



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:28 AM UTC

PDB ID : 3HMJ / pdb_00003hmj
Title : Saccharomyces cerevisiae FAS type I
Authors : Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.;
Grininger, M.
Deposited on : 2009-05-29
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

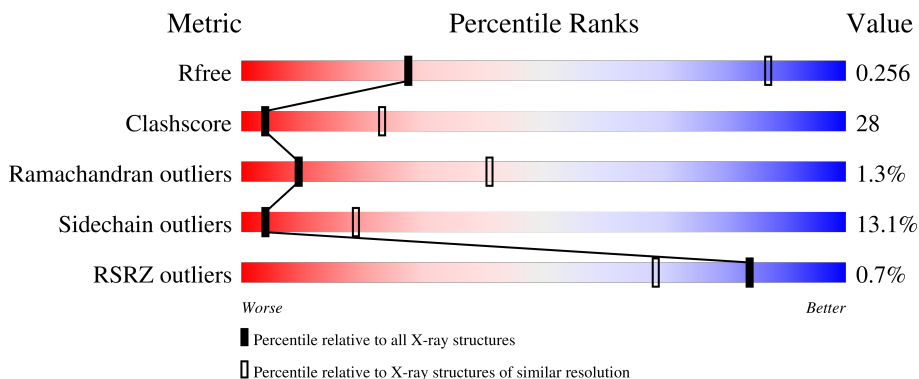
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1887	
1	B	1887	
1	C	1887	
2	G	2051	
2	H	2051	

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Mol	Chain	Length	Quality of chain
2	I	2051	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '49%', a yellow segment in the middle labeled '40%', and a red segment on the right labeled '10%'. A small red square is positioned at the beginning of the bar, and a small black dot is at the end. A '%' symbol is located above the bar.</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 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.

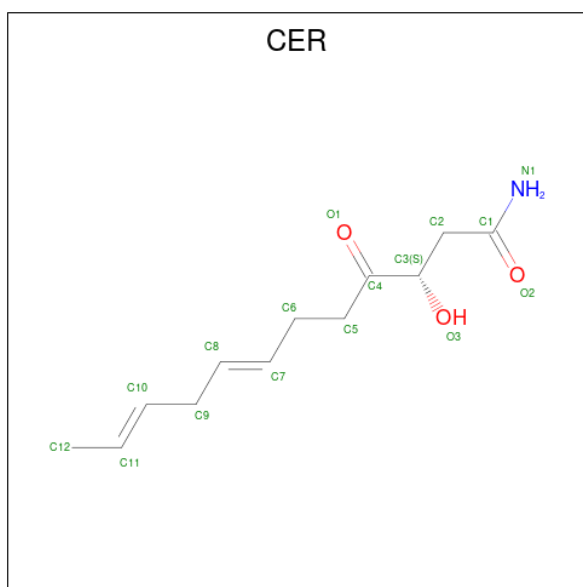
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1750	13572	8594	2292	2637	49	0	0	0
1	B	1750	13572	8594	2292	2637	49	0	0	0
1	C	1750	13572	8594	2292	2637	49	0	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

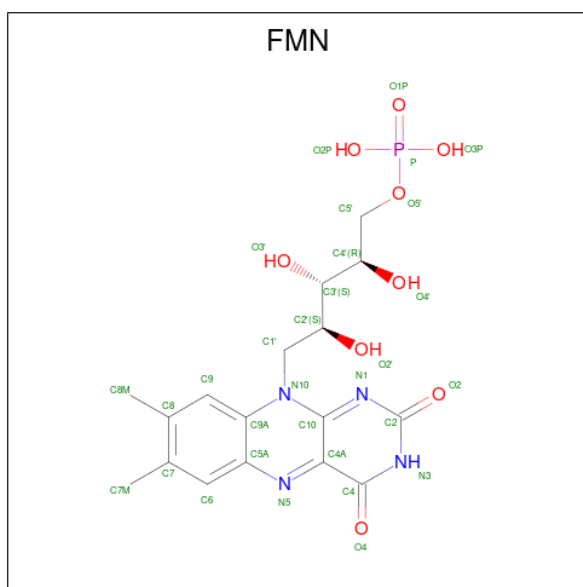
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	2033	15995	10253	2660	3026	56	0	0	0
2	H	2033	15995	10253	2660	3026	56	0	0	0
2	I	2033	15995	10253	2660	3026	56	0	0	0

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (CCD ID: CER) (formula: C₁₂H₁₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		
3	C	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

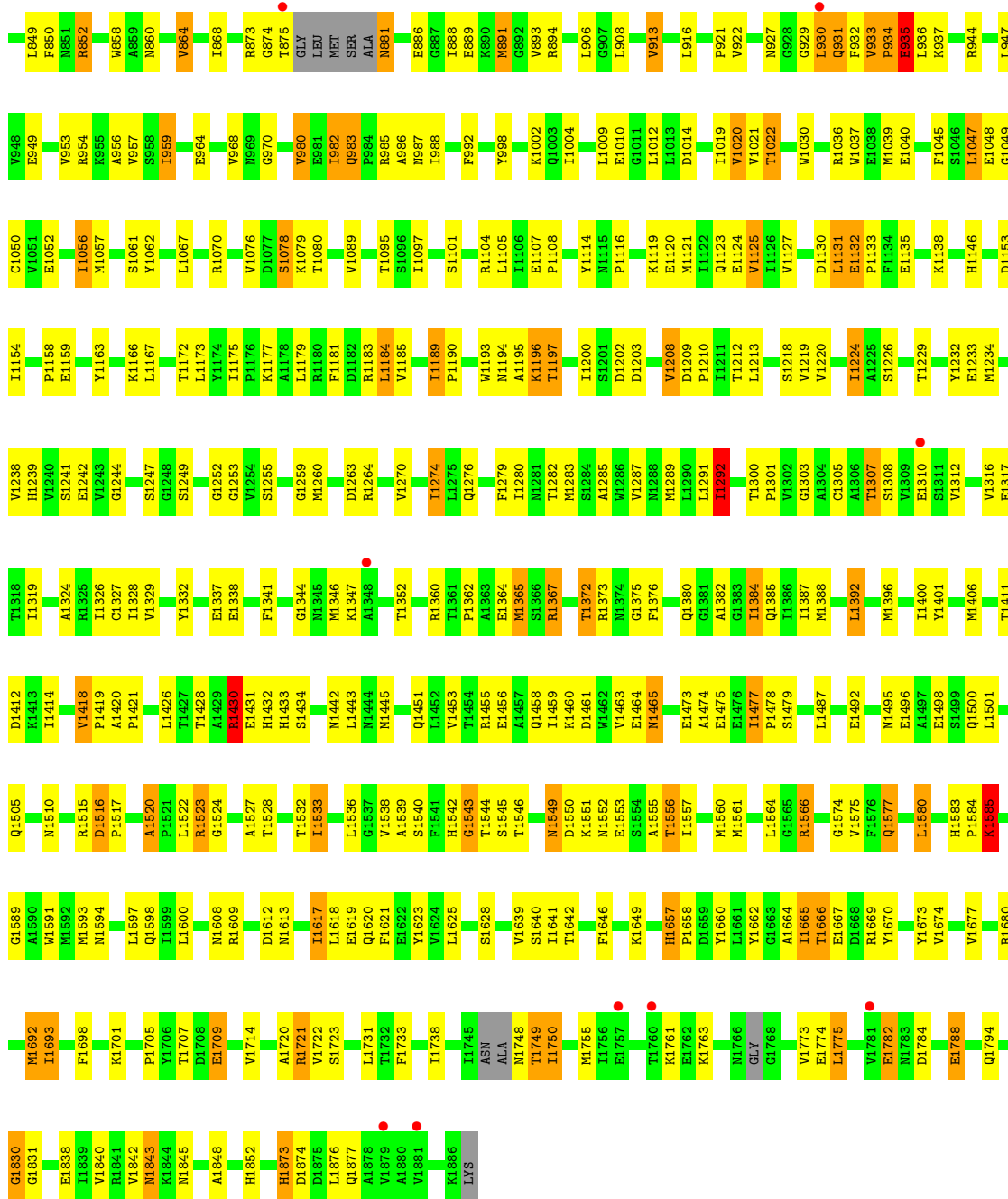


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

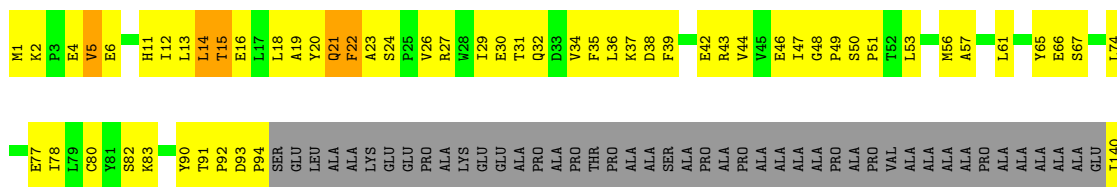
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		



● Molecule 1: Fatty acid synthase subunit alpha



A1324	A1325	I1326	C1327	I1328	V1329	Y1332	G1252	G1253	E1337	E1338	F1341	G1344	M1345	M1346	K1347	T1352	R1360	T1361	P1362	E1364	M1365	S1366	R1367	T1370	I1371	R1372	R1373	M1374	G1375	F1376	Q1380	I1384	Q1385	I1386	I1387	M1388	L1392	M1396	P1399	I1400	Y1401	M1406	T1411	D1412	K1413	I1414																																																													
V1293	G1244	S1247	G1248	S1249	G1252	G1253	V1254	S1255	A1256	L1257	R1258	G1259	M1260	D1261	R1264	R1264	V1270	I1274	L1275	Q1276	F1279	N1280	N1281	T1282	M1283	S1284	A1285	W1286	V1287	N1288	M1289	V1289	V1289	P1297	T1300	P1300	V1302	G1303	A1304	C1305	A1306	T1307	S1308	E1310	Y1311	V1312	V1316	E1317	V1240	I1318	I1319	I1414																																																							
E1052	Y1163	K1166	L1167	T1172	L1173	Y1174	L1175	P1176	K1177	A1178	L1179	R1180	F1181	D1182	R1183	L1184	V1185	Q1188	I1189	P1190	W1193	A1194	A1195	K1196	T1197	I1200	S1201	D1202	Y1114	M1115	P1116	L1116	E1117	K1118	K1119	Q1123	E1124	S1218	V1219	I1224	A1225	S1226	L1229	Y1232	E1233	M1234	V1238	H1239	V1240	I1318	I1414																																																								
S951	E952	V953	R954	K955	A956	I959	E984	V988	V989	V990	E991	I992	O993	R994	R995	F992	L1009	E1010	G1011	L1012	L1013	D1014	I1019	V1020	V1021	T1022	G1028	P1029	W1030	R1036	W1037	E1038	M1039	E1040	F1045	L1047	E1048	G1049	C1050	V1051	L980	Q931	F932	V933	P934	K937	E938	F939	R944	L947	V948	O949	C1050	V1051																																																					
A141	D142	E143	P144	V145	L149	H152	V155	A156	H157	K158	L163	D164	S165	I166	F167	M168	S169	K170	T171	L175	V176	G177	G178	K179	S180	I181	V182	Q183	E185	I186	L187	L190	T196	T197	P198	P201	E202	E203	T204	P205	L206	L209	F213	F217	L221	S225	L228	L232	L233	S234	S235	K236	M237	P238	F241	T242	L243	T244	V245	A246	R247	L250	Q251	T252	R253	W254	C255	L256	P257	R260	G263	L266	V267	A268	L269	S270	N271	E272	P273	Q341	Q342	R276	E280	P201	A283	K284	A285	F286	M290	A291	Q292	K293	Y294	F217	I297	V298	G299										
L531	S456	N457	T458	D459	E460	T461	K462	N465	R400	T401	A402	D403	W406	N407	W408	A409	K410	Q411	S412	L413	L414	S415	L416	F417	F418	E419	L420	L421	V424	N427	V428	H335	K336	V337	L338	A339	R340	Q341	Q342	L343	Q344	V345	L350	K351	M352	D353	L354	N444	D445	A446	S523	Q527	E528	M529	A530	T501	V433	G507	S434	N508	A435	A436	L437	N438	E513	L439	M440	R441	R442	S443	R520	K521	L522	A446	S523	Q527	E528	M529	A530																												
T485	S486	N487	T488	D489	E490	T491	K492	N495	R400	T401	A402	D403	W406	N407	W408	A409	K410	Q411	S412	L413	L414	S415	L416	F417	F418	E419	L420	L421	V424	N427	V428	H335	K336	V337	L338	A339	R340	Q341	Q342	L343	Q344	V345	L350	K351	M352	D353	L354	N444	D445	A446	S523	Q527	E528	M529	A530	T501	V433	G507	S434	N508	A435	A436	L437	N438	E513	L439	M440	R441	R442	S443	R520	K521	L522	A446	S523	Q527	E528	M529	A530																												
L531	T536	F537	E538	S539	Q540	P501	R502	I503	R504	L505	T506	A507	D508	E509	D603	A604	L605	D606	K607	D608	S609	W610	G611	E612	S615	T621	L622	S623	K624	T625	W626	S627	I628	F629	L630	P631	T634	I635	P636	F637	L638	T644	L645	L655	D661	S662	L663	E664	F668	R669	G670	V671	F672	R673	L674	I675	T676	R677	L678	R679	L679	K680	R681	C685	W686	K687	R688	I689	R690	A691	N681	O682	N683	I683	R684	R685	E686	G687	I688	O689	F692	Y998	I1004	L1009	E1010	G1011	L1012	L1013	D1014	I1019	V1020	V1021	T1022	G1028	P1029	W1030	R1036	W1037	E1038	M1039	E1040	F1045	L1047	E1048	G1049	C1050	V1051
T485	S486	N487	T488	D489	E490	T491	K492	N495	R400	T401	A402	D403	W406	N407	W408	A409	K410	Q411	S412	L413	L414	S415	L416	F417	F418	E419	L420	L421	V424	N427	V428	H335	K336	V337	L338	A339	R340	Q341	Q342	L343	Q344	V345	L350	K351	M352	D353	L354	N444	D445	A446	S523	Q527	E528	M529	A530	T501	V433	G507	S434	N508	A435	A436	L437	N438	E513	L439	M440	R441	R442	S443	R520	K521	L522	A446	S523	Q527	E528	M529	A530																												
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T485	S486	N487	T488	D489	E490	T491	K492	N495	R400	T401	A402	D403	W406	N407	W408	A409	K410	Q411	S412	L413	L4																																																																																						

Y1090	F1017	I932	V846	Y702	G622	N560	I479	F304	V157	F80	MET
G1091	V1018	W938	E852	L703	G623	W561	V480	F305	A158	L84	ASP
D1092	P1019	F939	P853	G704	Y624	L562	C481	I306	I159	M85	ALA
D1093	L1021	L1021	I854	L705	A774	E563	I483	R309	F160	L86	TYR
K1096	R1024	T942	H855	P707	G629	Y565	I484	P315	G161	T89	T6
I1097	F1025	W943	K856	A712	M630	H566	R485	P315	G162	P8	R7
P1098	F1026	R944	I857	F713	A632	K567	L486	L319	Q163	N93	L9
A1099	I1027	T945	A858	L714	I634	L569	V488	C238	T166	C94	L8
V1100	F946	S714	L781	Q715	I634	L570	S417	P239	D167	C95	T10
Y1101	T947	W795	E784	Q716	V638	K571	W490	L240	D168	Y95	L11
Y1102	G948	W785	I716	W717	I641	N572	E491	L241	Y169	F170	S15
F1103	D1032	S786	H718	H718	I641	K573	T492	L328	F170	D100	L16
S1107	L1040	I787	I719	S574	G644	S574	T493	E332	L173	I101	V22
P1108	E1041	K788	A720	G644	G644	G575	T494	L246	R174	H102	V22
V1109	A1042	F789	K721	S645	S645	K576	T494	L246	D175	A105	P23
ASP	V1043	E870	D790	E722	E722	I577	A424	H248	L176	A105	T24
VAL	V1044	Y791	H723	G648	G648	F578	S425	Y249	V177	L109	A25
GLN	D1045	F782	H723	I649	I649	V579	A426	V256	Q178	L109	S28
SER	Q1046	F793	F726	M650	M650	E590	F427	V251	T179	M112	F27
GLN	V1047	W794	P727	L651	L651	T581	H428	I391	Y180	M112	F28
VAL	D1048	K879	I728	I652	I652	K582	S429	S342	H181	D113	F28
ASP	Q1049	L880	A729	Y653	Y653	F583	H430	L344	V182	T114	L33
SER	R1050	V881	L730	V654	V654	S584	H431	T345	L183	T115	L33
SER	T1051	P882	Q731	G505	G505	K585	L432	Q346	V184	T115	L40
SER	C1052	T883	W732	M658	M658	L586	L438	E347	G185	V117	L41
VAL	L1053	L884	F733	L659	L659	I587	L439	Q348	D186	K118	P42
SER	L1054	F734	Q735	Q660	Q660	G588	M440	P260	L187	V119	P42
GLU	H1055	R736	R736	G662	G662	R589	M441	Q350	E262	K120	E43
D1123	V1058	Y970	G739	I663	I663	P591	D442	V853	L063	E121	T45
S1124	A1059	S971	H740	L665	L665	L592	L443	N594	S191	L122	E46
K1128	A1060	L972	H741	I666	I666	L593	L444	K355	A192	L123	G47
A1129	Q1061	L973	E810	V811	V811	P595	M446	T357	T194	K124	F48
T1130	F1062	Y871	S742	K667	K667	G596	M447	N357	E193	A49	A49
T1133	T1063	Y871	D745	E668	E668	G596	D521	H359	T194	M127	D51
D1134	I1066	E992	A746	L669	L669	M597	D521	L360	S198	T128	D52
E1135	E1067	Q993	H747	R670	R670	T598	R526	L360	E197	I131	D52
W1138	F1068	Q993	T748	Y674	Y674	C900	G531	Q365	L198	M132	E53
S1145	I1070	Q998	P749	P675	P675	T901	T532	Q365	I199	M132	P54
M1148	I1071	Q998	M750	I676	I676	V602	L533	I368	K134	K134	T55
W1149	M1074	D999	L751	Q677	Q677	S603	L533	S369	L203	R135	T55
R1150	D1075	I1000	L752	F678	F678	F606	D540	L370	E206	P136	E59
H1151	G1076	H1000	M753	L679	L679	V607	D540	V371	F209	F137	L60
F1158	H1078	H1000	G826	T680	T680	V607	F543	A374	T210	D138	L60
I1159	D1079	H1006	V828	I681	I681	T610	K544	K375	G272	K139	V61
Q1160	H1081	M1006	W832	G682	G682	T611	Q545	A374	T286	K140	G62
Q1161	I1082	P1010	T835	A683	A683	M612	V550	K375	L213	K140	K63
D1162	K1083	P1010	T840	V690	V690	A613	V550	A374	N214	S141	F64
K1163	L1084	P1012	T840	E693	E693	G614	S552	K375	L214	F146	F64
F1166	L1085	K1013	G841	Y694	Y694	Y615	N553	N376	N214	L145	V68
I1167	H1086	P1014	G842	T697	T697	E618	K556	L377	N214	L145	V68
M1168	H1087	P1016	I843	L698	L698	L519	K557	L377	L215	L145	V68
			T845	G699	G699	E477	N558	L391	L216	F146	V72
						R478	P559	T392	E217	K149	E73
									W218	M142	E73
									L219		
									I300	M153	K76
									T225	A154	V77
									W302	Q155	G78
									L303	L156	Q79

T1417	V1328	S1252	I1170	L1085	Q1012	V846	G772	Y702	A620	R553	V480	L393	F304
D1418	V1329	E1253	R1171	L1086	V1015	E852	S773	L703	G621	K556	D481	R394	F305
F1419	V1330	V1254	K1172	H1087	P1016	E853	A774	G704	G622	K557	C482	K397	I306
E1420	W1331	M1255	V1173	F1091	F1017	P853	T777	L705	G623	N558	I483	K399	R309
M1421	I1335	E1256	K1175	G1091	F1018	H855	T778	K706	Y624	N559	L484	L402	R309
T1422	R1258	R1257	P1176	D1092	P1019	K856	P779	P707	G629	L562	L486	D403	P315
F1423	I1338	Q1289	S1177	D1093	L1020	I857	Y780	A712	M630	L563	Q404	D404	P315
T1426	F1339	M1280	M1180	F1103	L1021	A858	F781	I713	T631	Y665	F488	F416	L319
V1427	R1340	R1261	M1181	I1097	R1024	T859	E784	S714	A632	H566	H489	H416	L324
A1428	M1341	I1262	K1184	R944	F1025	R860	S785	Q715	A633	P567	W490	S417	L324
Y1431	T1342	K1263	I1189	E1101	E1026	L864	S786	V716	I634	K568	E491	M418	L328
Q1432	D1344	M1265	T1189	Y1102	I1027	W665	T787	I717	V638	L569	T492	R419	L328
M1433	L1347	Y1266	V1194	F1103	K1031	R866	K788	W718	V639	N572	T494	F420	E332
H1434	L1348	W1267	V1195	D1108	D1032	E948	F789	I719	I641	N573	T494	L421	E332
L1435	L1349	K1268	M1196	P1109	F950	R868	Y791	A720	P422	Q495	P422	L421	P335
K1436	K1349	L1269	T1196	V1109	L951	D869	P792	K721	S574	G575	F496	V423	P335
T1437	L1350	M1270	L1197	ASP	R952	E870	P793	A722	S645	K576	T499	S425	M338
S1438	H1351	I1271	S1198	VAL	E1041	T871	K794	H723	G643	I577	H500	P426	L339
I1441	M1355	D1272	E1199	GLN	A1042	I872	P795	F726	I649	I578	H501	F427	L339
A1442	L1356	P1274	L1205	GLN	V1043	F873	D796	P727	I652	Y579	L502	H428	I341
V1443	G1357	F1275	K1206	GLN	V1044	N874	D797	I728	I653	E580	D503	S429	S342
R1445	Y1357	F1275	K1206	VAL	D1045	L875	G798	A729	V654	T581	F504	H430	N343
S1446	K1358	F1279	I1210	ASP	Q1046	L875	G799	L730	G654	K582	G505	L431	L344
L1452	M1359	R1282	K1211	SER	D1047	K879	L800	Q731	M658	F583	P506	L432	T345
L1453	I1360	R1282	K1212	SER	V1048	L880	R804	W732	Q660	S584	G507	L438	Q346
L1454	V1368	V1283	L1213	VAL	K1050	V881	R805	I733	L665	L659	L443	L438	E347
F1457	G1369	V1284	L1214	SER	T1051	P882	M806	S742	I666	N591	V444	V444	Q348
D1458	D1370	V1284	L1214	GLU	C1052	K887	I807	R736	K667	L593	N446	N446	N440
L1459	F1290	E1291	M1217	D1123	I1053	L886	I807	G739	G662	G588	L512	K441	V349
K1462	T1374	I1292	I1218	A1129	L1054	I982	E810	H740	P664	R589	T516	D442	Q350
T1463	V1377	T1293	Q1220	M1230	H1055	S893	R811	H741	L665	P591	H517	D442	V388
T1468	I1378	E1296	M1221	A1130	V1058	R894	K812	S742	I666	N592	R518	V444	M354
E1469	V1381	F1300	M1223	E1135	A1060	L896	T813	D745	K667	L593	N519	N445	K355
V1470	V1382	A1303	R1227	E1135	Q1061	D898	D816	A746	L669	V594	K520	N447	T357
V1472	I1389	A1303	M1229	W1138	F1062	F899	A817	H747	R670	G596	G524	N447	M357
T1473	M1229	D1230	M1229	S1145	T1063	Q900	K818	T748	Y674	N597	R526	L455	S358
F1474	G1231	K1231	D1230	S1145	I1066	K901	I821	P749	P675	T598	R526	Q456	L360
K1475	K1232	K1232	K1232	M1448	D1067	P902	A822	M750	I676	P599	G530	V459	P361
S1481	L1396	F1311	V1233	W1149	E1068	F904	A823	L751	Q677	C600	A530	V460	F367
S1482	S1397	S1313	V1234	M1149	P1069	A905	C824	Q752	Q677	T601	G531	Y460	I368
V1483	L1403	R1314	S1235	H1151	P1070	V907	T825	Y754	F678	V602	T532	D461	S389
F1486	M1404	T1314	L1236	H1151	K1071	V907	G826	Y754	T680	S603	L533	T462	L370
V1491	E1405	M1319	L1238	F1158	M1074	Q910	P828	R758	G682	F606	P537	D464	V371
E1492	L1406	L1320	L1239	I1159	D1075	A911	W832	R759	A683	V607	D538	D465	A374
L1493	T1407	A1321	Y1240	T1160	G1076	R912	T835	H760	V690	T610	D539	D467	K376
S1494	S1408	P1322	M1241	Q1161	I1077	D913	T835	N762	V690	T611	D540	L468	N376
T1495	S1409	M1323	F1242	D1162	H1078	L914	T835	I763	E693	N612	N612	L468	L377
K1496	F1410	D1324	M1243	K1163	D1079	A915	T840	M764	Y694	G613	F543	R469	L377
F1499	F1411	E1325	P1244	M1006	S1005	T916	G842	L765	T697	V615	Q545	L471	S380
V1499	F1411	A1326	G1247	M1006	H1081	E921	V844	S769	T697	T616	V550	S476	L389
		I1327		P1010	K1082	R943	V844	G769	G699	L617	T551	R477	M390
				M1011	K1084	L926	T845			L619	S552	R478	L391
												L479	T392

G2034	E1560
S2035	I1501
E2036	G1502
P2037	I1503
I2038	V1504
K2039	G1509
E2040	A1510
I2041	S1511
I2042	H1512
D2043	G1513
N2044	N1514
W2045	P1515
E2046	T1526
K2047	L1527
Y2048	E1528
E2049	L1533
Q2050	D1543
SER	P1547
	S1548
	T1549
	H1550
	E1551
	P1552
	Y1553
	V1556
	L1560
	N1561
	P1562
	I1563
	H1564
	V1565
	S1566
	R1567
	H1568
	M1574
	L1575
	I1579
	T1580
	M1583
	F1584
	S1585
	S1586
	V1589
	R1590
	L1592
	I1593
	E1594
	A1597
	A1598
	D1599
	S1600
	V1601
	S1602
	V1605
	R1606
	G1607
	Y1608
	T1609
	M1615
	V1616
	K1623
	E1624
	S1625
	Q1626
	Q1627
	G1630
	M1631
	I1632
	L1637
	O1638
	K1639
	F1640
	E1641
	T1642
	L1651
	T1652
	G1653
	I1657
	V1661
	T1662
	T1663
	F1666
	G1670
	S1671
	Q1672
	E1673
	Q1674
	G1675
	M1676
	G1677
	M1678
	D1679
	L1680
	T1683
	M1784
	S1684
	Q1688
	L1774
	Q1775
	F1776
	T1777
	Q1778
	P1779
	A1780
	L1781
	T1782
	L1783
	M1784
	E1785
	G1722
	G1726
	A1735
	M1736
	I1737
	F1738
	E1739
	T1740
	I1741
	F1742
	K1745
	L1746
	K1747
	I1751
	I1755
	H1756
	E1757
	S1761
	E1764
	R1765
	L1770
	T1774
	Q1775
	F1776
	R1761
	M1854
	I1855
	A1856
	I1857
	H1858
	P1859
	G1860
	R1861
	V1862
	F1866
	S1867
	Q1868
	L1871
	Q1872
	Q1896
	Q1897
	Y1898
	L1898
	V1899
	A1900
	A1901
	R1905
	A1906
	L1907
	D1908
	M1909
	V1910
	V1913
	L1914
	I1917
	K1918
	L1919
	Q1920
	K1921
	I1922
	D1923
	I1924
	L1927
	Q1928
	K1929
	S1930
	L1931
	S1932
	E1935
	V1936
	E1937
	L1940
	F1941
	D1945
	K1949
	V1953
	P1955
	R1956
	P1957
	L1958
	K1959
	F1964
	V1970
	S1973
	F1976
	H1977
	Y1980
	L1981
	M1982
	K1986
	P1987
	F1988
	K1989
	K1993
	I1996
	I1997
	K1998
	V2003
	A2004
	R2005
	K2009
	Y2010
	I2011
	P2012
	N2013
	L2014
	T2015
	A2016
	K2017
	Q2020
	Y2021
	T2022
	Y2025
	F2026
	V2029
	Y2030
	T2033

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	231.88Å 231.88Å 756.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-4.00) 96.4 (20.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.94Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.267 0.255 , 0.256	Depositor DCC
R_{free} test set	8521 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	130.2	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	88830	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, CER

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	0.58	5/13822 (0.0%)	0.93	38/18682 (0.2%)
1	B	0.57	9/13822 (0.1%)	0.96	37/18682 (0.2%)
1	C	0.57	8/13822 (0.1%)	0.92	30/18682 (0.2%)
2	G	0.56	12/16360 (0.1%)	0.94	43/22198 (0.2%)
2	H	0.55	10/16360 (0.1%)	0.93	47/22198 (0.2%)
2	I	0.54	10/16360 (0.1%)	0.94	53/22198 (0.2%)
All	All	0.56	54/90546 (0.1%)	0.94	248/122640 (0.2%)

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
2	G	0	1
2	H	0	2
2	I	0	1
All	All	0	4

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	PHE	C-N	21.92	1.59	1.33
1	C	992	PHE	C-N	21.64	1.59	1.33
2	I	842	GLY	C-N	19.10	1.59	1.33
2	G	315	PRO	C-N	18.47	1.58	1.33
1	C	485	ASP	C-N	16.78	1.56	1.33

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	992	PHE	CA-C-N	-17.47	102.73	120.03
1	B	992	PHE	C-N-CA	-17.47	102.73	120.03
1	B	992	PHE	O-C-N	14.71	137.19	121.60
1	A	992	PHE	CA-C-N	-14.65	105.95	120.31
1	A	992	PHE	C-N-CA	-14.65	105.95	120.31

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
2	H	1256	GLU	Mainchain
2	I	1108	PRO	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	13572	0	13489	696	15
1	B	13572	0	13491	643	6
1	C	13572	0	13491	672	22
2	G	15995	0	15978	1067	32
2	H	15995	0	15978	1074	7
2	I	15995	0	15977	1021	26
3	A	12	0	10	3	0
3	B	12	0	10	4	0
3	C	12	0	10	4	0
4	G	31	0	19	8	0
4	H	31	0	19	5	0
4	I	31	0	19	4	0
All	All	88830	0	88491	4991	54

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 28.

The worst 5 of 4991 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:1749:THR:CB	1:A:1874:ASP:HB3	1.53	1.37
1:B:1749:THR:CB	1:B:1874:ASP:HB3	1.56	1.34
1:B:1749:THR:CB	1:B:1873:HIS:O	1.75	1.32
1:A:1464:GLU:HG3	1:A:1773:VAL:CG1	1.58	1.32
1:C:1749:THR:CB	1:C:1874:ASP:HB3	1.62	1.29

The worst 5 of 54 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:C:1784:ASP:CA	2:G:1087:HIS:CE1[7_655]	0.16	2.04
1:A:1784:ASP:CG	2:I:1087:HIS:CE1[7_545]	0.52	1.68
1:C:1784:ASP:C	2:G:1087:HIS:NE2[7_655]	0.54	1.66
1:C:1784:ASP:CB	2:G:1087:HIS:ND1[7_655]	0.56	1.64
1:A:1784:ASP:OD2	2:I:1087:HIS:ND1[7_545]	0.58	1.62

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	1736/1887 (92%)	1614 (93%)	100 (6%)	22 (1%)	9	41
1	B	1736/1887 (92%)	1619 (93%)	100 (6%)	17 (1%)	12	45
1	C	1736/1887 (92%)	1618 (93%)	96 (6%)	22 (1%)	9	41
2	G	2029/2051 (99%)	1825 (90%)	173 (8%)	31 (2%)	8	38
2	H	2029/2051 (99%)	1826 (90%)	173 (8%)	30 (2%)	8	38
2	I	2029/2051 (99%)	1829 (90%)	174 (9%)	26 (1%)	9	41
All	All	11295/11814 (96%)	10331 (92%)	816 (7%)	148 (1%)	9	41

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	PRO
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY

5.3.2 Protein sidechains [i](#)

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	1460/1566 (93%)	1283 (88%)	177 (12%)	5	21
1	B	1460/1566 (93%)	1288 (88%)	172 (12%)	5	21
1	C	1460/1566 (93%)	1280 (88%)	180 (12%)	4	20
2	G	1772/1789 (99%)	1521 (86%)	251 (14%)	3	17
2	H	1772/1789 (99%)	1524 (86%)	248 (14%)	3	17
2	I	1772/1789 (99%)	1526 (86%)	246 (14%)	3	17
All	All	9696/10065 (96%)	8422 (87%)	1274 (13%)	4	19

5 of 1274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1227	ARG
2	I	945	THR
2	H	1446	SER
2	H	1219	ILE
2	I	109	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 311 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	572	ASN
2	I	855	HIS
2	H	752	GLN
2	H	1896	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1421	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	CER	A	2748	-	11,11,15	4.18	3 (27%)	11,13,17	4.44	4 (36%)
4	FMN	G	3051	-	33,33,33	6.45	22 (66%)	48,50,50	1.36	6 (12%)
4	FMN	H	3051	-	33,33,33	6.35	21 (63%)	48,50,50	1.36	7 (14%)
3	CER	B	2748	-	11,11,15	4.17	3 (27%)	11,13,17	4.27	4 (36%)
3	CER	C	2748	-	11,11,15	4.19	3 (27%)	11,13,17	4.43	4 (36%)
4	FMN	I	3051	-	33,33,33	6.45	24 (72%)	48,50,50	1.36	8 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CER	A	2748	-	-	4/12/12/16	-
4	FMN	G	3051	-	-	5/18/18/18	0/3/3/3
4	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
3	CER	B	2748	-	-	4/12/12/16	-
3	CER	C	2748	-	-	4/12/12/16	-
4	FMN	I	3051	-	-	5/18/18/18	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3051	FMN	C6-C7	13.44	1.57	1.39
4	I	3051	FMN	C6-C7	13.08	1.57	1.39
4	H	3051	FMN	C6-C7	12.77	1.57	1.39
4	I	3051	FMN	C6-C5A	12.55	1.59	1.40
4	I	3051	FMN	C9-C8	12.37	1.56	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2748	CER	O1-C4-C3	-11.11	108.66	120.07
3	C	2748	CER	O1-C4-C3	-11.09	108.69	120.07
3	B	2748	CER	O1-C4-C3	-10.73	109.06	120.07
3	C	2748	CER	O1-C4-C5	-8.10	107.97	121.68
3	A	2748	CER	O1-C4-C5	-8.05	108.06	121.68

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2748	CER	C2-C3-C4-O1
3	B	2748	CER	C2-C3-C4-O1
3	C	2748	CER	C2-C3-C4-O1
4	G	3051	FMN	C2'-C3'-C4'-C5'
4	G	3051	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

6 monomers are involved in 28 short contacts:

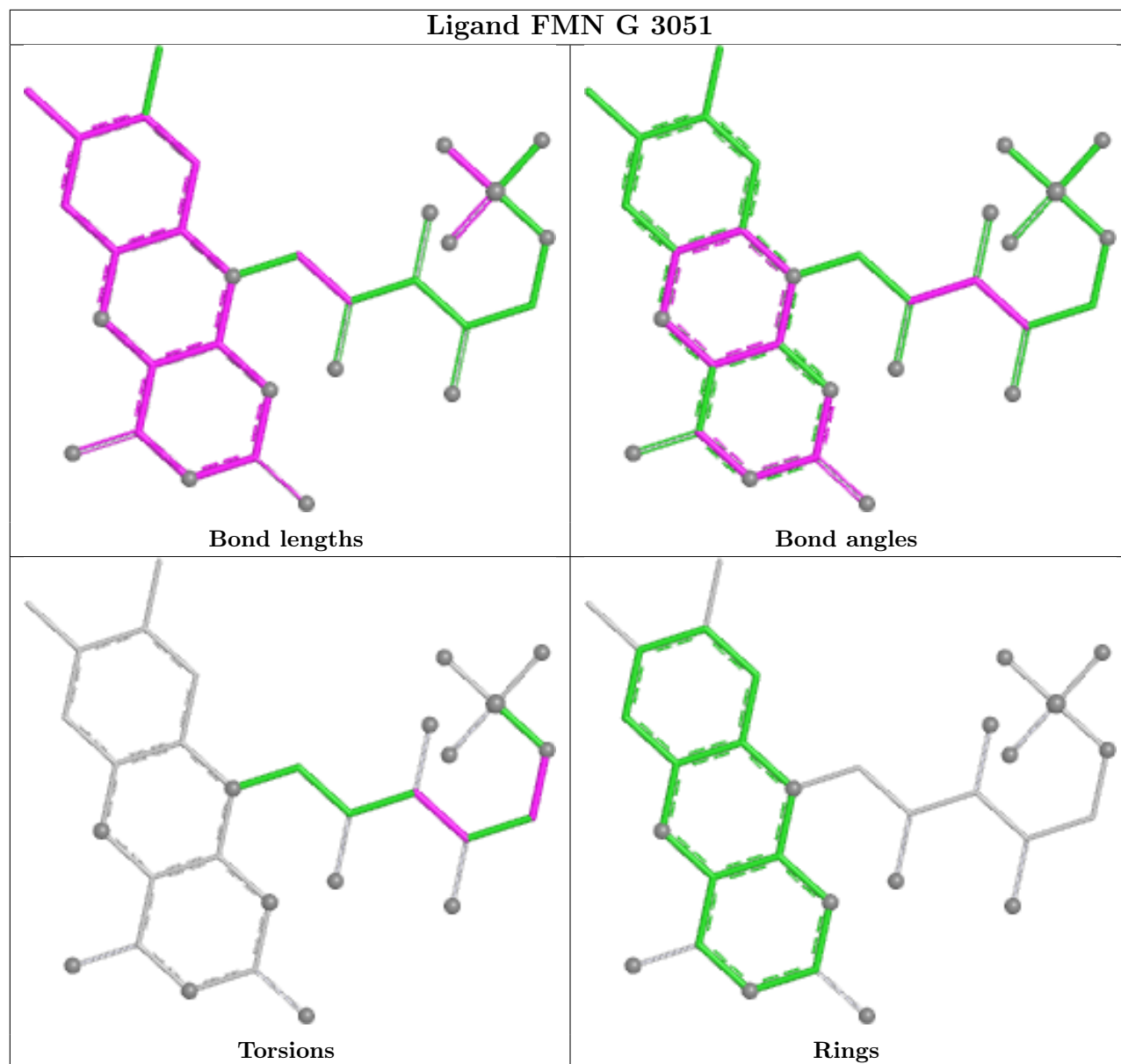
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2748	CER	3	0

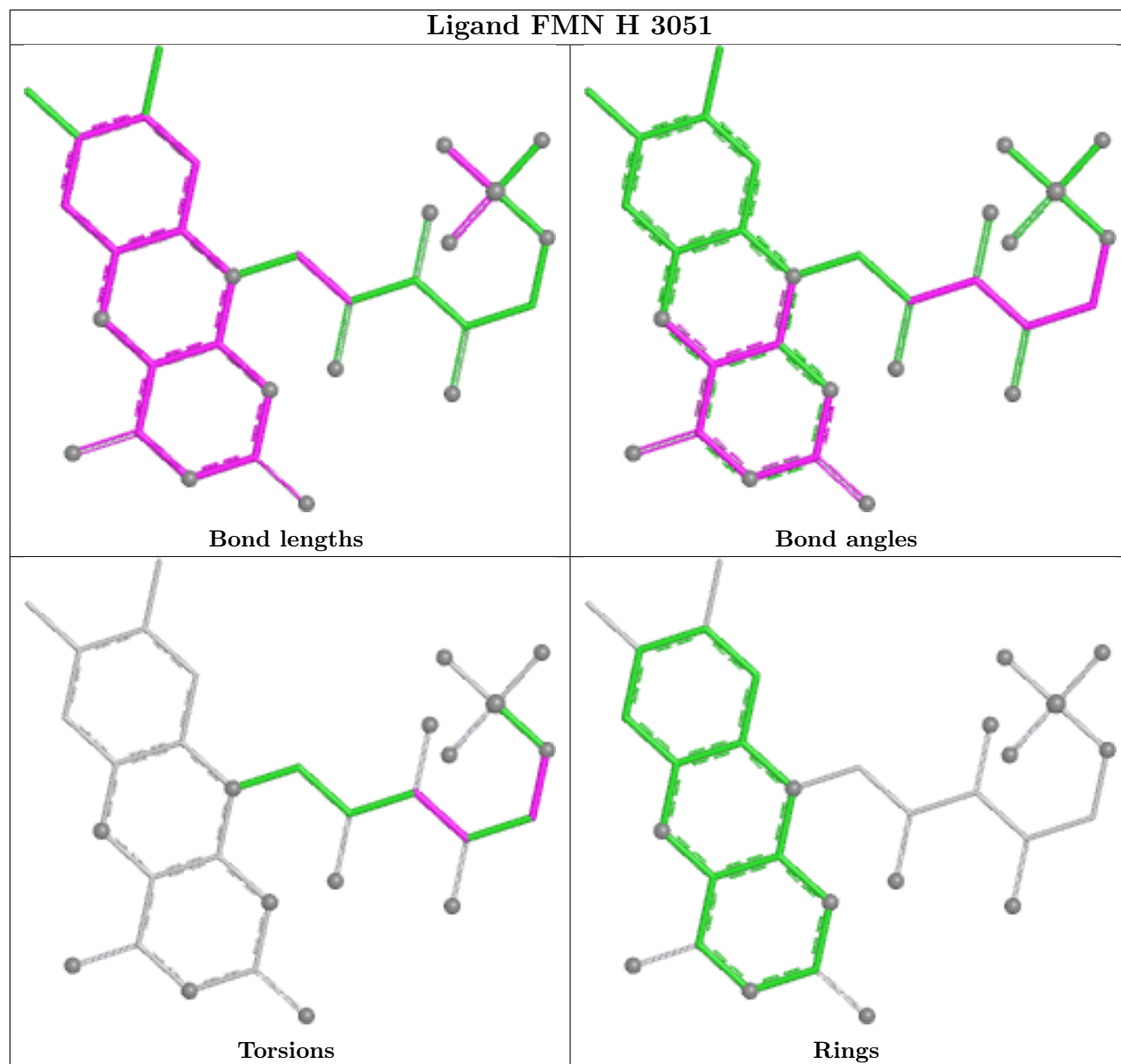
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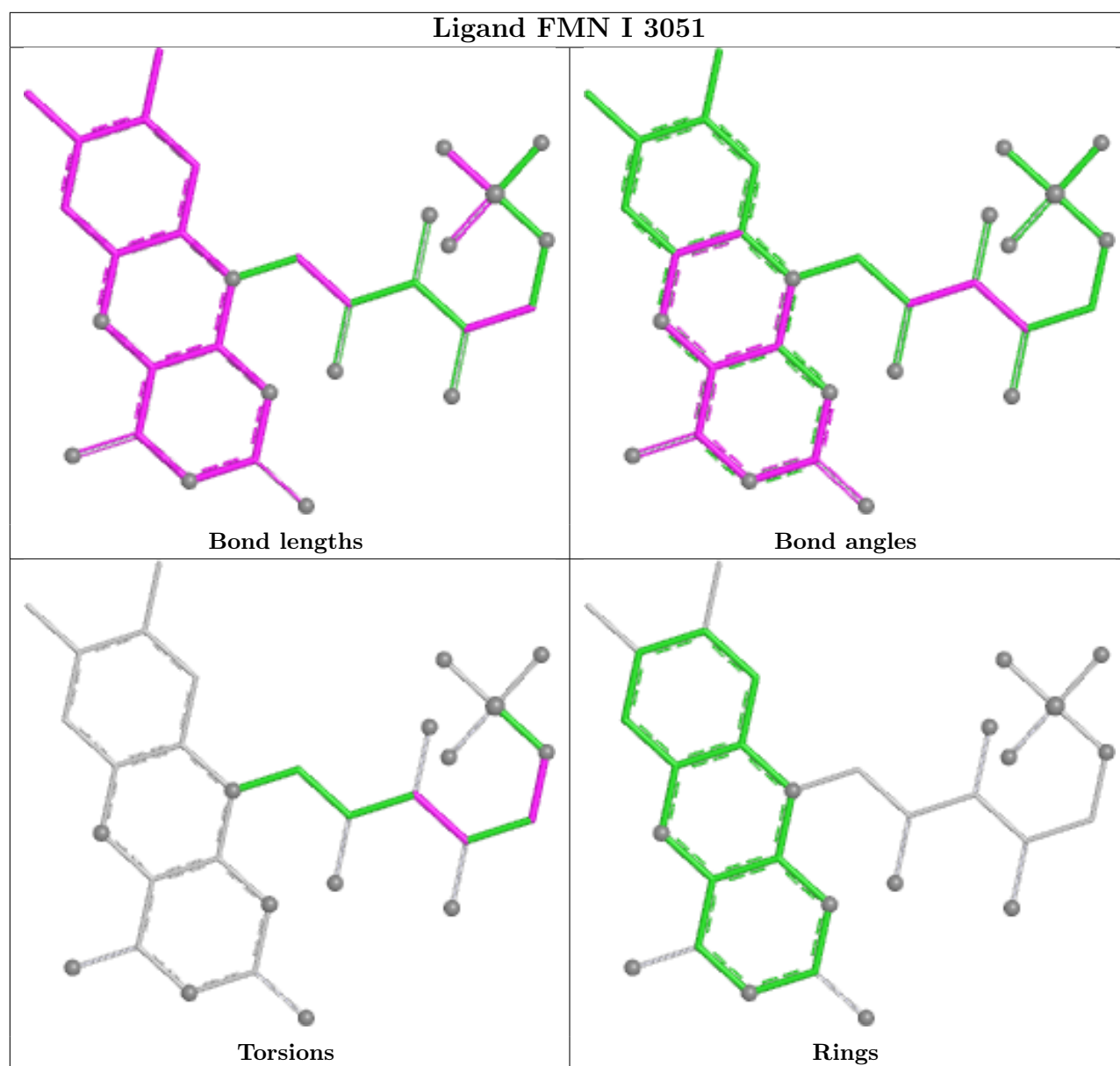
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	3051	FMN	8	0
4	H	3051	FMN	5	0
3	B	2748	CER	4	0
3	C	2748	CER	4	0
4	I	3051	FMN	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [\(i\)](#)

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	1750/1887 (92%)	-0.03	10 (0%) 85 71	95, 134, 347, 457	0
1	B	1750/1887 (92%)	-0.06	10 (0%) 85 71	96, 132, 302, 419	0
1	C	1750/1887 (92%)	-0.01	15 (0%) 81 64	98, 135, 423, 568	0
2	G	2033/2051 (99%)	-0.10	13 (0%) 85 71	131, 169, 218, 267	0
2	H	2033/2051 (99%)	-0.05	11 (0%) 87 73	130, 170, 215, 265	0
2	I	2033/2051 (99%)	-0.07	15 (0%) 84 68	131, 171, 215, 261	0
All	All	11349/11814 (96%)	-0.05	74 (0%) 84 68	95, 162, 239, 568	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1924	ILE	6.9
2	I	205	ALA	4.8
2	H	2014	LEU	4.6
1	B	1837	ILE	3.9
2	G	1958	LEU	3.4

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

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

6.3 Carbohydrates [i](#)

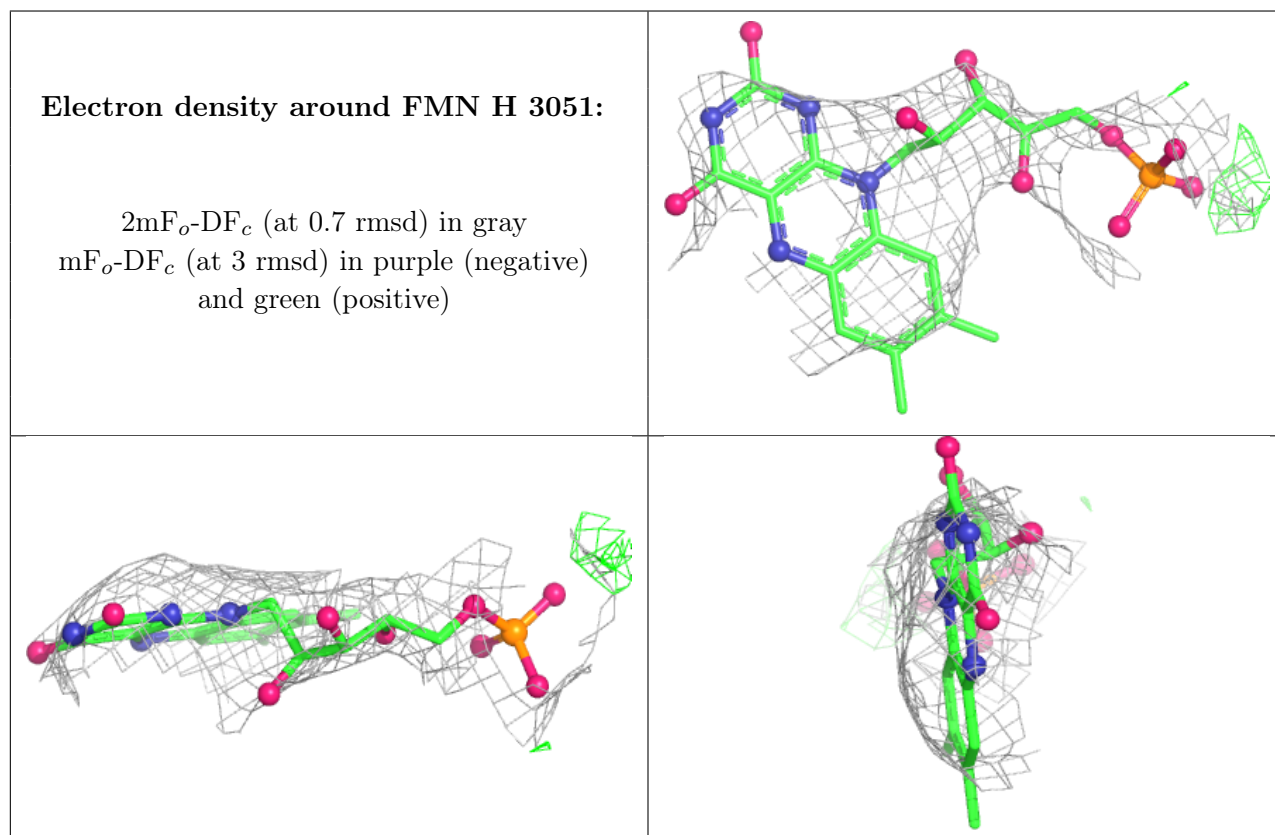
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

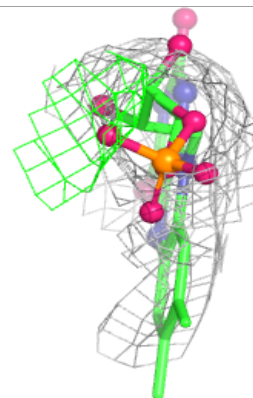
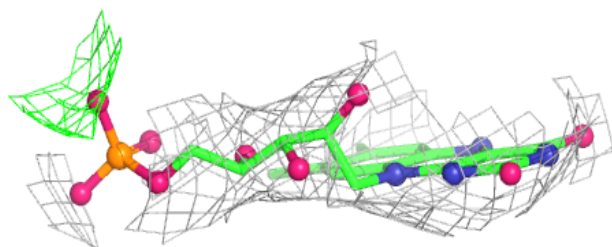
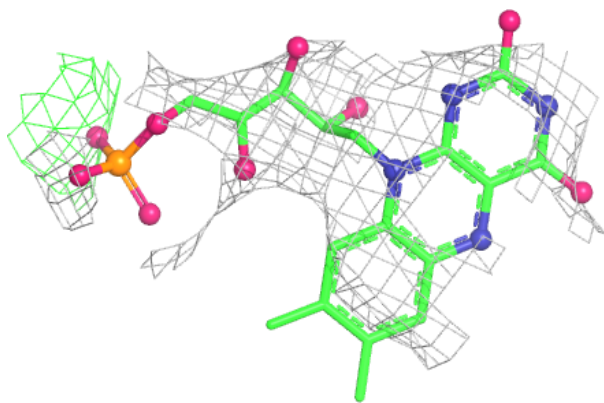
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CER	A	2748	12/16	0.80	0.17	67,131,240,249	0
4	FMN	H	3051	31/31	0.84	0.10	131,157,181,186	0
4	FMN	G	3051	31/31	0.85	0.11	135,158,184,203	0
4	FMN	I	3051	31/31	0.88	0.11	129,161,178,201	0
3	CER	B	2748	12/16	0.90	0.12	67,131,249,250	0
3	CER	C	2748	12/16	0.91	0.22	67,131,249,250	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

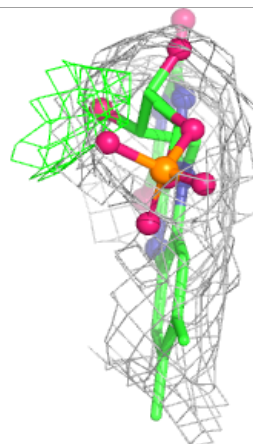
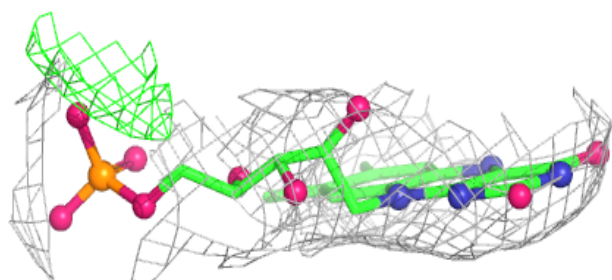
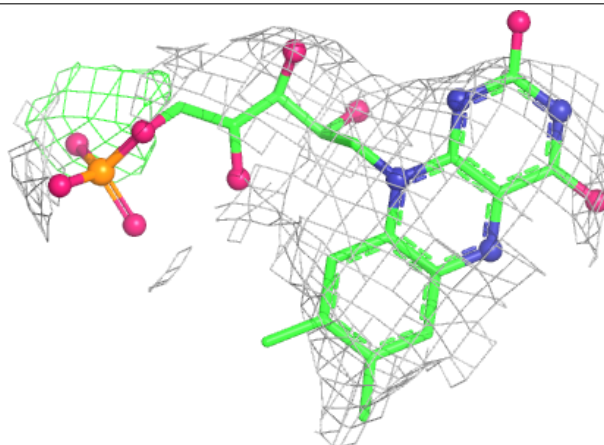


Electron density around FMN G 3051:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMN I 3051:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.