACID SYNTHASE ALPHA SUBUNITS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1457	Total	C	N	O	S	0	0	0
			11514	7290	2005	2170	49			
1	B	1464	Total	C	N	O	S	0	0	0
			11571	7323	2015	2183	50			
1	C	1462	Total	C	N	O	S	0	0	0
			11555	7312	2012	2181	50			
1	D	1467	Total	C	N	O	S	0	0	0
			11593	7336	2021	2186	50			
1	E	1456	Total	C	N	O	S	0	0	0
			11506	7285	2004	2169	48			
1	F	1461	Total	C	N	O	S	0	0	0
			11546	7307	2010	2179	50			

- Molecule 2 is a protein called FATTY ACID SYNTHASE BETA SUBUNITS.

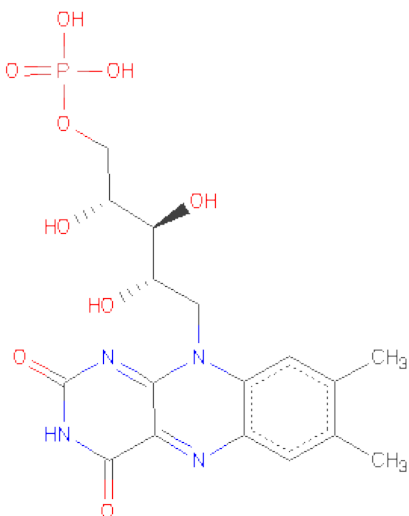
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	H	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	I	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	J	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	K	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			
2	L	2060	Total	C	N	O	S	0	0	0
			16200	10314	2781	3051	54			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		





A1323	I1249	F1156	H1075	N989	Q906	N835	D741	G647	I574	S491	T418	K330	THR
A1327	L1250	D1157	I1078	L990	F907	T836	Y742	L648	R575	I492	F419	D931	ASP
E1330	Q1251	R1158	R1079	V994	P908	L837	F746	A655	A576	P493	G420	Q332	VAL
R1333	S1253	V1160	L1080	V995	P909	T838	A747	A655	M579	T498	R421	R333	ILE
R1334	F1254	A1161	L1081	V996	D910	I839	A747	A655	M579	T498	L422	A334	ARG
R1335	T1257	G1162	E1082	T997	K912	V843	R754	G661	T584	D501	R423	L345	ALA
R1336	M1258	Q1163	P1083	G998	G913	W846	E755	A662	M585	A502	V424	F336	PRO
P1337	A1259	L1164	P1084	L999	L914	T847	I756	A667	M586	R503	V426	K337	VAL
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I1339	G1167	G1165	F1086	E1001	T916	R848	S758	V669	GLY	N505	E428	L340	GLN
M1340	M1168	G1167	F1086	E1001	K917	R848	I759	V669	LYS	N505	E428	E341	LEU
S1341	M1264	G1167	F1086	E1001	L918	T850	D760	G671	ASP	O507	V430	F342	LYS
R1342	L1265	M1168	G1167	E1001	R919	G851	S761	G672	ARG	Y508	V430	I343	LYS
P1343	L1266	R1171	P1091	G1006	R919	L852	A766	L673	ARG	R513	C433	I343	LEU
T1344	L1267	R1172	M1092	M1007	I922	M853	A766	L673	ARG	R513	C433	I343	LEU
S1345	S1268	Y1173	K1093	A1008	I922	M853	A766	L673	ARG	R513	C433	I343	LEU
T1346	S1269	G1174	K1094	A1008	S926	S854	A766	L673	ARG	R513	C433	I343	LEU
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F1351	I1273	E1177	L1096	W1012	Q930	L858	T772	T683	GLY	Y522	M441	A353	PRO
M1352	K1274	D1178	V1100	M1014	I933	A860	L777	T683	ASN	V523	P442	K356	SER
E1353	T1275	I1179	V1101	M1014	I933	A860	L777	T683	ASN	V523	P442	K356	LEU
S1354	P1276	I1180	E1103	Y1017	N940	G862	L777	T683	GLY	M526	L444	A357	ALA
G1355	P1277	Q1104	F1103	L1022	V943	V863	A780	F687	ASN	A527	L444	F358	ILE
P1356	G1278	D1105	E1103	E1023	V943	V863	A780	F687	HIS	A527	L444	F358	ILE
C1357	A1280	L1186	L1106	E1023	V943	V863	A780	F687	SER	A527	L444	F358	ILE
T1360	C1282	T1187	E1107	M1031	D947	V868	T783	T692	ARG	S533	E446	A360	ASP
I1361	I1283	L1191	P1108	M1032	H948	R869	K786	E693	PRO	Q534	M448	S361	VAL
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M1363	Y1291	Y1207	E1117	H1038	L951	Q873	R793	Q896	GLY	R538	Y450	L368	LYS
A1365	T1292	Y1207	E1118	M1039	Y952	Q873	R793	Q896	GLY	R538	Y450	L368	LYS
Q1366	T1293	F1209	K1120	L1042	I956	E875	L799	G697	ILE	N543	I452	I382	THR
L1367	Q1296	V1213	R1121	S1048	P959	M876	L801	G703	P614	R546	C455	Y383	LEU
M1371	G1297	H1214	I1129	G1049	R960	L880	S802	G703	P614	R546	C455	Y383	LEU
G1372	A1299	H1215	F1130	V1051	N962	L881	S802	G703	P614	R546	C455	Y383	LEU
V1373	L1215	S1216	E1131	D1052	L963	G882	L801	G703	P614	R546	C455	Y383	LEU
P1374	E1217	E1217	I1132	T1055	K964	L883	L801	G703	P614	R546	C455	Y383	LEU
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T1386	G1306	S1224	T1139	P1058	P967	V889	L813	Q716	N625	Q555	E468	V398	LYS
I1389	F1307	G1225	Y1140	V1059	P968	N890	Y814	G717	N625	Q555	E468	V398	LYS
V1393	D1308	V1226	E1141	D1060	W973	L891	S815	S718	Y628	R556	G470	Y399	PHE
P1394	F1309	T1229	L1142	D1063	K978	C892	S817	V726	S629	R556	G470	Y399	PHE
A1395	Q1311	L1232	A1146	V1064	P979	Q893	S817	V726	S629	R556	G470	Y399	PHE
P1396	E1312	L1233	T1147	K1065	L980	F898	L821	V726	S629	R556	G470	Y399	PHE
L1401	E1313	R1233	L1148	Y1068	Q983	A899	T823	V730	G634	F566	L481	D409	PRO
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	Y1236	M1235	L1150	E1069	L984	L901	L824	D731	I635	N567	P484	M413	GLU
	Y1237	Y1237	K1070	K1070	R985	N302	W828	G735	Y636	A568	P485	M413	GLU
	D1238	D1238	Y1071	Y1071	G986	G903	L736	G735	Y636	A568	P485	M413	GLU
			L1154	L1154	N987	G904	W833	L736	Y636	A568	P485	M413	GLU
			Q1155	Q1155	V988	L905	G834	L740	L640	Y570	Y487	Y415	THR
												I325	PRO
												I417	LEU
												I417	ASP





- Molecule 1: FATTY ACID SYNTHASE ALPHA SUBUNITS





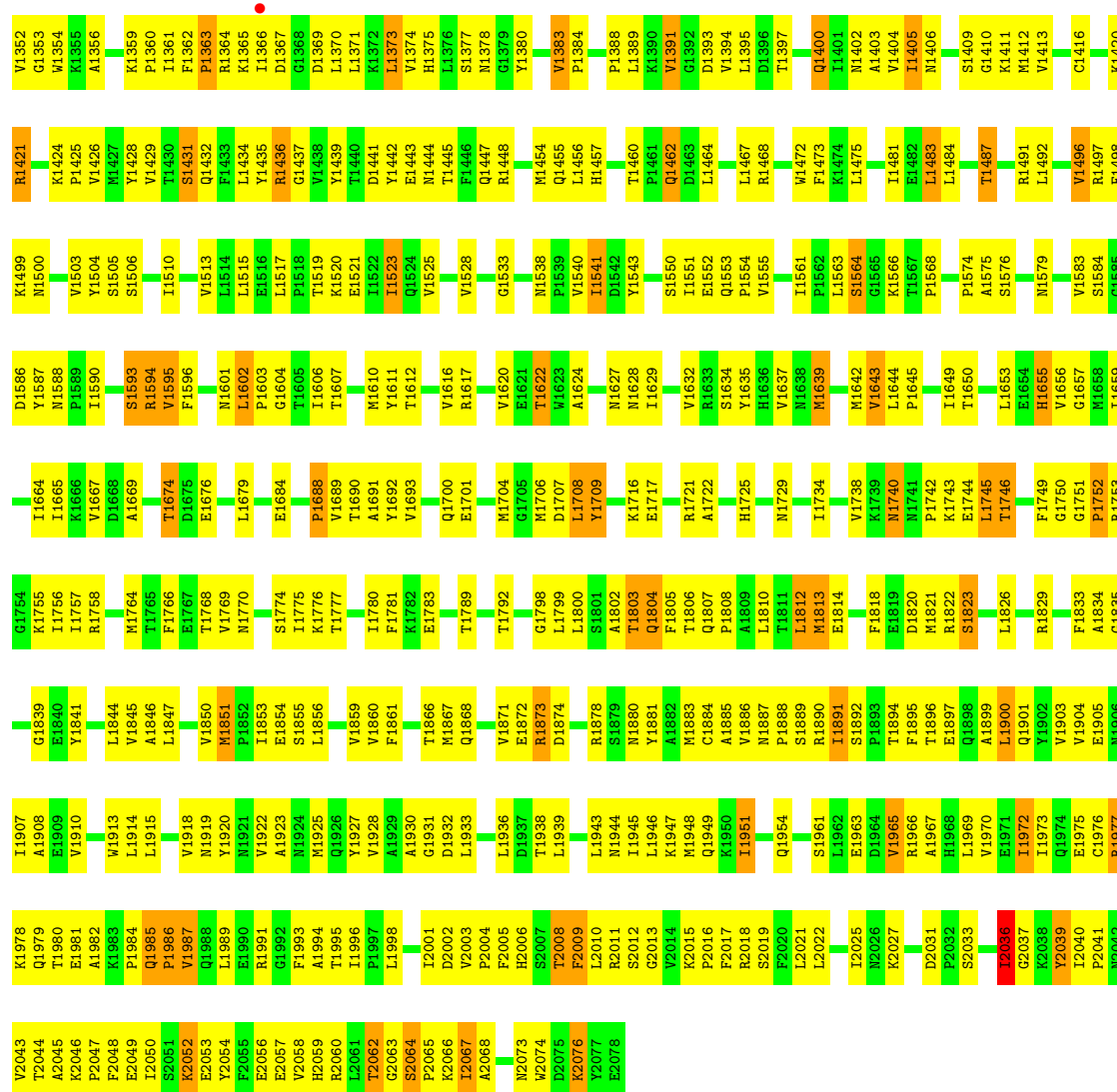
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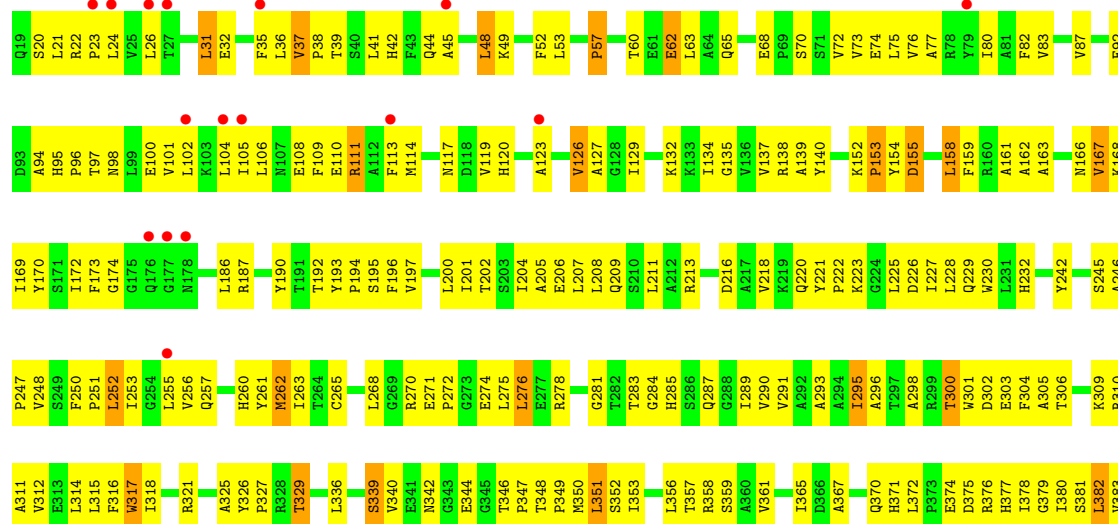


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I1217	Q1059	A123	Q1060	Q911	F910	D841	T776	N623	K473	P395	R321	L252
S1218	V1061	T1124	V1062	Q912	Q912	Q842	T777	Y626	K474	S397	A325	G254
Y1219	G1063	P1128	G1064	N913	N913	E844	Q778	R627	T475	L398	Y326	L255
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R1262	L1098	L1098	K956	K956	K956	S889	H751	I674	P518	I451	E374	R299
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K1338	F1030	F1030	T959	T959	T959	E890	H753	L676	G520	D454	R376	W301
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F1335	Y1102	Y1102	F962	F962	F962	E894	F755	P686	S522	V455	I378	E303
E1336	D1104	D1104	R963	R963	R963	K897	D756	I687	G523	G379	G379	F304
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F1342	E1107	E1107	E967	E967	E967	R899	L762	T691	P461	A462	L382	T306
G1343	P1111	P1111	Y969	Y969	Y969	D900	L763	W664	N529	S464	V383	K309
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D1347	I1113	I1113	S1050	S1050	S1050	K904	I768	V701	K532	V466	F389	E313
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V1351												

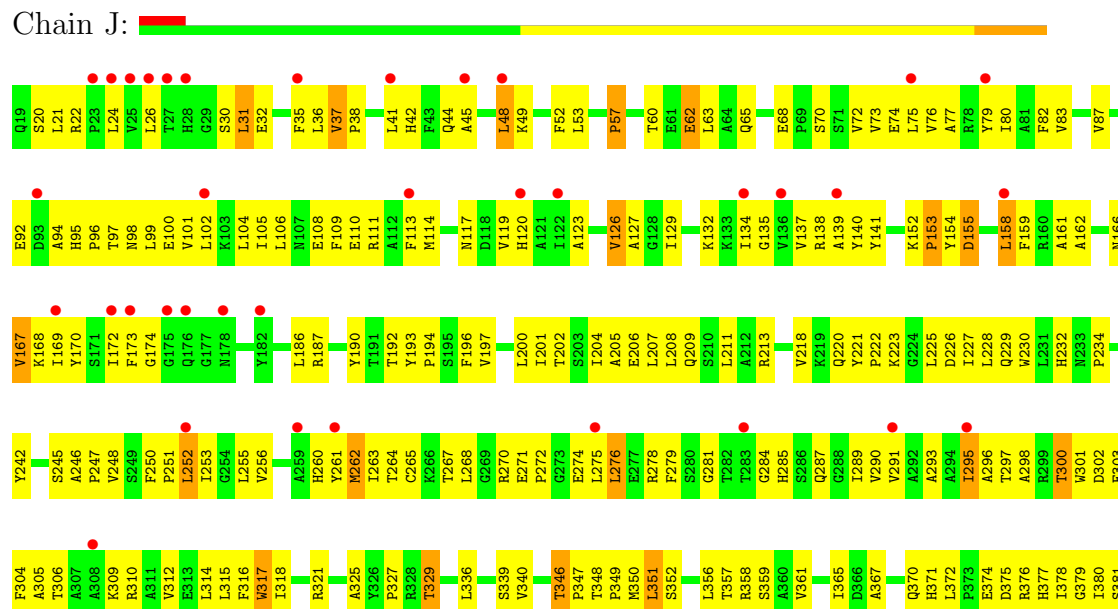
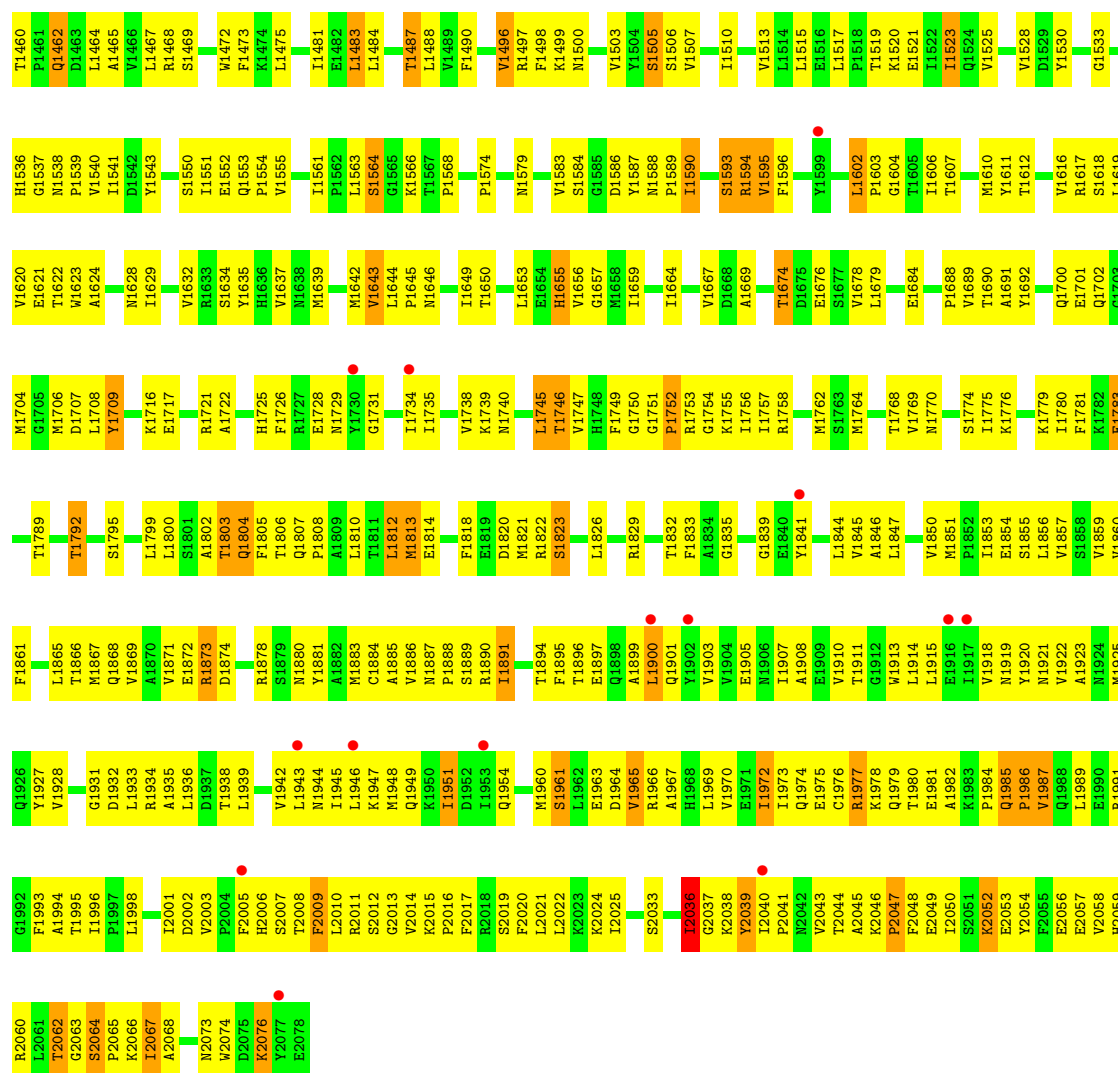




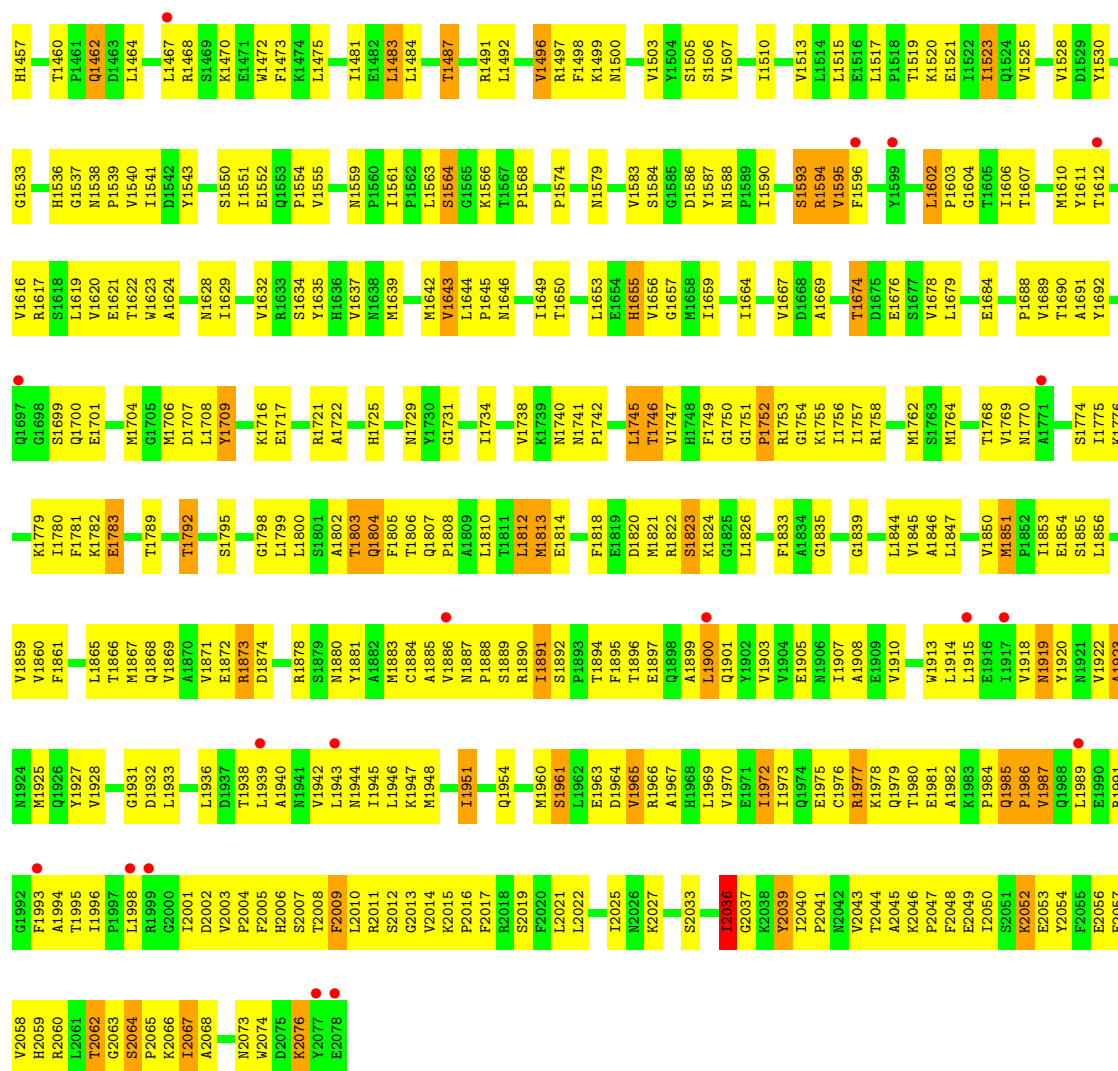
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F1343	F1343	E1268	V1103	E1036	E967	K897	S825	I687	M608	T535	I467	V383	L314
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P1345	G1270	G1105	G1106	S1046	R969	R899	K827	L762	P610	V537	V469	R387	F316
D1346	Y1271	F1106	F970	W1041	R969	D900	A828	L763	T611	L541	Y470	N388	W317
D1347	E1107	E1107	T971	K1044	T971	Y901	K829	M764	T612	A542	D471	F389	I318
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Y1116	F1116	F1116	Q837	E1051	Q881	D909	G837	I706	M622	E551	L481	S397	T329
P1212	D1082	D1082	F910	E1082	Q881	F910	V838	I707	M623	V552	G482	L398	A332
T1215	I1083	I1083	Q911	I1083	S984	Q911	D839	T708	V626	K555	D483	G400	P333
V1216	Y1087	Y1087	D985	Y1087	D985	K912	D840	L709	H627	K555	D483	L401	S334
I1217	G1058	G1058	D987	G1058	D987	Y913	Q842	G781	I628	D560	E484	N402	T335
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K1230	I1066	I1066	L996	I1066	L996	L926	V854	Y789	A638	D571	D497	Q416	G345
T1231	L1067	L1067	L997	L1067	L997	E927	V854	I724	M641	N572	D497	P420	T346
V1232	Q1068	Q1068	D928	Q1068	D928	N929	T856	I792	V573	K574	P498	P420	P347
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K1235	A1071	A1071	Y931	E1071	E1002	Y931	L858	G794	V581	N500	N500	K425	P349
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F1247	F1176	F1176	H1015	I1086	H1015	V944	T870	P806	V581	N500	N500	F432	L353
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G1249	L1088	L1088	L1017	L1088	L1017	N951	F875	D808	V581	N500	N500	F432	L353
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S1377	Y1169	Y1169	H1008	S1076	L1007	H936	E863	K799	A651	K582	V506	F432	L353
N1378	S1170	S1170	N1009	V1078	N1009	N938	I865	G801	V581	N500	N500	F432	L353
G1379	W1171	W1171	A1010	I1079	A1010	A1010	H866	Y802	V581	N500	N500	F432	L353
Y1380	R1172	R1172	Q1011	I1079	Q1011	L941	H866	P803	V581	N500	N500	F432	L353
V1383	H1173	H1173	D1012	E1083	D1012	N942	K867	P804	V581	N500	N500	F432	L353
P1384	A1174	A1174	V1013	D1085	Q1014	Y943	L868	P738	V581	N500	N500	F432	L353
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V1391	T1177	T1177	F1016	I1086	F1016	N950	R871	F807	V581	N500	N500	F432	L353
G1392	L1178	L1178	L1017	L1088	L1017	N951	F875	D808	V581	N500	N500	F432	L353
D1393	E1179	E1179	L1018	G1089	L1018	D952	K876	P804	V581	N500	N500	F432	L353
V1394	V1180	V1180	L1019	G1089	L1018	D952	K876	P804	V581	N500	N500	F432	L353
L1395	F1181	F1181	H1091	H1091	G1020	P953	K877	M811	V581	N500	N500	F432	L353
D1396	N1092	N1092	Q1021	H1091	G1020	L955	E878	M811	V581	N500	N500	F432	L353
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Q1400	F1187	F1187	H1094	H1094	R1022	K956	I853	M816	V581	N500	N500	F432	L353
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V382	V383	R387	F389	I318	V390	L318	V390	L318	V390	L318	V390	L318	V390
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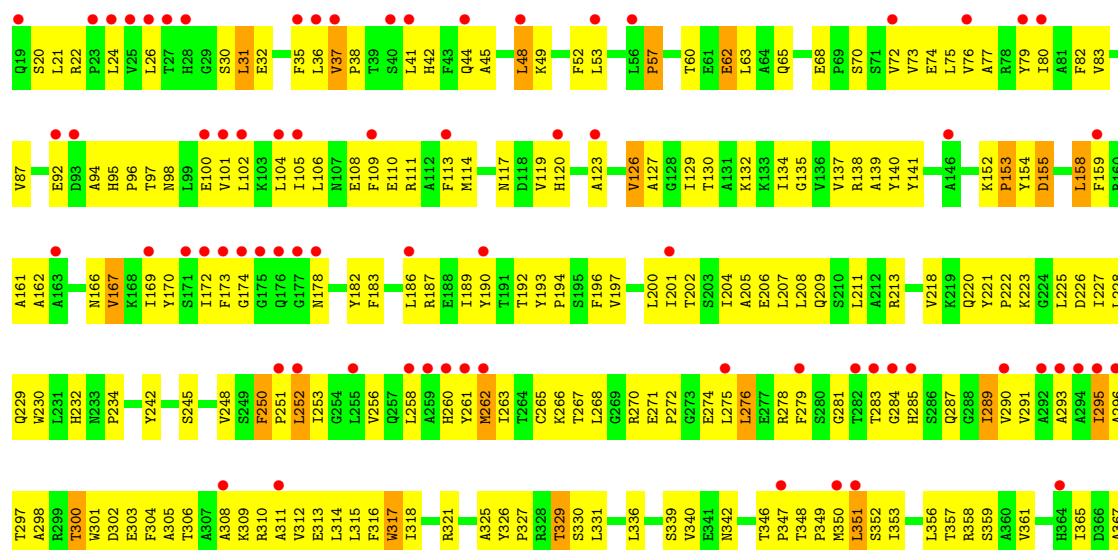


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D1393	V1179	T1251	V1179	K1095	F1031	P962	S889	T818	E754	V685	G608	G536	V469	T392
V1394	V1180	V1257	V1180	K1096	F1030	R963	S890	R819	E755	P686	T609	V537	V470	G393
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Q1400	Q1188	Q1188	Q1188	Y1103	Y1040	E967	E884	H823	P760	P601	V613	G543	T474	S397
I1401	T1189	T1189	T1189	D1104	Y1041	E968	R897	T824	S698	S698	G544	G543	T474	S397
N1402	N1190	N1190	N1190	Y1105	Y1042	R969	R898	S825	L761	I761	P614	A544	D477	L398
A1403	H1191	H1191	H1191	F1047	Q976	R970	R899	S826	L762	T699	W615	I545	D477	Y399
V1404	L1192	L1192	L1192	K1043	Q1049	S978	D900	Q827	H764	V701	D816	R478	R478	G400
I1405	E1114	E1114	E1114	Y1115	S1050	S979	Y901	A828	Y765	T708	F617	T550	R479	L401
N1406	F1116	F1116	F1116	F1051	E051	L980	B966	A835	I774	L709	V618	E551	E480	N402
K1410	R1200	R1200	R1200	D1052	P1052	Q981	D909	G836	I774	L709	V618	E551	E480	N402
K1411	Y1203	Y1203	Y1203	I1053	I1053	L986	F910	G837	L776	G710	I628	V552	L481	L403
M1412	V1204	V1204	V1204	Y1057	Y1057	P989	Q911	Q830	L777	I711	M622	K555	D483	K409
V1413	T1207	T1207	T1207	G1058	G1058	P990	Y913	A831	A778	H713	G632	K555	E484	A410
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P1425	T1212	T1212	T1212	Y1061	Y1061	A992	Y916	V834	M773	T708	Y626	L558	D485	P411
V1426	E1126	E1126	E1126	G1062	G1062	R995	R917	A846	I774	L709	H627	F559	L486	L414
M1427	P1212	P1212	P1212	P1063	P1063	R995	N918	Y847	G781	K717	I628	F559	L487	L414
Y1428	T1215	T1215	T1215	T1064	T1064	L996	Y924	T851	G782	P718	A631	D560	P488	P415
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V1292	V1219	V1219	V1219	G1069	G1069	E1002	D928	T856	Y790	V727	I648	G577	T505	I435
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K1297	Q1224	Q1224	Q1224	S1143	S1143	T1005	T930	L858	L792	N729	I652	V681	V506	T436
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P1300	D1302	D1302	D1302	L1146	L1146	T1006	A932	E860	G794	A731	G655	S584	T511	A437
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L1306	E1233	E1233	E1233	S1143	S1143	T1009	Y935	E863	S797	P735	T659	Q587	V514	L444
F1309	D1157	D1157	D1157	Y1076	Y1076	A1010	R936	E864	S797	P735	T659	Q587	V514	L444
D1310	S1159	S1159	S1159	K1077	K1077	A1011	R937	P864	T798	T736	V660	T588	F516	A447
G1311	F1160	F1160	F1160	Y1078	Y1078	Q1011	N938	I865	K799	F737	N661	F589	G517	H448
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G1313	E1081	E1081	E1081	Y1013	Y1013	Y1014	L941	K867	G801	I739	I663	V590	G519	I451
G1314	L1163	L1163	L1163	Q1014	Q1014	H1015	N942	L868	H802	I740	Y664	D520	G520	L452
G1315	I1164	I1164	I1164	F1016	F1016	F1016	N943	L868	P803	L741	V665	M594	V521	G453
E1314	L1084	L1084	L1084	L1017	L1017	L1017	Y944	T870	P804	O742	N666	M594	V521	G453
E1315	Y1169	Y1169	Y1169	L1018	L1018	L1018	R871	M805	M805	W743	M670	L597	I524	V455
V1316	S1170	S1170	S1170	L1019	L1019	L1019	G872	G872	F807	T744	M670	L597	I524	V455
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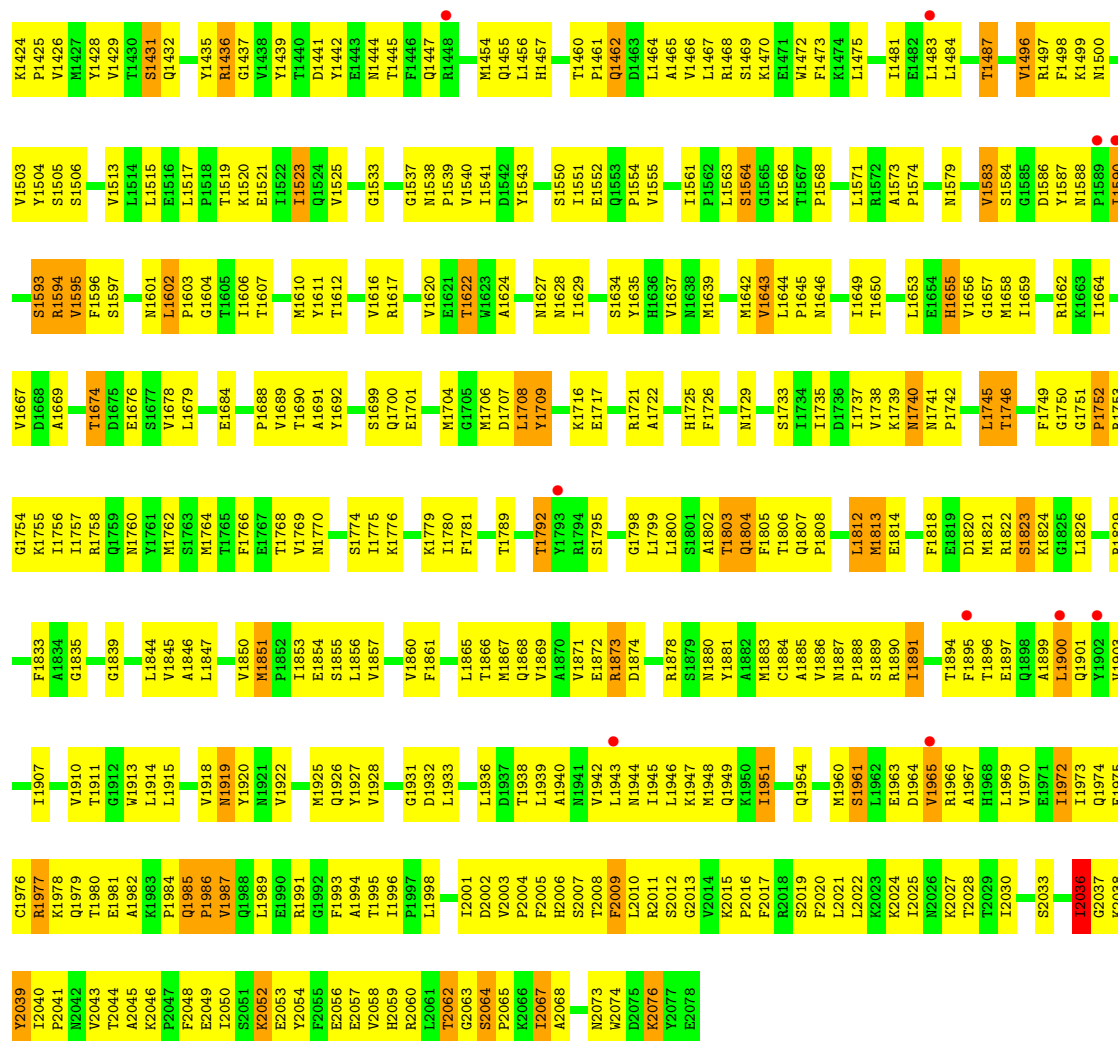
## ● Molecule 2: FATTY ACID SYNTHASE BETA SUBUNIT

Chain K:

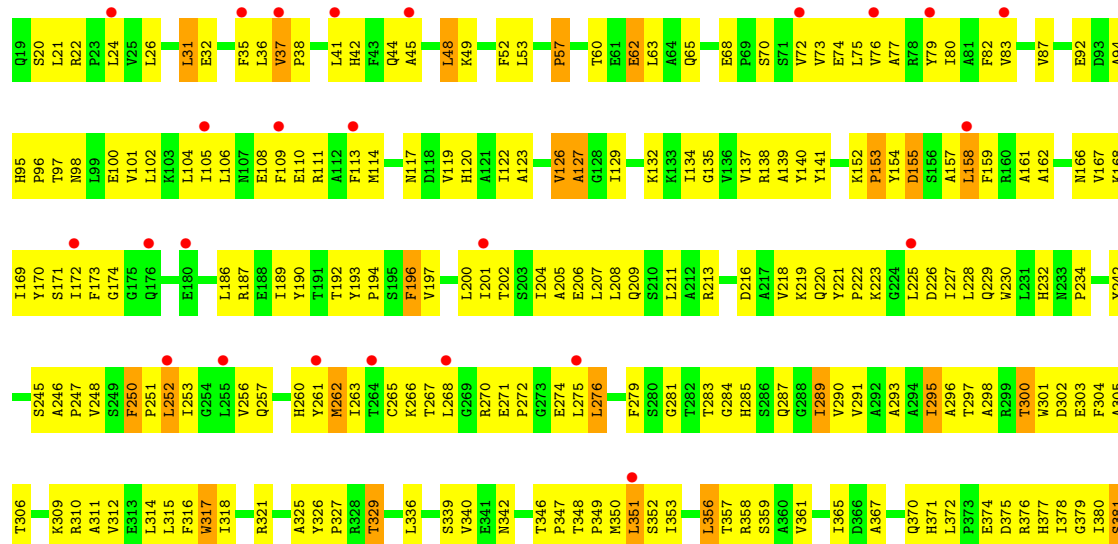


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I1357	R1291	V1219	S1143	G1089	Y1000	E928	L858	S795	G795	T652	S585	F516	A447	P373
T1358	T1292	R1220	L1146	V1071	E1002	M929	S859	W796	A731	P653	Q586	F517	H448	E374
K1359	W1293			I1070	E1002	T930	E860	S797	K732	P654	Q587	F518	D375	D376
P1360	F1294			A1072	A1003	Y931	M861	T798		G655	T588	G519	I451	D377
I1361		Q1224	A1149	A1073	S1004	E932	G662	K799	P735	F589	F589	G520	D451	K376
F1362	V1299	S1225	P1150	K1074	T1005	E933	E863	F800	T736	V660	S590	G521	D454	K377
P1363	P1300	K1227	K1074	Y1075	Q1006	Y934	T865	G802	F737	G661	D591	S521	V455	K378
R1364	F1301	D1228	D1156	S1076	Q1007	Y935	R865	Y802	F738	T663	M594	S522	D456	K379
K1365	D1302	V1229	P1157	K1077	L1007	H936	R866	P803	T739	T664	R596	G523	K458	I380
I1366		K1230	D1158	V1078	N1008	R937	K867	P804	I740	T663	L597	G524	K459	I381
	L1305	T1231	S1159	I1079	A1010	M938	L868	M805	L741	V665	R596	G525	K459	L382
D1369		V1232	F1160	I1079	A1011		A869	P806	Q742	V665	L597	V526	L460	V383
F1370	F1309	E1233		D1080	Q1011	L941	T870	F807	W743	G666	L598	G527	P461	N384
L1371	D1310	E1233		E1081	D1012	M942	R871	D808	T744	T666	G599	T528	A462	A385
K1372	G1311	K1235	L1163	I1082	V1013	Y943	G872	G809	G745	M670	V600	N529	S463	A386
L1373	G1312	L1236	L1164	K1084	H1015	Y944	V873	C810	G746	G871	P601	R530	S464	R387
V1374	R1313	V1237	Y1169	D1085	F1016	K945	L874	M811	R747	M672	P602	R531	L465	N388
H1375	E1314	G1238	S1170	I1086	L1017	R946	F875	F812	G748	Q673	R603	K532	V466	F389
L1376	I1315	D1239	W1171	L1087	L1018	W950	K876	G813	G749	T674	M604	D533	T467	V390
S1377	V1316	N1240	R1172	D1088	L1019	R815	K877	S814	G750	P675	V605	T535	P468	V391
K1378	N1317	E1241	H1173	G1089	Q1020	I951	E878	R816	H751	L676	A606	T392	Y469	T392
V1379	A1318	I1242	A1174	I1090	G1021	D952		M817	H752		G507	G536	Y470	G393
Y1380	Q1319	A1243	M1175	H1091	R1022	P953	K882	M817	S753	V685	M608	V537	D471	P394
	A1320	T1244		N1092	K1026	S954	L883	T818	F754	P686	T609	L541	T472	P395
V1383	F1321	T1245	T1177	D1093	P1027	L955	D887	A819	E755	P687	K473	A542	T474	I396
P1384	A1322	L1246	T1178	H1094	V1028	K956	R888	K820	T756		T611	G543		L398
	D1323	F1247	E1179	I1095	P1029	T959	K889	E821	F757	L690	T612	F544	D477	L401
F1324	F1324	E1248	V1180	K1096	F1030	R962	K890	H823	Q759	T691	P614	I545	R479	
L1389	H1325	G1249	F1181	P1097	F1031	F963	R891	T824	T760	G693	W615	D546	E480	R406
K1390	H1326	R1250		L1098	P1032	R964	K892	K825	L762	S698	F617	T550	L481	K409
V1391	A1327	T1251	H1185	L1099	A1033	R965	E894	S826	L763	E700	V618	E551	E480	A410
G1392	V1328		R1186	L1102	E1036	V966	K897	Q827	K764	V701		V552	E484	P411
D1393	G1329	V1257	Q1187	Y1103		E967	R898	K829	Y765		T621	K555	D485	L414
V1394	Q1330	P1258	Q1188	D1104	Y1041	R969	R899	Q830			M622	F558	L487	D415
L1395	T1331	L1259	T1199	G1105	F1042	R970	D900	I832	N773	E704	N623	F559	P488	Q416
D1396	G1332	T1260	M1190	E1107	K1043	T971	Y901	V833	W774	Y705	Y626	D560	E489	N417
	E1333		K1193	K1106	D1044	S972	I902	D834	V775	Q707	I628	R561	L490	R418
Q1400	F1335	Y1265	R1194	V1110	D1045	Q976	K905	P836	L776	T708	E629	R561	V491	I419
I1401	F1336	H1266	R1195	P1111	S1046	L979	D908	G837	A778	G710	A631	A565	R492	P420
N1402	D1337	P1267	L1196	V1112	L1047	Q981	K904	D840	G779	I711	G632	V566	M493	K425
A1403	R1338	E1268	F1196	V1113	W1048			D841	G781	H713	G633	A569	D497	K426
V1404	G1339	A1269	A1197	I1113	Q1049	P977	I906	Q842			G634	A569	P498	F428
I1405	K1340	G1270	P1198	E1114	Q1049	S978	N907	W843	G783	F716	Y635	V570	V499	F429
	D1341	Y1271	T1199	Y1115	S1050	L979	D908	N845	G784	K717	A638	D571	N500	F432
S1409	F1342	A1272	R1200	F1116	E1051	L980	D909	T846	V775	P718	E502	V573	E502	L433
G1410	F1343	P1273			D1052	Q981	F910	Y847	L776	G719	M641	K574	T505	P434
K1411	A1344	I1274	Y1203	R1119	I1053	L986	Q911	T851		A723	D642	P578	T506	I435
M1412	M1346	R1275	V1204	I1120	Y1057	D987	K912	Y851	G783		A644	R579	V506	A437
V1413	T1347	M1278	T1207	A1123	G1058	E988	V913	T851	G784	F716	Y635	L580	F507	F438
	F1348	E1279	N1208	Q1059	Q1058	P989	N914	T846	S785	P718	A638	V573	E502	L433
C1416	A1349	G1280	P1209	E1126	D1060	Y990	F915	Y847	E786	G719	M641	K574	T505	P434
L1419	I1350	R1281	P1212	E1127	V1061	P991	G916	T851	D787	S720	D642	P578	T506	I435
R1420	V1351	K1286	T1215	P1128	C1065	A992	N919	T851	T788	A723	D642	R579	V506	A437
	F1352	E1287		A1135		R995	Y924	V854	Y791	Q726	I648	L580	F507	F438





Chain L:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.78Å 412.67Å 220.90Å 90.00° 111.57° 90.00°	Depositor
Resolution (Å)	12.00 – 3.10 96.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.10) 92.6 (96.48-3.10)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, $R_{free}$	0.270 , 0.300 0.254 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.1	EDS
Estimated twinning fraction	0.078 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 645017 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	167247	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.43	0/11744	0.60	1/15873 (0.0%)
1	B	0.43	0/11801	0.60	1/15949 (0.0%)
1	C	0.44	0/11785	0.59	0/15928
1	D	0.43	0/11824	0.60	0/15980
1	E	0.42	0/11736	0.59	0/15863
1	F	0.44	0/11776	0.60	5/15916 (0.0%)
2	G	0.36	0/16573	0.53	0/22516
2	H	0.35	0/16573	0.53	0/22516
2	I	0.35	0/16573	0.53	0/22516
2	J	0.36	0/16573	0.54	0/22516
2	K	0.39	0/16573	0.55	0/22516
2	L	0.36	0/16573	0.54	0/22516
All	All	0.39	0/170104	0.56	7/230605 (0.0%)

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	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	585	MET	N-CA-C	9.44	136.48	111.00
1	B	608	LYS	N-CA-C	-8.94	86.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	614	PHE	N-CA-C	6.04	127.30	111.00
1	F	613	PRO	CA-C-N	5.57	129.46	117.20
1	A	579	MET	N-CA-C	5.39	125.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	ALA	Peptide
1	F	613	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11514	0	11476	746	1
1	B	11571	0	11529	708	1
1	C	11555	0	11507	717	0
1	D	11593	0	11552	725	0
1	E	11506	0	11467	754	0
1	F	11546	0	11499	701	0
2	G	16200	0	16081	1290	1
2	H	16200	0	16081	1326	1
2	I	16200	0	16081	1344	0
2	J	16200	0	16081	1326	0
2	K	16200	0	16081	1391	0
2	L	16200	0	16081	1366	0
3	A	48	0	25	5	0
3	B	48	0	25	5	0
3	C	48	0	25	4	0
3	D	48	0	25	6	0
3	E	48	0	25	4	0
3	F	48	0	25	4	0
3	G	48	0	25	4	0
3	H	48	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	48	0	25	4	0
3	J	48	0	25	4	0
3	K	48	0	25	4	0
3	L	48	0	25	4	0
4	G	31	0	19	17	0
4	H	31	0	19	16	0
4	I	31	0	19	16	0
4	J	31	0	19	15	0
4	K	31	0	19	15	0
4	L	31	0	19	15	0
All	All	167247	0	165930	11767	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 11767 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:542:GLN:HB3	1:D:579:MET:HE2	1.25	1.17
1:F:1443:LEU:HD21	1:F:1470:ARG:HB3	1.18	1.17
1:B:1268:SER:HB3	1:D:1389:ILE:HG13	1.23	1.16
1:F:1504:ARG:HH11	1:F:1504:ARG:HG3	1.04	1.15
1:D:1504:ARG:HH11	1:D:1504:ARG:HG3	1.02	1.15

All (2) 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	Distance(Å)	Clash(Å)
1:A:575:ARG:NH1	2:H:164:GLU:O[2.555]	2.01	0.19
1:B:1452:SER:O	2:G:1092:ASN:ND2[1.556]	2.18	0.02

## 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	1451/1878 (77%)	1270 (88%)	164 (11%)	17 (1%)	19	62
1	B	1458/1878 (78%)	1278 (88%)	160 (11%)	20 (1%)	16	58
1	C	1456/1878 (78%)	1283 (88%)	156 (11%)	17 (1%)	19	62
1	D	1461/1878 (78%)	1276 (87%)	161 (11%)	24 (2%)	14	55
1	E	1450/1878 (77%)	1276 (88%)	155 (11%)	19 (1%)	18	60
1	F	1455/1878 (78%)	1282 (88%)	153 (10%)	20 (1%)	16	58
2	G	2058/2060 (100%)	1789 (87%)	237 (12%)	32 (2%)	14	55
2	H	2058/2060 (100%)	1791 (87%)	230 (11%)	37 (2%)	13	52
2	I	2058/2060 (100%)	1787 (87%)	238 (12%)	33 (2%)	14	55
2	J	2058/2060 (100%)	1784 (87%)	240 (12%)	34 (2%)	14	54
2	K	2058/2060 (100%)	1785 (87%)	239 (12%)	34 (2%)	14	54
2	L	2058/2060 (100%)	1780 (86%)	241 (12%)	37 (2%)	13	52
All	All	21079/23628 (89%)	18381 (87%)	2374 (11%)	324 (2%)	15	57

5 of 324 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	PHE
1	A	1566	LYS
1	B	614	PHE
1	B	624	GLY
1	B	1566	LYS

### 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	1220/1527 (80%)	1107 (91%)	113 (9%)	13	44
1	B	1227/1527 (80%)	1117 (91%)	110 (9%)	14	47
1	C	1225/1527 (80%)	1110 (91%)	115 (9%)	13	43
1	D	1229/1527 (80%)	1107 (90%)	122 (10%)	11	39
1	E	1219/1527 (80%)	1106 (91%)	113 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	1224/1527 (80%)	1111 (91%)	113 (9%)	13	45
2	G	1752/1752 (100%)	1569 (90%)	183 (10%)	10	36
2	H	1752/1752 (100%)	1569 (90%)	183 (10%)	10	36
2	I	1752/1752 (100%)	1565 (89%)	187 (11%)	10	35
2	J	1752/1752 (100%)	1567 (89%)	185 (11%)	10	35
2	K	1752/1752 (100%)	1566 (89%)	186 (11%)	10	35
2	L	1752/1752 (100%)	1563 (89%)	189 (11%)	9	34
All	All	17856/19674 (91%)	16057 (90%)	1799 (10%)	11	38

5 of 1799 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1436	ARG
2	H	1564	SER
2	L	726	GLN
2	G	1707	ASP
2	H	616	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 492 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	1500	ASN
2	H	1655	HIS
2	L	448	HIS
2	G	1725	HIS
2	H	388	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

18 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	NAP	A	1901	-	52,52,52	1.09	3 (5%)	80,80,80	1.73	8 (10%)
3	NAP	B	1901	-	52,52,52	1.08	3 (5%)	80,80,80	1.69	10 (12%)
3	NAP	C	1901	-	52,52,52	1.14	3 (5%)	80,80,80	1.76	7 (8%)
3	NAP	D	1901	-	52,52,52	1.24	3 (5%)	80,80,80	1.81	7 (8%)
3	NAP	E	1901	-	52,52,52	1.09	3 (5%)	80,80,80	1.81	9 (11%)
3	NAP	F	1901	-	52,52,52	1.11	3 (5%)	80,80,80	1.72	8 (10%)
4	FMN	G	2101	-	33,33,33	6.09	22 (66%)	46,50,50	1.76	8 (17%)
3	NAP	G	2102	-	52,52,52	1.07	4 (7%)	80,80,80	1.71	6 (7%)
4	FMN	H	2101	-	33,33,33	6.07	20 (60%)	46,50,50	1.67	8 (17%)
3	NAP	H	2102	-	52,52,52	1.07	4 (7%)	80,80,80	1.71	7 (8%)
4	FMN	I	2101	-	33,33,33	6.08	20 (60%)	46,50,50	1.75	10 (21%)
3	NAP	I	2102	-	52,52,52	1.01	3 (5%)	80,80,80	1.72	5 (6%)
4	FMN	J	2101	-	33,33,33	6.30	22 (66%)	46,50,50	1.73	6 (13%)
3	NAP	J	2102	-	52,52,52	1.09	4 (7%)	80,80,80	1.72	9 (11%)
4	FMN	K	2101	-	33,33,33	6.31	22 (66%)	46,50,50	1.93	10 (21%)
3	NAP	K	2102	-	52,52,52	1.04	4 (7%)	80,80,80	1.68	7 (8%)
4	FMN	L	2101	-	33,33,33	6.14	20 (60%)	46,50,50	1.71	8 (17%)
3	NAP	L	2102	-	52,52,52	1.05	4 (7%)	80,80,80	1.69	6 (7%)

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	NAP	A	1901	-	-	0/35/67/67	0/5/5/5
3	NAP	B	1901	-	-	0/35/67/67	0/5/5/5
3	NAP	C	1901	-	-	0/35/67/67	0/5/5/5
3	NAP	D	1901	-	-	0/35/67/67	0/5/5/5
3	NAP	E	1901	-	-	0/35/67/67	0/5/5/5
3	NAP	F	1901	-	-	0/35/67/67	0/5/5/5
4	FMN	G	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	G	2102	-	-	0/35/67/67	0/5/5/5
4	FMN	H	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	H	2102	-	-	0/35/67/67	0/5/5/5
4	FMN	I	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	I	2102	-	-	0/35/67/67	0/5/5/5
4	FMN	J	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	J	2102	-	-	0/35/67/67	0/5/5/5
4	FMN	K	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	K	2102	-	-	0/35/67/67	0/5/5/5
4	FMN	L	2101	-	-	0/18/18/18	0/3/3/3
3	NAP	L	2102	-	-	0/35/67/67	0/5/5/5

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2101	FMN	O2-C2	15.44	1.41	1.21
4	L	2101	FMN	O2-C2	15.03	1.41	1.21
4	G	2101	FMN	O2-C2	15.00	1.41	1.21
4	I	2101	FMN	O2-C2	14.84	1.40	1.21
4	J	2101	FMN	O2-C2	14.80	1.40	1.21

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2102	NAP	N3A-C2A-N1A	-10.77	119.41	128.89
3	D	1901	NAP	N3A-C2A-N1A	-10.73	119.45	128.89
3	G	2102	NAP	N3A-C2A-N1A	-10.36	119.78	128.89
3	J	2102	NAP	N3A-C2A-N1A	-10.33	119.80	128.89
3	L	2102	NAP	N3A-C2A-N1A	-10.24	119.88	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1457/1878 (77%)	0.14	4 (0%)	91 53	16, 50, 103, 146	0
1	B	1464/1878 (77%)	0.16	8 (0%)	88 39	17, 50, 106, 157	0
1	C	1462/1878 (77%)	0.16	8 (0%)	88 39	15, 48, 107, 155	0
1	D	1467/1878 (78%)	0.14	3 (0%)	93 61	17, 52, 106, 151	0
1	E	1456/1878 (77%)	0.14	5 (0%)	91 53	17, 50, 106, 152	0
1	F	1461/1878 (77%)	0.17	4 (0%)	91 53	17, 47, 106, 156	0
2	G	2060/2060 (100%)	0.25	28 (1%)	72 17	24, 83, 128, 156	0
2	H	2060/2060 (100%)	0.31	67 (3%)	44 6	24, 85, 129, 155	0
2	I	2060/2060 (100%)	0.27	51 (2%)	54 9	20, 85, 129, 158	0
2	J	2060/2060 (100%)	0.34	95 (4%)	31 5	27, 88, 132, 157	0
2	K	2060/2060 (100%)	0.46	143 (6%)	17 3	25, 90, 133, 157	0
2	L	2060/2060 (100%)	0.32	72 (3%)	42 6	22, 86, 131, 158	0
All	All	21127/23628 (89%)	0.25	488 (2%)	57 9	15, 74, 125, 158	0

The worst 5 of 488 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	176	GLN	11.3
2	K	175	GLY	7.5
2	K	516	PHE	6.7
2	H	24	LEU	6.6
2	K	517	GLY	6.5

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	A	1901	48/48	0.32	0.39	19,76,121,169	0
3	NAP	B	1901	48/48	0.31	0.31	23,78,115,145	0
3	NAP	F	1901	48/48	0.31	0.24	19,78,125,159	0
3	NAP	D	1901	48/48	0.32	0.05	21,83,127,174	0
3	NAP	C	1901	48/48	0.32	0.04	23,81,130,171	0
3	NAP	L	2102	48/48	0.30	-0.07	37,84,116,120	0
3	NAP	K	2102	48/48	0.28	-0.36	43,94,127,131	0
3	NAP	E	1901	48/48	0.26	-0.36	24,77,123,157	0
3	NAP	H	2102	48/48	0.25	-0.40	37,85,113,122	0
4	FMN	J	2101	31/31	0.32	-0.42	23,61,101,113	0
3	NAP	I	2102	48/48	0.26	-0.47	29,80,104,116	0
4	FMN	G	2101	31/31	0.32	-0.56	26,63,101,111	0
4	FMN	I	2101	31/31	0.30	-0.59	22,56,87,103	0
4	FMN	L	2101	31/31	0.29	-0.59	19,59,102,114	0
4	FMN	H	2101	31/31	0.32	-0.60	25,49,105,113	0
3	NAP	G	2102	48/48	0.23	-0.65	42,87,119,128	0
4	FMN	K	2101	31/31	0.34	-0.69	27,66,110,123	0
3	NAP	J	2102	48/48	0.21	-0.83	35,88,118,120	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.