



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 11:35 PM EDT

PDB ID : 3G61
Title : Structure of P-glycoprotein Reveals a Molecular Basis for Poly-Specific Drug Binding
Authors : Aller, S.G.; Yu, J.; Ward, A.; Weng, Y.; Chittaboina, S.; Zhuo, R.; Harrell, P.M.; Trinh, Y.T.; Zhang, Q.; Urbatsch, I.L.; Chang, G.
Deposited on : 2009-02-05
Resolution : 4.35 Å(reported)

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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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

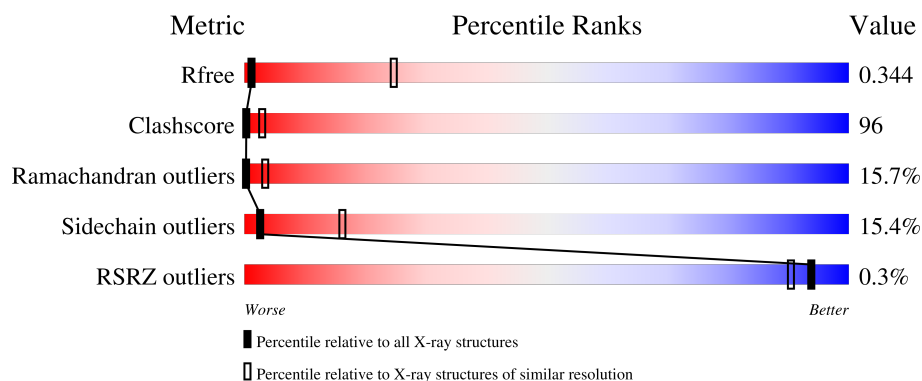
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.35 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}	130704	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)
RSRZ outliers	127900	1078 (4.92-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1284	
1	B	1284	

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	2J8	A	6002	-	-	-	X
2	2J8	B	6003	-	-	-	X
2	2J8	B	6004	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18448 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.

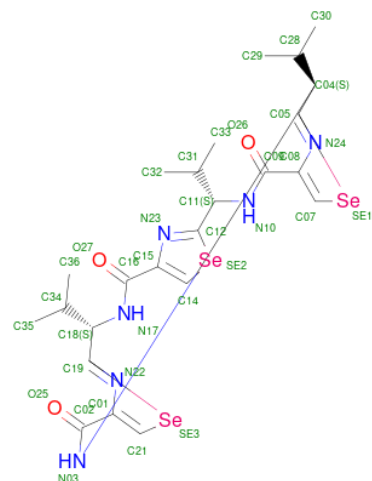
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			
1	B	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TYR	-	expression tag	UNP Q5I1Y5
A	1278	VAL	-	expression tag	UNP Q5I1Y5
A	1279	HIS	-	expression tag	UNP Q5I1Y5
A	1280	HIS	-	expression tag	UNP Q5I1Y5
A	1281	HIS	-	expression tag	UNP Q5I1Y5
A	1282	HIS	-	expression tag	UNP Q5I1Y5
A	1283	HIS	-	expression tag	UNP Q5I1Y5
A	1284	HIS	-	expression tag	UNP Q5I1Y5
B	1277	TYR	-	expression tag	UNP Q5I1Y5
B	1278	VAL	-	expression tag	UNP Q5I1Y5
B	1279	HIS	-	expression tag	UNP Q5I1Y5
B	1280	HIS	-	expression tag	UNP Q5I1Y5
B	1281	HIS	-	expression tag	UNP Q5I1Y5
B	1282	HIS	-	expression tag	UNP Q5I1Y5
B	1283	HIS	-	expression tag	UNP Q5I1Y5
B	1284	HIS	-	expression tag	UNP Q5I1Y5

- Molecule 2 is (4S,11S,18S)-4,11,18-tri(propan-2-yl)-6,13,20-triseleno-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1.5,8.1.12,15]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri-one (three-letter code: 2J8) (formula: C₂₄H₃₀N₆O₃Se₃).

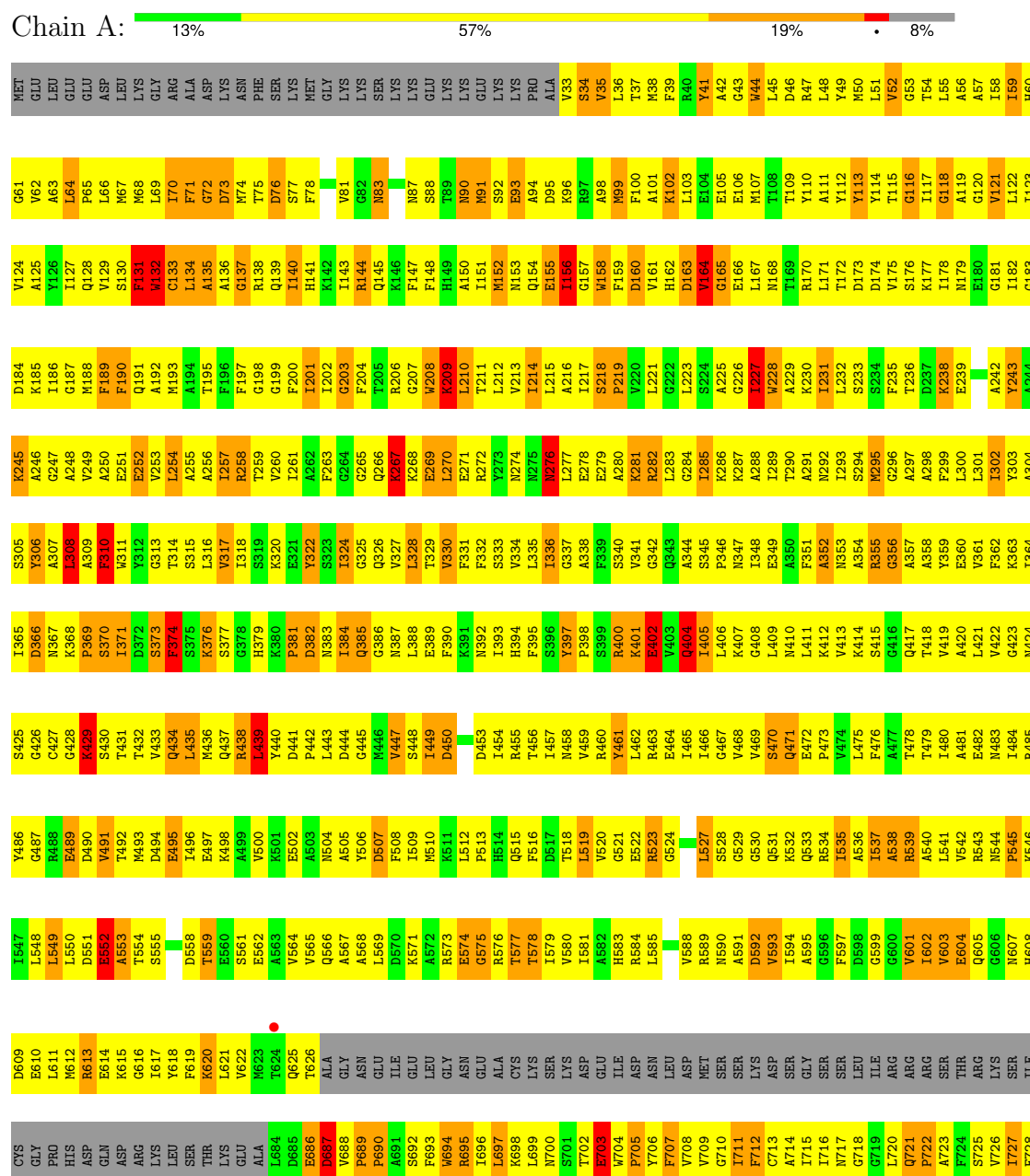


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 24	N 6	O 3	Se 3	0	0
2	A	1	Total 17	C 11	N 3	O 1	Se 2	0	0
2	B	1	Total 36	C 24	N 6	O 3	Se 3	0	0
2	B	1	Total 17	C 11	N 3	O 1	Se 2	0	0

3 Residue-property plots

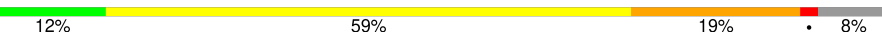
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Multidrug resistance protein 1a



S729	M792	L853	Y916	A976	Y1040	V1102	C1223	G61	V124	D184	K245	S305
K730	L793	T854	A917	I977	P1041	Q1103	I1224	V62	A125	K185	A246	Y306
V732	R794	L856	Q918	V978	T1042	W1104	V1226	A63	Y126	I186	G247	A307
V731	R795	L857	Q919	F979	R1043	L1105	V1225	L64	I127	G187	A248	L308
V734	R796	L858	Q920	G980	P1044	A1106	A1227	P65	Q128	M188	V249	A309
V733	V797	L859	Q921	A981	S1045	A1107	H1228	L66	V129	F189	A250	F310
F735	S798	A859	T922	M982	T1046	Q1108	R1229	M67	S130	F190	E251	V311
T736	W799	I860	P923	Q986	P1047	L1109	L1230	M68	F131	Q191	E252	Y312
	F800	V861	Y924	Q987	V1048	G1110	L1231	L69	Y132	A192	E253	G313
P740	D801	P862	R925	V987	Q1050	I1111	T1232	I70	C133	M193	L254	T314
P741	D802	I863	N926	S988	Q1051	V1112	T1233	F71	L134	A194	A255	S315
E742	P803	I864	A927	S989	G1052	S1113	A1234	G72	A135	T195	A256	L316
T743	K804	A865	M928	F990	L1052	Q1114	M1235	D73	A136	F196	I257	V317
	N805	I866	K929	A991	S1053	E1115	A1236	M74	G137	F197	R258	I318
Q746	T806	A867	K930	P992	L1054	P1116	I1239			G198	T259	S319
N747	T807	V870	A931	D993	E1055	Q1117	V1240	T75	Y138	G199	V260	K320
S748	G808	V871	H932	Y994	V1056	L1118	V1241	S77	I140	F200	I261	E321
N749	A809	A895	V933	Y994	K1057	T1119	L148	F78	H141	I201	A262	Y322
L750	L810	K872	F934	K996	L1058	D1120	I1242	V81	K142	G202	F263	S323
F751	T811	L875	Q985	A997	G1059	C1121	Q1243		I143	G203	G284	I324
S752	T812		T998	T998	Q1060	I1122	M1244	V81	R144	T204	G285	G325
L753	R813	Q878	V999	V999	T1061	I1123	K1245	G82	Q145	Q138	G286	Q326
L754	L814	F938	S1000	S1000	L1062	A1124	K1246	N83	K146	R139	Q267	V327
F755	A815	A879	S939	A1001	A1063	E1125	V1247	K86	F147	G207	K268	L328
L756	L816	F940	S940	A1001	L1064	N1126	K1248	N87	F148	W208	E269	L329
I757	D817	K881	T941	H1003	V1065	I1127	E1249	S88	H149	K209	L270	V330
L758	A818	D882	Q942	H1004	G1066	A1128	L1250	I89	A150	K210	E271	F331
G759	A819	K883	Y949	I1005	S1067	Y1129	G1251	N90	I151	T211	R272	F332
I760	K820	K884	A950	I1006	G1068	G1130	Q1252	M91	M152	L212	Y273	S333
I761	V821	E885	N945	I1008	S1069	E1131	H1253	S92	N153	V213	N274	V334
S762	K822	L886	Y946	I1009	L1070	N1132	Q1254	E83	Q154	I214	K275	L335
F763	G823	E887	F947	K1010	L1071	S1133	Q1255	A94	E155	L215	K276	I336
I764	I764	G888	S948	I1011	V1075	R1134	L1257	D95	I156	A216	L277	G337
T765	T825	S889	Y949	P1012	V1076	V1135	L1257	A98	W158	I217	A338	A338
F766	G826	E890	E1013	A950	Q1077	Y1136	Q1258	M99	F159	S218	E279	F339
F767	S827	K891	A951	I1014	Q1078	S1137	K1260	F100	D160	P219	A280	S340
L768	R828	L892	C952	I1017	L1079	E1138	G1261	A101	V161	W220	K281	V341
Q769	L829	A893	F983	S1018	E1080	E1139	I1262	K102	H162	L221	R282	G342
G770	A830	T894	A954	T1019	R1081	I1141	Y1262	R40	D163	G222	L283	Q343
T772	I832	E896	F955	T1019	F1082	V1142	F1264	Y41	E104	L223	A344	A344
F773	F833	I897	G956	G1021	Y1083	R1143	S1265	A42	E105	S224	I285	S345
G774	Q834	E898	A957	L1022	D1084	A1144	M1266	G43	E106	G225	K286	P346
K775	N835	N899	L959	K1023	P1085	A1145	V1267	W44	M107	L167	A288	N347
A776	I836	F900	V960	P1024	H1086	K1146	E1207	L45	T108	N168	I289	I348
G777	A837	R901	T961	N1025	A1087	E1147	K1208	V52	T169	T175	T290	A350
E778	N838	T902	Q962	M1026	G1088	A1148	V1209	D46	Y110	R170	A291	F351
I779	L839	V903	Q963	L1027	S1089	N1149	Q1211	R47	A111	L171	N292	A352
L780	G840	V904	L964	E1028	V1090	I1150	H1151	L48	T172	T172	K293	N353
T781	T841	S905	M965	G1029	F1091	H1151	E1212	M50	D173	G173	S294	A354
K782	G842	L906	T966	N1030	L1092	Q1152	A1213	L51	Y113	Y113	K295	R355
R783	I843	T907	F967	Q1031	D1093	F1153	L1214	V52	T115	V175	G296	G356
L784	I844	R908	E968	Q1032	G1094	I1154	D1215	G53	G116	S176	A297	A357
R785	E909	E909	F1033	K1095	K1095	D1155	K1216	T54	I117	K177	A298	A358
Y786	S846	Q910	V970	S1034	E1096	S1156	A1217	L55	G118	N178	F299	V359
M787	K911	L971	L971	G1035	L1097	L1157	E1218	A56	A119	N179	E239	E360
V788	I848	F912	L972	V1036	K1038	F1158	E1219	A57	G120	I179	L301	V361
F789	Y849	E913	V973	V1037	Q1099	D1159	HIS	I58	V121	G181	I302	F362
K790	T914	F974	S975	I1038	L1100	K1160	R1220	I59	L122	I182	Y303	K363
S791	Q852	M915	N1039	N1039	N1101	Y1161	T1222	H60	I123	G183	A304	I364

• Molecule 1: Multidrug resistance protein 1a

Chain B:  12% 59% 19% 8%

MET	V124	D184	K245	S305
GLU	A125	K185	A246	Y306
LEU	A63	I186	G247	A307
GLU	L64	G187	A248	L308
GLU	P65	M188	V249	A309
ASP	L66	F189	A250	F310
LEU	M67	F190	E251	V311
LVS	M68	Q191	E252	Y312
GLY	L69	A192	E253	G313
ARG	I70	C133	L254	T314
ALA	F71	L134	A255	S315
ASP	G72	A135	A256	L316
LVS	D73	F196	I257	V317
ASN	M74	G137	R258	I318
PHE	T75	G198	T259	S319
SER	T76	Q139	V260	K320
LVS	S77	I140	I261	E321
MET	F78	H141	A262	Y322
GLY	V81	K142	F263	S323
LVS	G82	I143	G284	I324
SER	N83	Q145	G285	G325
LVS	K86	K146	Q266	Q326
LVS	M91	K147	K267	V327
PRO	E83	F148	K268	L328
ALA	A94	Q154	E269	T329
V33	D95	E155	L270	V330
S34	A98	I156	E271	F331
L36	M99	W158	R272	F332
T37	F100	F159	K273	S333
M38	A101	D160	N274	V334
F39	K102	V161	K275	L335
R40	L103	H162	K276	I336
Y41	E104	G163	L277	G337
A42	E105	G165	A338	A338
G43	E106	G166	E279	F339
W44	M107	L167	A280	S340
L45	T108	N168	K281	V341
T109	T109	T169	R282	G342
Y110	Y110	R170	L283	Q343
A111	A111	L171	A344	A344
Y112	Y112	T172	I285	S345
Y113	Y113	D173	K286	P346
Y114	Y114	D174	G287	N347
T115	T115	V175	A288	I348
G53	G53	S176	I289	E349
T54	T54	K177	T290	A350
L55	L55	D237	A291	F351
A56	A56	N178	N292	A352
A57	A57	E239	K293	N353
I58	I58		S294	A354
I59	I59		K295	R355
H60	H60		G296	G356
			A297	A357
			A298	A358
			F299	V359
			E360	L300
			V361	L301
			I302	F362
			Y303	K363
			A304	I364

C1223	G1223	Y1181	N1101	Y1040	1977	A917	T854	R794	G733	GLY	D609	E547	Y486	S425	I365
I1224	I1224	R1164	V1102	P1041	V978	Q818	L855	Q795	V794	PRO	E610	L548	G487	G426	D366
V1225	V1225	V1165	Q1103	T1042	F979	S919	L856	Q796	V796	HIS	L611	L549	C427	C427	N367
I1226	I1226	V1166	W1104	R1043	G980	S920	L857	Q797	T736	ASP	M612	L550	E488	G428	K368
A1227	A1227	D1167	L1105	P1044	A981	Q921	L858	Q798	H737	GLN	R613	D551	K429	K429	P369
H1228	H1228	K1168	R1106	S1045	M982	I922	S1045	Q799	G738	ASP	E614	V491	S430	S430	S370
R1229	R1229	G1169	A1107	T1046	Q985	P923	T860	F800	G739	ARG	K615	T492	T431	I371	I371
L1230	L1230	T1170	Q1108	P1047	Q986	V924	V861	D801	P740	LYS	G616	M493	T432	D372	D372
S1231	S1231	G1171	L1109	V1048	R925	R925	P862	D802	P741	LEU	P617	D494	V433	S373	S373
T1232	T1232	G1172	G1110	L1049	S987	N926	P863	F803	T742	THR	F618	E495	Q434	F374	F374
I1233	I1233	L1172	I1111	Q1050	S988	A927	T864	K804	T743	LYS	F619	I496	Q435	S375	S375
Q1234	Q1234	S1173	V1112	G1051	S989	N928	T865	R805	Q746	GLY	K620	E497	M436	K376	K376
R1235	R1235	G1174	S1113	L1052	F980	Q929	T866	R806	G747	LYS	L621	K498	Q437	S377	S377
A1236	A1236	Q1175	Q1114	S1053	A991	K930	A867	T807	N747	ALA	V622	E561	R438	G378	G378
I1239	I1239	Q1176	E1115	L1054	P992	A931	V870	Q909	S748	ALA	Q625	V500	R438	H379	H379
V1240	V1240	K1177	P1116	E1055	D993	H932	N749	A809	N749	ALA	T626	A501	L439	Y440	K380
I1241	I1241	Q1178	I1117	V1056	Y994	V933	E871	L810	L750	ALA	ALA	E502	D441	P381	P381
L1242	L1242	R1179	L1118	K1057	A995	F934	T811	T811	G751	GLY	GLY	V564	P442	D382	D382
I1243	I1243	I1180	F1119	K1058	K996	G935	T812	T812	S752	ASN	ASN	Q566	L443	N383	N383
Q1243	Q1243	A1181	D1120	G1059	A997	I936	L875	R813	L753	ASN	ASN	A505	D444	I384	I384
N1244	N1244	I1182	C1121	Q1060	T998	T937	Q942	R814	L753	GLY	GLY	A506	G445	Q385	Q385
G1245	G1245	R1183	S1122	T1061	V999	F938	Q878	A815	L755	LEU	LEU	D507	M446	G386	G386
K1246	K1246	R1184	I1123	A1063	S1000	S939	A879	N816	L756	LEU	LEU	D507	V447	N387	N387
V1247	V1247	A1185	A1124	A1063	A1001	T941	K881	D817	L757	GLY	GLY	K571	S448	L388	L388
K1248	K1248	L1186	E1125	L1064	S1002	F940	K881	A818	L758	GLY	GLY	A572	I449	E389	E389
E1249	E1249	V1187	N1126	V1065	H1003	Q942	D882	A819	G759	ASN	ASN	R573	D450	F390	F390
H1250	H1250	R1188	I1127	G1066	I1004	A943	K883	Q820	L760	GLY	GLY	E574	Q391	K391	K391
G1251	G1251	K1189	A1128	S1067	I1005	N944	K884	R821	L761	ALA	ALA	G575	D453	N392	N392
T1252	T1252	P1190	Y1129	S1068	R1006	K945	E885	K822	S762	CYS	CYS	H514	I454	I393	I393
H1253	H1253	H1191	G1130	G1069	I1007	Y946	L886	C823	F763	LYS	LYS	T577	R455	H394	H394
Q1254	Q1254	I1192	D1131	C1070	I1008	F947	E887	A824	L764	SER	SER	T578	T456	F395	F395
Q1255	Q1255	L1193	N1132	G1071	E1009	S943	G888	T825	L765	LYS	LYS	I579	I457	S386	S386
L1256	L1256	L1194	S1133	K1072	K1010	Y949	S889	G826	F766	ASP	ASP	V580	M468	Y397	Y397
A1258	A1258	L1195	R1134	T1011	P1012	A950	G890	S827	F767	GLY	GLY	L519	V459	P398	P398
Q1259	Q1259	E1197	V1136	V1076	E1013	C952	K891	R828	L768	ILE	ILE	V520	R460	S399	S399
K1260	K1260	A1198	S1137	Q1077	I1014	F953	L892	L829	Q769	ASP	ASP	G521	Y461	R400	R400
G1261	G1261	T1199	Y1138	L1078	D1015	R954	T894	R831	G770	ASN	ASN	E522	L462	K401	K401
I1262	I1262	S1200	E1139	L1079	S1016	F955	E895	L832	T772	ASP	ASP	R523	R463	E402	E402
Y1263	Y1263	A1201	E1140	E1080	G956	G956	A896	F833	F773	MET	MET	G524	E464	V403	V403
F1264	F1264	L1202	T1141	R1081	T1019	Q962	L897	Q834	G774	SER	SER	L527	I465	Q404	Q404
S1265	S1265	D1203	V1142	F1082	Q1020	Y958	E398	N835	K775	SER	SER	S528	I466	I405	I405
M1266	M1266	T1204	R1143	Y1083	G1021	Q963	E398	N835	K775	LYS	LYS	G529	G467	L406	L406
V1267	V1267	E1205	A1144	D1084	L1022	V960	F900	A837	A776	ASP	ASP	G530	V468	K407	K407
Q1270	Q1270	S1206	A1145	P1085	K1023	T961	R901	N838	G777	ASP	ASP	D592	V469	G408	G408
A1271	A1271	E1207	K1146	M1086	P1024	Q962	T902	L839	E778	SER	SER	Q531	S470	L409	L409
GLY	GLY	K1208	E1147	A1087	M1025	Q963	V903	G840	L780	GLY	GLY	K532	Q471	N410	N410
ALA	ALA	V1209	A1148	G1088	M1026	L964	V904	T841	K781	SER	SER	Q533	E472	L411	L411
LYS	LYS	V1210	N1149	S1089	N965	N965	S905	G842	T782	SER	SER	R534	P473	K412	K412
ARG	ARG	Q1211	T1150	V1090	E1028	T966	L906	T843	K783	LEU	LEU	I535	V474	V413	V413
THR	THR	E1212	H1151	F1091	V1031	F967	T907	T844	L784	ILE	ILE	A536	L475	K414	K414
VAL	VAL	L1214	F1153	D1093	Q1032	N968	R908	T845	R785	ARG	ARG	I537	F476	S415	S415
HIS	HIS	D1215	I1154	G1094	F1033	N969	E909	S846	Y786	ARG	ARG	G600	A477	G416	G416
HIS	HIS	K1216	D1155	K1095	S1034	V970	Q910	L847	N787	SER	SER	V601	T478	Q417	Q417
HIS	HIS	A1217	S1156	E1096	G1035	L971	K911	T848	V788	THR	THR	I541	T479	T418	T418
HIS	HIS	R1218	L1157	I1097	V1036	L972	E912	F889	F789	ARG	ARG	V542	I480	V419	V419
HIS	HIS	P1153	P1153	K1098	V1037	V973	E913	G850	K790	LYS	LYS	Q605	E482	A420	A420
HIS	HIS	D1159	D1159	Q1099	F1038	F974	T914	K851	S791	SER	SER	G606	N463	V422	V422
HIS	HIS	T1221	N1159	S975	N915	N915	N915	M792	M792	ILE	ILE	P545	G423	G423	G423
HIS	HIS	T1222	K1160	L1100	N1039	A976	Y916	L853	L793	CYS	CYS	H608	R485	N424	N424

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.74Å 114.98Å 375.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 4.35 19.95 – 4.35	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.95-4.35) 93.2 (19.95-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 4.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.308 , 0.356 0.298 , 0.344	Depositor DCC
R_{free} test set	2807 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	195.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18448	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: 2J8

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	0.40	0/9339	0.72	12/12626 (0.1%)
1	B	0.39	0/9339	0.71	14/12626 (0.1%)
All	All	0.40	0/18678	0.72	26/25252 (0.1%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	SER	N-CA-C	10.10	138.27	111.00
1	B	1159	ASP	N-CA-C	-8.41	88.29	111.00
1	A	374	PHE	N-CA-C	8.32	133.47	111.00
1	A	450	ASP	N-CA-C	-8.05	89.26	111.00
1	A	1098	LYS	N-CA-C	-7.76	90.04	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	916	TYR	Sidechain

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	9171	0	9344	1807	0
1	B	9171	0	9344	1791	0
2	A	53	0	36	5	0
2	B	53	0	36	20	0
All	All	18448	0	18760	3588	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 96.

The worst 5 of 3588 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:B:718:GLY:O	1:B:722:PRO:HD2	1.44	1.17
1:A:718:GLY:O	1:A:722:PRO:HD2	1.43	1.15
1:B:858:LEU:O	1:B:862:PRO:HD2	1.47	1.15
1:A:195:THR:HB	1:A:340:SER:HB2	1.27	1.14
1:B:35:VAL:HG23	1:B:36:LEU:H	1.13	1.11

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	1178/1284 (92%)	685 (58%)	305 (26%)	188 (16%)	0	3
1	B	1178/1284 (92%)	678 (58%)	318 (27%)	182 (15%)	0	3
All	All	2356/2568 (92%)	1363 (58%)	623 (26%)	370 (16%)	0	3

5 of 370 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	88	SER
1	A	131	PHE
1	A	133	CYS

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	976/1065 (92%)	823 (84%)	153 (16%)	2	16
1	B	976/1065 (92%)	829 (85%)	147 (15%)	3	17
All	All	1952/2130 (92%)	1652 (85%)	300 (15%)	2	16

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	711	ILE
1	B	1140	GLU
1	B	751	PHE
1	B	912	PHE
1	A	853	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	721	GLN

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Mol	Chain	Res	Type
1	B	1099	GLN
1	B	749	ASN
1	B	878	GLN
1	B	1235	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 monosaccharides 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
2	2J8	A	6002	-	9,18,39	1.49	1 (11%)	8,24,57	1.30	2 (25%)
2	2J8	B	6003	-	21,39,39	1.50	3 (14%)	24,57,57	1.25	3 (12%)
2	2J8	B	6004	-	9,18,39	1.62	1 (11%)	8,24,57	1.43	2 (25%)
2	2J8	A	6001	-	21,39,39	1.49	3 (14%)	24,57,57	1.32	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2J8	A	6002	-	-	0/8/16/48	0/2/2/4
2	2J8	B	6003	-	-	0/24/48/48	0/3/4/4
2	2J8	B	6004	-	-	0/8/16/48	0/2/2/4
2	2J8	A	6001	-	-	0/24/48/48	0/3/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6004	2J8	C16-N17	4.45	1.44	1.34
2	A	6002	2J8	C16-N17	4.17	1.43	1.34
2	B	6003	2J8	C16-N17	4.10	1.43	1.34
2	A	6001	2J8	C16-N17	3.66	1.42	1.34
2	A	6001	2J8	C02-N03	3.57	1.42	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	2J8	C36-C34-C18	2.70	114.63	111.33
2	B	6004	2J8	C18-N17-C16	2.65	127.28	121.94
2	A	6001	2J8	C11-N10-C09	2.65	127.26	121.94
2	B	6004	2J8	C36-C34-C18	2.59	114.50	111.33
2	A	6002	2J8	C36-C34-C18	2.50	114.38	111.33

There are no chirality outliers.

There are no torsion outliers.

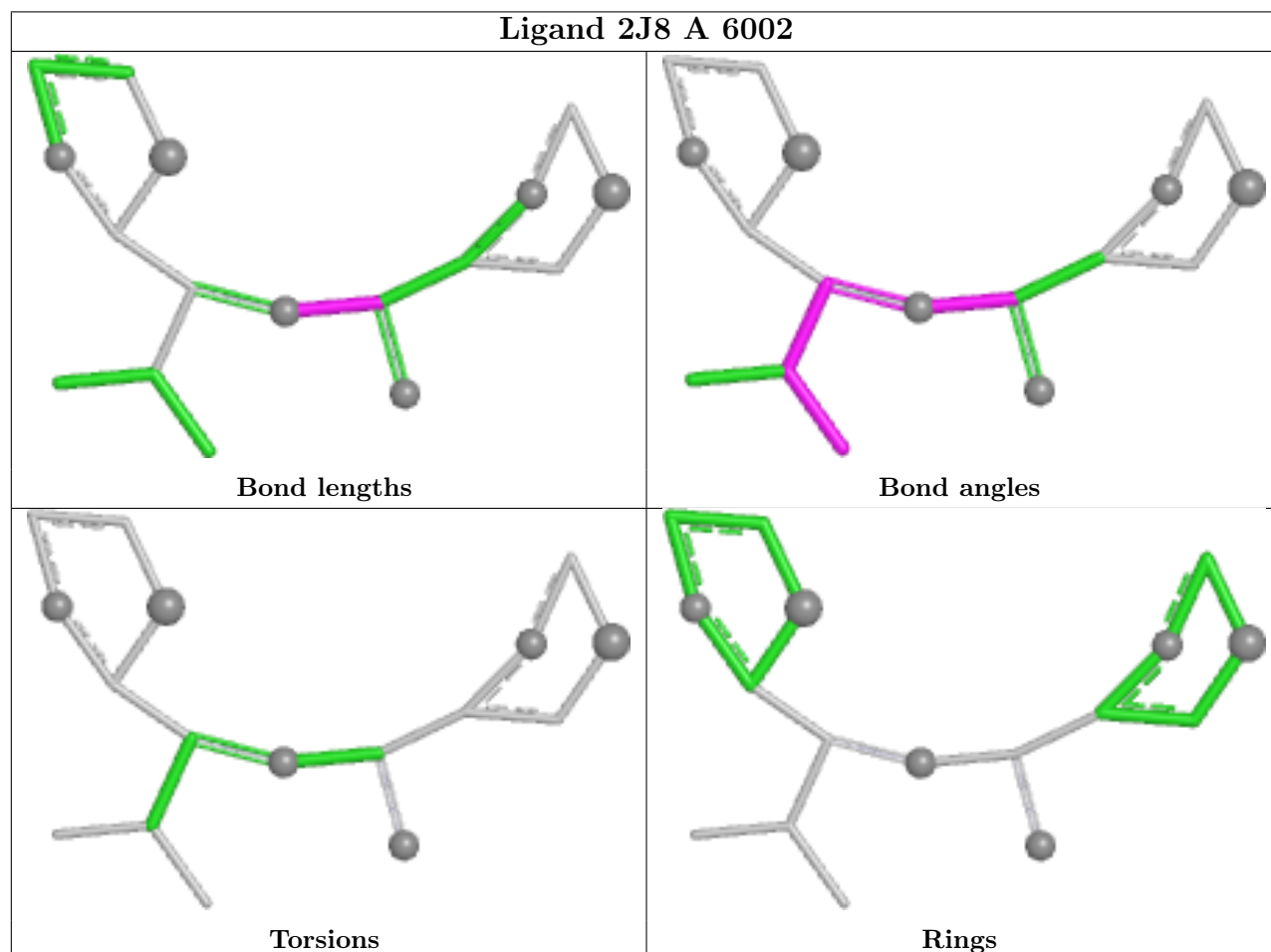
There are no ring outliers.

4 monomers are involved in 25 short contacts:

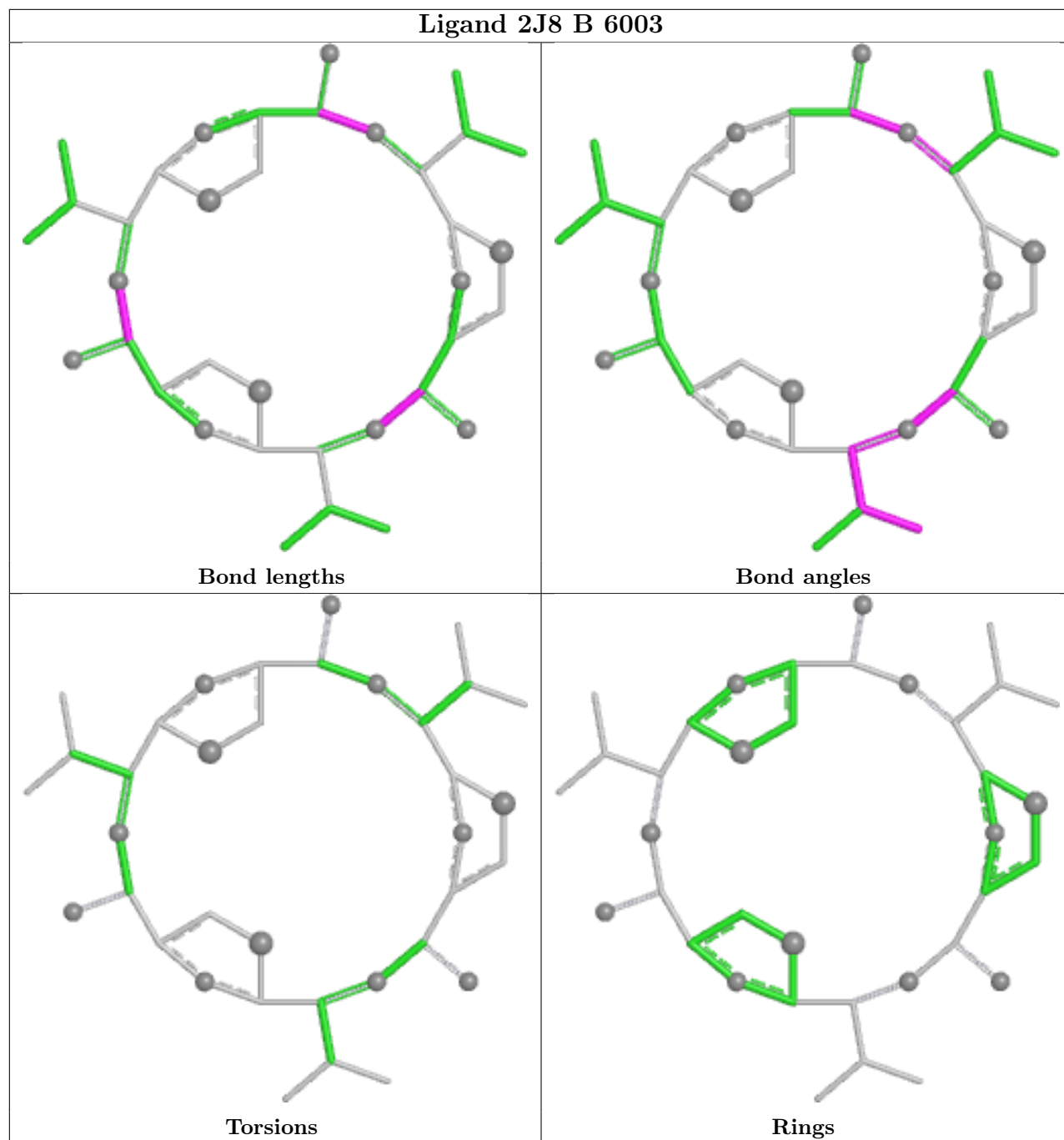
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6002	2J8	1	0
2	B	6003	2J8	16	0
2	B	6004	2J8	4	0
2	A	6001	2J8	4	0

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

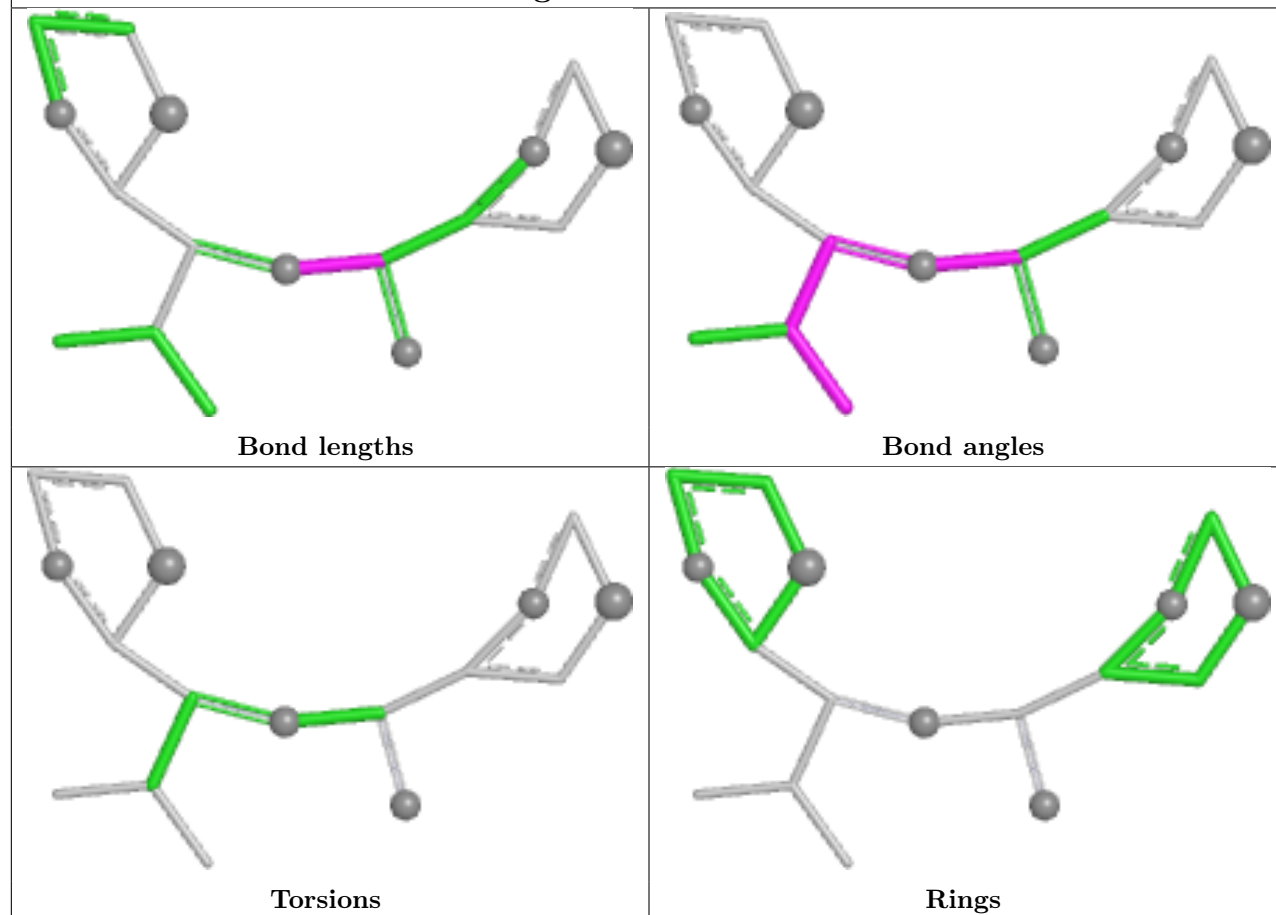
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

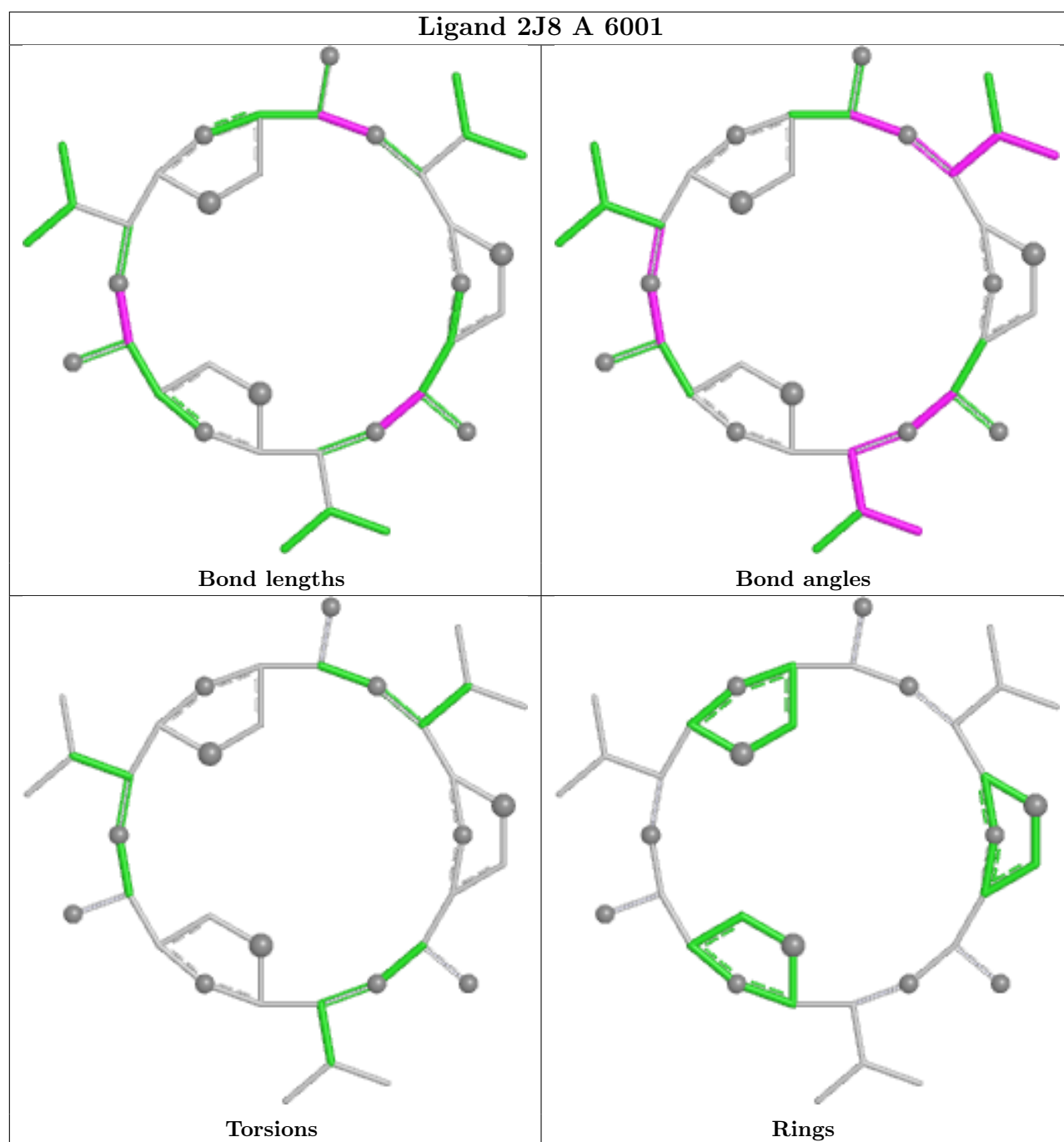


Ligand 2J8 B 6003



Ligand 2J8 B 6004





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	1182/1284 (92%)	-0.58	3 (0%) 94 90	115, 180, 210, 247	0
1	B	1182/1284 (92%)	-0.56	3 (0%) 94 90	97, 183, 214, 303	0
All	All	2364/2568 (92%)	-0.57	6 (0%) 94 90	97, 182, 212, 303	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1024	PRO	3.7
1	A	962	GLN	3.4
1	B	1244	ASN	3.0
1	A	1228	HIS	2.4
1	A	624	THR	2.1

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](#)

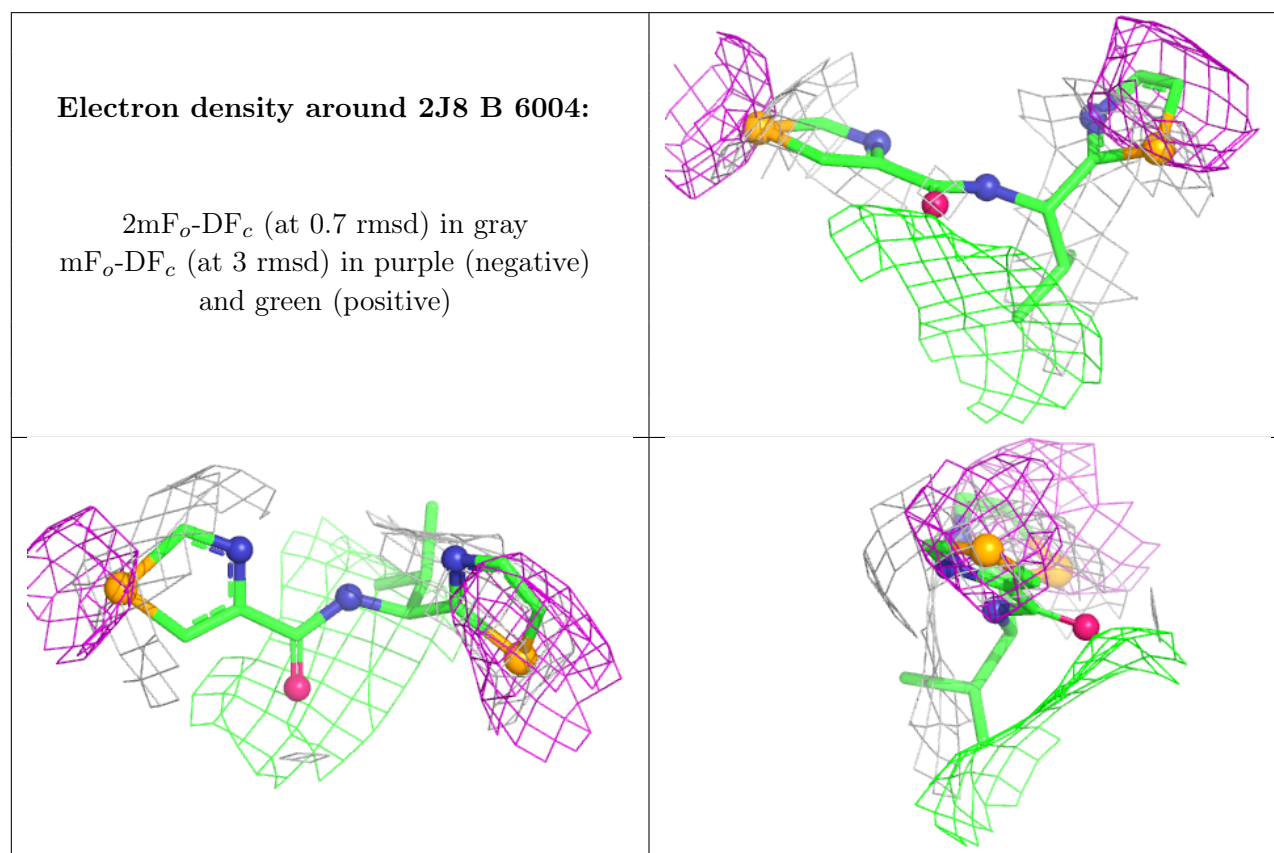
There are no monosaccharides in this entry.

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.

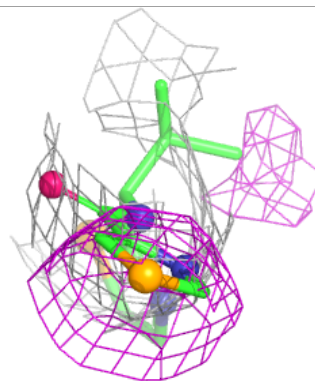
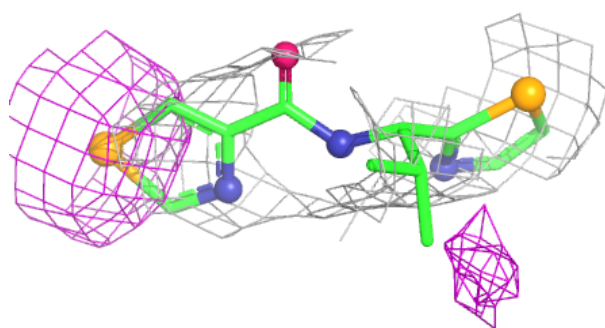
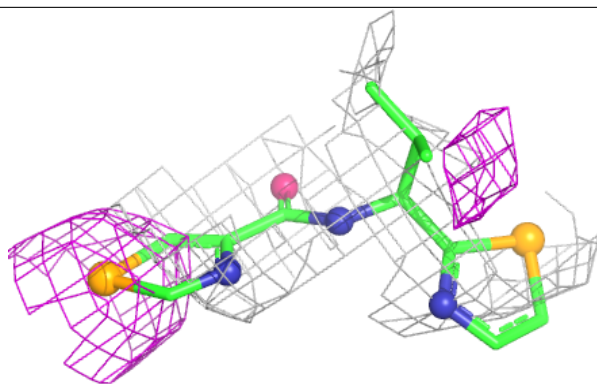
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2J8	B	6004	17/36	0.52	0.48	185,185,185,185	0
2	2J8	A	6002	17/36	0.68	0.52	185,185,185,185	0
2	2J8	B	6003	36/36	0.69	0.44	185,185,185,185	0
2	2J8	A	6001	36/36	0.80	0.36	185,185,185,185	0

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.



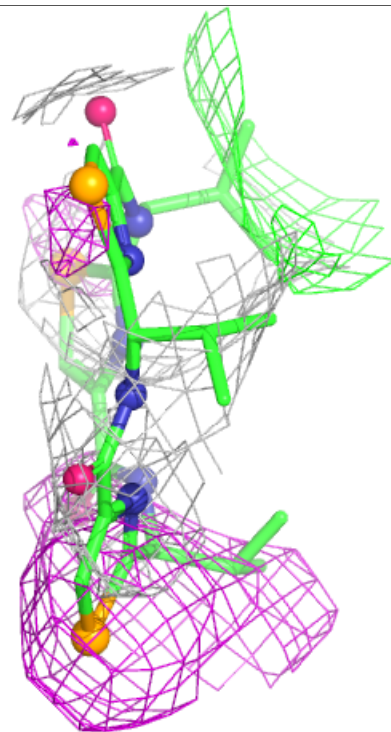
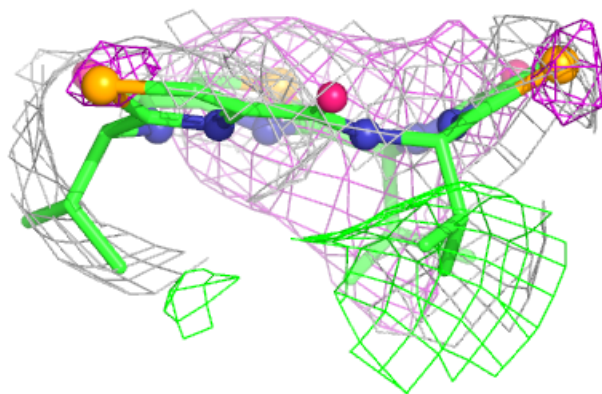
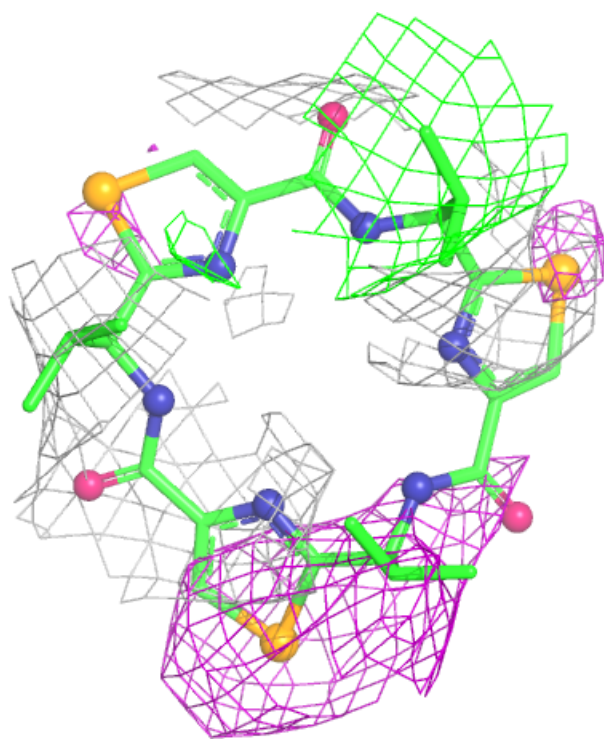
Electron density around 2J8 A 6002:

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



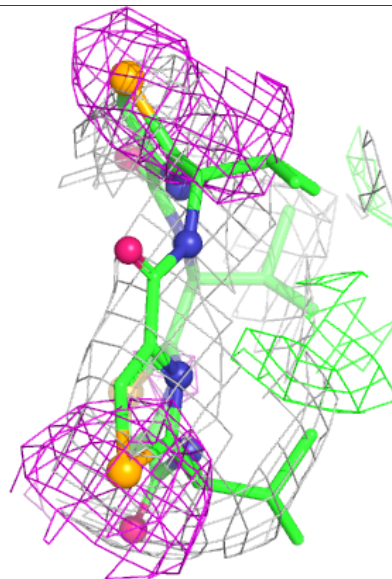
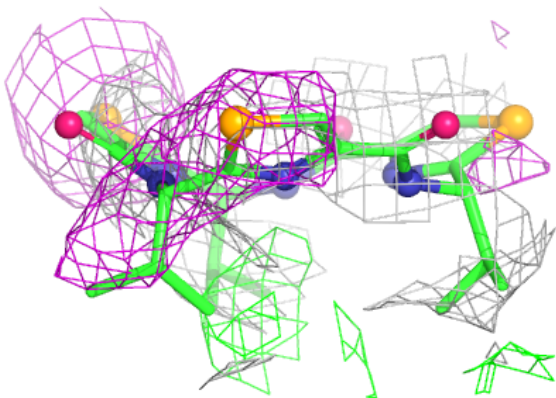
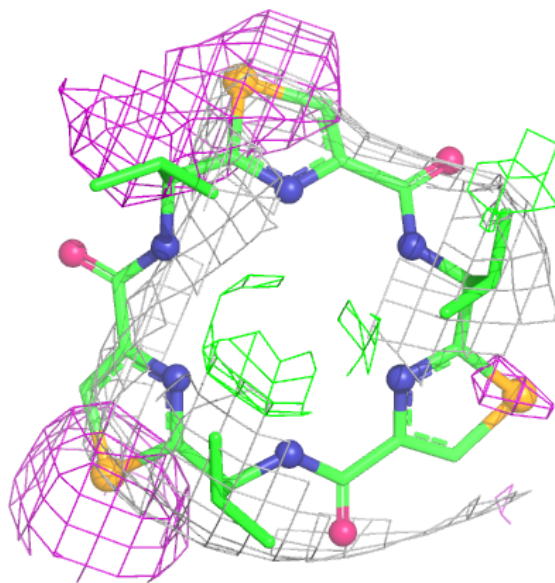
Electron density around 2J8 B 6003:

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



Electron density around 2J8 A 6001:

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 ⓘ

There are no such residues in this entry.