



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 3G60 / pdb_00003g60
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 : 4.40 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

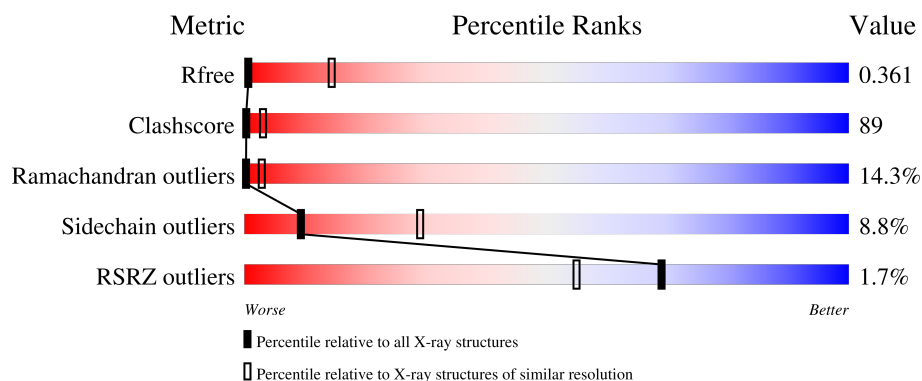
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	2% 14% 57% 19% 8%
1	B	1284	% 14% 57% 19% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18414 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.

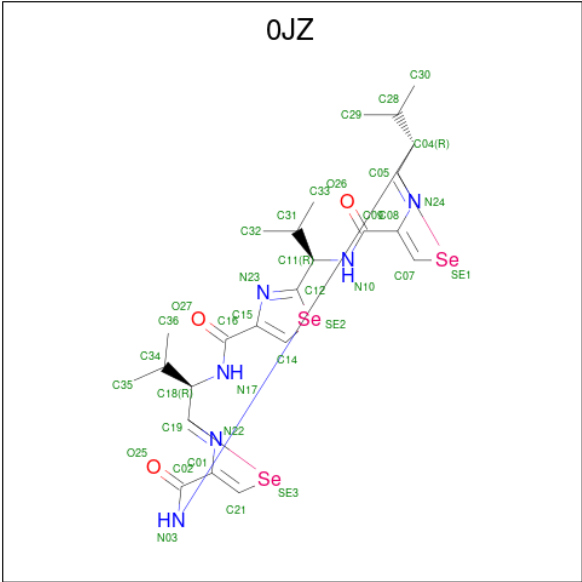
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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			

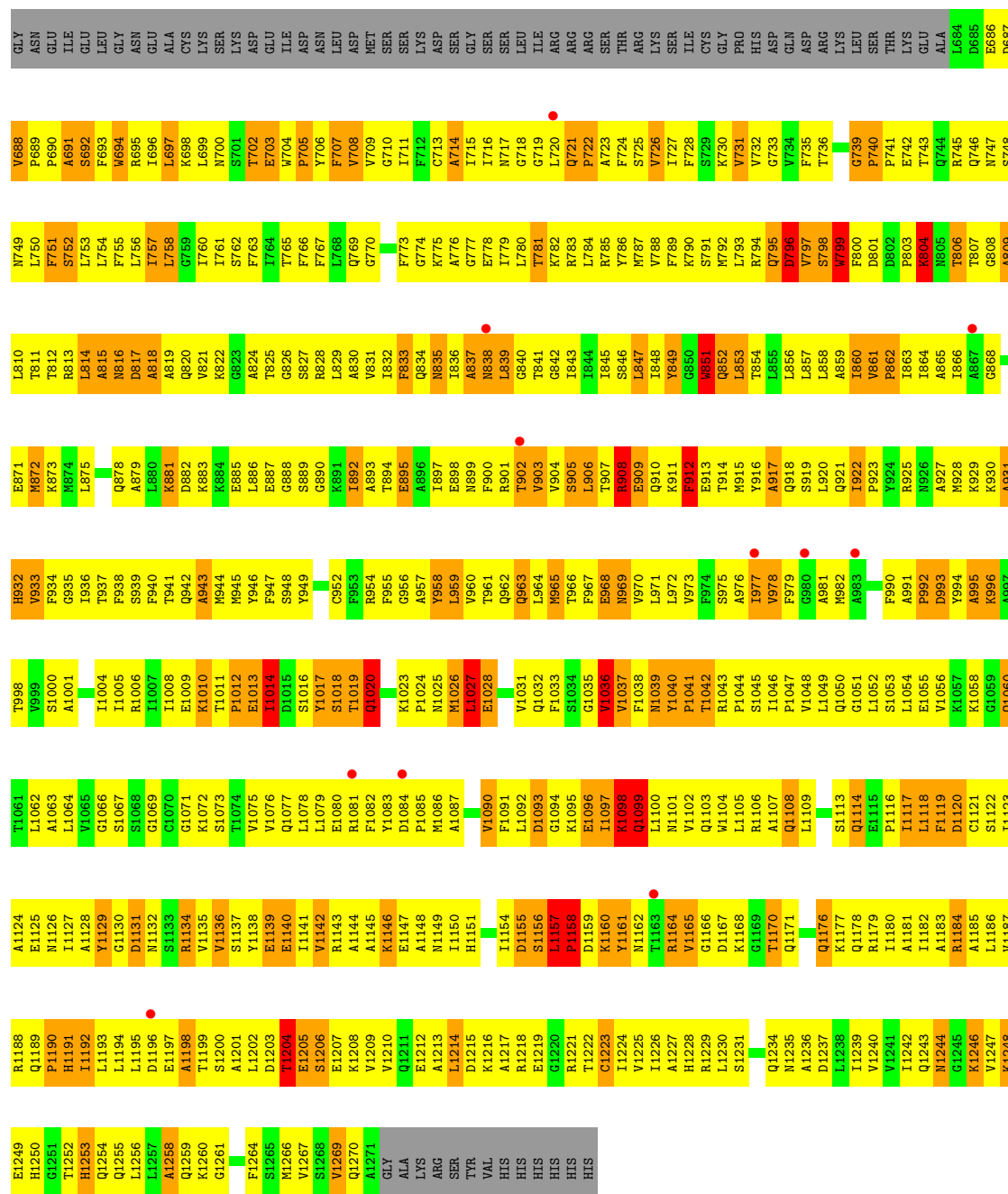
There are 16 discrepancies between the modelled and reference sequences:

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 (4R,11R,18R)-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 (CCD ID: 0JZ) (formula: C₂₄H₃₀N₆O₃Se₃).



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



S1122	G1059	A995	N928	I863	P803	T743	ALA	M623	T554	M493	T432	D372	H311	E251	G187
I1123	Q1060	K996	K929	I864	K804	Q744	L684	T624	S855	D494	V433	S373	Y312	E252	M188
A1124	T1051	A997	A930	I865	K805	Q745	D685	Q625	E935	E935	Q434	F374	T314	E253	F189
E1125	L1062	T998	A931	I866	T806	Q746	E686	T626	L557	L496	L435	S375	T314	L254	F190
N1126	A1063	V999	H932	A867	T807	N747	D687	ALA	D558	E497	M436	K376	A255	A255	Q191
T1127	L1064	G988	G808	G868	G808	S748	G688	GLY	T559	K498	Q437	S377	L316	A256	A192
A1128	V1065	A1001	A809	G869	A809	N749	P689	ASN	E560	A499	R438	G378	V317	L257	M193
Y1129	G1066	G935	L810	E871	L810	L750	P690	GLU	S661	V500	L439	H379	I318	R258	A194
G1130	H1003	I936	T811	M872	T811	F751	A691	ILE	S662	K501	Y440	K380	T259	T195	T195
N1131	S1068	T937	T812	K873	T812	S692	S692	LEU	A563	E502	P442	P381	K320	V260	F196
D1132	G1069	F938	L753	M874	L753	L753	F693	LEU	V564	A503	P442	E321	E321	T261	F197
S1133	L1070	S939	L814	L875	L814	W694	W694	ASN	V665	N504	L443	N383	Y322	A262	G198
L1134	G1071	F940	A815	G876	A815	F755	G695	ASN	Q566	A505	D444	L384	S323	G199	G199
V1135	K1072	T941	N816	Q878	N816	L756	I696	GLU	A567	Y506	G445	Q385	I324	F200	F200
Y1136	S1073	Q942	D817	A879	D817	L757	L697	ALA	A568	D507	M446	G386	G325	G285	T201
S1137	T1074	A943	L758	K880	L758	F759	K698	CYS	L569	F508	V447	N387	Q326	Q266	T202
Y1138	V1075	N944	I699	K881	I699	T760	L699	LYS	D570	M510	S448	L388	V327	K267	G203
E1139	P1076	N945	K820	D882	K820	N700	N700	SER	D570	K511	I449	I389	L328	K268	F204
L1140	Q1077	Y946	W821	K883	W821	T761	S701	LYS	R573	L512	D450	F390	T329	E269	T205
I1141	L1078	F947	K822	K884	K822	S762	T702	ASP	E574	L513	D453	K391	V330	L270	R206
S948	L1079	S948	G823	E885	G823	F763	E703	GLU	G575	P513	I454	N392	F331	L271	G207
D1015	S1016	I744	A824	L886	A824	I764	W704	ILE	T577	H514	I454	I393	F332	R272	V208
T1019	C952	F953	T825	E887	T825	T765	P705	ASP	T578	Q515	R455	K394	S333	Y273	K209
Q1020	F954	R954	G826	Q888	G826	F766	T706	ASN	T579	T518	T456	F395	V334	N274	L211
G1082	F1082	K1023	S827	S889	S827	F767	F707	LEU	I579	L519	I457	S396	L336	N276	L212
E1083	Y1083	K1026	R828	S890	R828	L768	V708	ASP	V880	L519	M458	Y397	I336	N276	L212
D1084	E1084	G1021	L829	T892	L829	Q769	V709	MET	L581	V520	V459	P398	G337	L277	V213
P1085	P1085	K1022	A830	T894	A830	G770	G710	SER	A582	G521	R460	F399	F332	E278	T214
M1086	A1087	K1023	W831	T894	W831	F771	I711	SER	H583	E522	Y461	R400	S333	E279	L215
L1087	L1087	M1026	L832	S895	L832	T772	F712	LYS	R584	R523	L462	K401	V341	A290	A216
V1090	F1090	L1027	F833	A896	F833	F773	G713	ASP	L585	G524	R463	E402	G342	K281	T217
F1091	L1092	V1031	Q834	I897	Q834	G774	A714	SER	A525	Q526	E464	V403	Q343	R282	S218
D1155	L1092	V1031	K835	E898	K835	K775	I715	GLY	V588	Q526	I465	Q404	A344	L283	P219
S1156	D1093	Q1032	T836	N899	T836	A776	I716	SER	R589	L527	I466	I405	S345	G284	V220
L1157	G1094	Q963	A837	F900	A837	G777	N717	SER	V593	S528	G467	L406	P346	T285	L221
P1158	K1095	L964	N838	R901	N838	E778	G718	LEU	V593	G529	V468	K407	N347	K286	G222
D1159	E1096	G1035	L839	T902	L839	I779	G719	ILE	F597	G530	V469	G408	I348	K287	L223
K1160	I1097	V1033	G840	V903	G840	L780	L720	ARG	F597	Q531	S470	L409	E349	A288	S224
Y1161	K1098	F1037	T841	V904	T841	T781	Q721	ARG	D598	K532	Q471	N410	A350	T289	T227
M1162	Q1099	F1038	G842	S905	G842	K782	P722	ARG	G599	Q533	E472	L411	F351	T290	W228
T1163	L1100	N1039	L843	L906	L843	R783	A723	SER	G600	R534	P473	K412	A352	A291	
N1164	V1101	Y1040	T907	T907	T844	L784	F724	THR	V601	I535	V474	V413	N353	N292	
V1165	V1102	P1041	L845	E908	L845	R785	S725	ARG	I602	A536	L475	K414	A354	T293	S233
G1166	Q1103	T1042	S846	E909	S846	Y786	V726	LYS	V603	I537	F477	S415	R355	S294	S234
D1167	L1104	R1043	L847	Q910	L847	M787	I727	SER	E604	A538	A477	G416	G356	N295	F235
G1168	S1045	P1044	T848	K911	T848	V788	F728	ILE	H608	R539	T478	Q417	A357	T296	T236
A1107	L1105	T1046	Y849	E913	Y849	F789	S729	CYS	L611	A540	T479	T418	A358	A297	D237
Q1108	Q1108	P1047	K851	T914	K851	K790	K730	GLY	L612	L541	I480	V419	Y359	A298	K238
L1109	L1109	V1048	Q852	N915	Q852	M792	V732	HIS	M612	R543	E482	L421	V361	F299	E239
S1113	Q1050	L1049	L853	Y916	L853	L793	G733	ASP	R613	N544	M483	V422	F362	L300	L240
Q1114	G1051	Q918	T854	A917	T854	V734	V734	GLN	E614	P545	I484	G423	K363	L301	H241
E1115	S1115	Q918	L855	Q918	L855	Q795	F735	ASP	K615	K546	R485	N424	Y303	I302	A242
P1116	L1052	N982	L856	S919	L856	T796	T736	ARG	G616	I547	Y486	S425	I365	Y303	Y243
L1180	S1053	L920	L857	L920	L857	V797	T737	LYS	I617	L548	G487	G426	A304	A244	A244
A1181	L1117	Q921	L858	O921	L858	S798	G738	LEU	V618	L549	R488	C427	S305	K245	K245
T1182	L1118	E1055	A859	I922	A859	V799	G739	SER	F619	L550	E489	G428	K388	A246	A246
A1183	P1119	P923	T860	F923	T860	P800	P740	THR	K620	D551	D490	K429	P369	A307	G247
R1184	K1057	G993	V861	L923	V861	L801	L621	LYS	L621	S430	S370	S430	L308	L308	A248
A1185	C1121	K1058	P862	A927	P862	D802	E742	GLU	V622	A553	T492	T431	I371	F310	A250

L1186	V1247
V1187	K1248
R1188	E1249
Q1189	H1250
P1190	G1251
H1191	T1252
I1192	H1253
L1193	Q1254
L1194	Q1255
L1195	L1256
D1196	L1257
E1197	A1258
A1198	Q1259
T1199	K1260
S1200	G1261
A1201	
L1202	F1264
D1203	S1265
T1204	M1266
E1205	V1267
S1206	S1268
E1207	V1269
K1208	Q1270
V1209	A1271
V1210	GLY
Q1211	ALA
E1212	LYS
A1213	ARG
L1214	SER
D1215	TYR
K1216	VAL
A1217	HIS
R1218	HIS
E1219	HIS
G1220	HIS
R1221	HIS
T1222	HIS
C1223	
I1224	
V1225	
I1226	
A1227	
H1228	
R1229	
L1230	
S1231	
Q1234	
N1235	
A1236	
D1237	
L1238	
I1239	
V1240	
V1241	
I1242	
Q1243	
N1244	
G1245	
K1246	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.63Å 115.09Å 374.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 4.40 19.99 – 4.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.5 (19.99-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 4.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.314 , 0.365 0.316 , 0.361	Depositor DCC
R_{free} test set	2835 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	201.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 119.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18414	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: 0JZ

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	0/9339	1.10	90/12626 (0.7%)
1	B	0.58	2/9339 (0.0%)	1.09	90/12626 (0.7%)
All	All	0.58	2/18678 (0.0%)	1.09	180/25252 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	VAL	C-O	-8.32	1.14	1.24
1	B	689	PRO	CA-C	5.39	1.57	1.52

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	CYS	N-CA-C	20.17	136.24	111.02
1	B	852	GLN	N-CA-C	-13.36	94.92	112.68
1	B	64	LEU	CA-C-N	-11.95	106.54	118.97
1	B	64	LEU	C-N-CA	-11.95	106.54	118.97
1	A	64	LEU	CA-C-N	-11.37	106.43	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9171	0	9344	1665	0
1	B	9171	0	9344	1636	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3298	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 89.

The worst 5 of 3298 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:797:VAL:O	1:B:801:ASP:HB2	1.45	1.15
1:A:523:ARG:HD3	1:A:524:GLY:H	0.99	1.13
1:B:523:ARG:HD3	1:B:524:GLY:H	0.98	1.12
1:B:858:LEU:O	1:B:862:PRO:HD2	1.51	1.11
1:B:1204:THR:O	1:B:1206:SER:N	1.83	1.10

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%)	704 (60%)	302 (26%)	172 (15%)	0	3
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0	3
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0	3

5 of 338 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	89	THR
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%)	889 (91%)	87 (9%)	9	28
1	B	976/1065 (92%)	892 (91%)	84 (9%)	10	29
All	All	1952/2130 (92%)	1781 (91%)	171 (9%)	9	29

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	310	PHE
1	B	892	ILE
1	B	397	TYR
1	B	697	LEU
1	B	978	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	878	GLN
1	B	515	GLN
1	B	795	GLN
1	B	1032	GLN

5.3.3 RNA ⓘ

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](#)

2 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	OJZ	B	6002	-	33,39,39	1.52	5 (15%)	51,57,57	1.62	11 (21%)
2	OJZ	A	6001	-	33,39,39	1.79	6 (18%)	51,57,57	1.77	9 (17%)

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	OJZ	B	6002	-	-	4/42/48/48	0/4/4/4
2	OJZ	A	6001	-	-	4/42/48/48	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	OJZ	C16-N17	5.70	1.46	1.34
2	B	6002	OJZ	C09-N10	4.62	1.43	1.34
2	A	6001	OJZ	C02-N03	4.57	1.43	1.34
2	A	6001	OJZ	C09-N10	4.04	1.42	1.34
2	B	6002	OJZ	C02-N03	3.85	1.42	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	OJZ	C04-N03-C02	4.67	131.07	121.57
2	A	6001	OJZ	C18-N17-C16	4.47	130.66	121.57
2	A	6001	OJZ	SE2-C14-C15	3.72	116.41	111.07
2	A	6001	OJZ	SE3-C21-C01	3.59	116.22	111.07
2	B	6002	OJZ	C01-C02-N03	3.57	120.29	115.22

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6001	OJZ	C19-C18-N17-C16
2	A	6001	OJZ	C34-C18-C19-N22
2	B	6002	OJZ	N03-C04-C05-N24
2	B	6002	OJZ	C28-C04-C05-N24
2	A	6001	OJZ	C34-C18-N17-C16

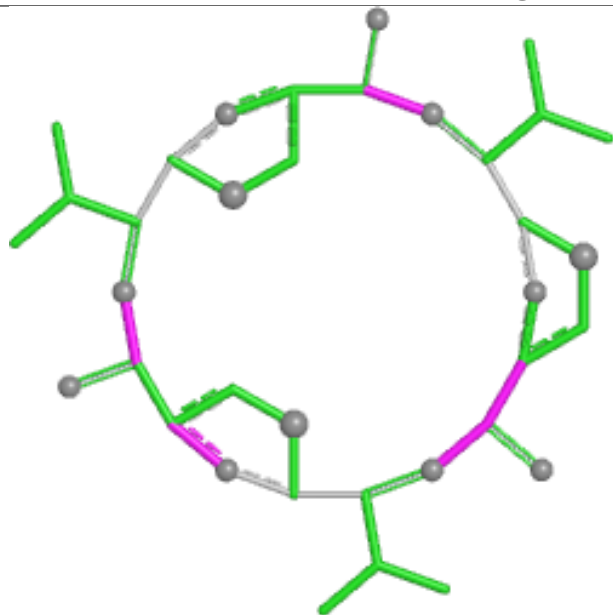
There are no ring outliers.

2 monomers are involved in 22 short contacts:

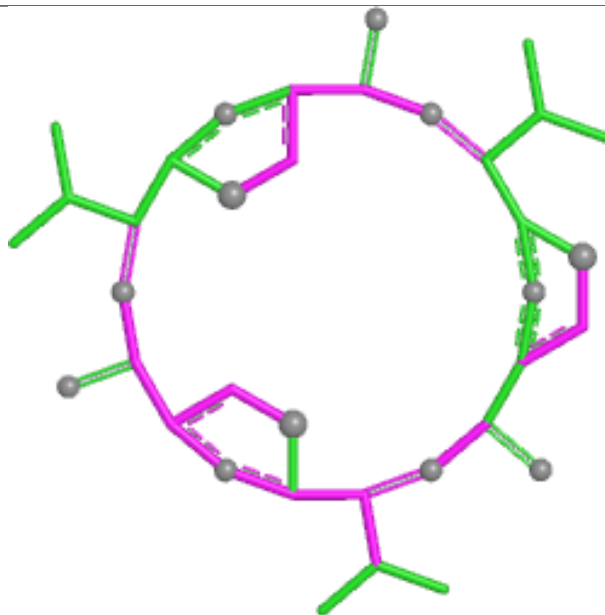
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	OJZ	10	0
2	A	6001	OJZ	12	0

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.

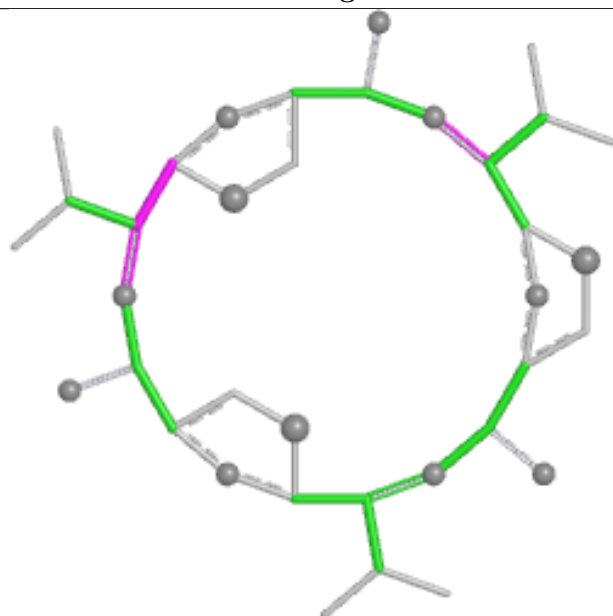
Ligand 0JZ B 6002



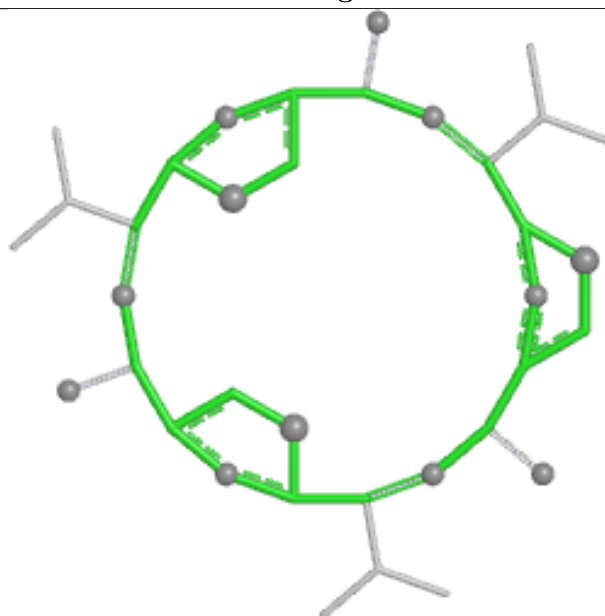
Bond lengths



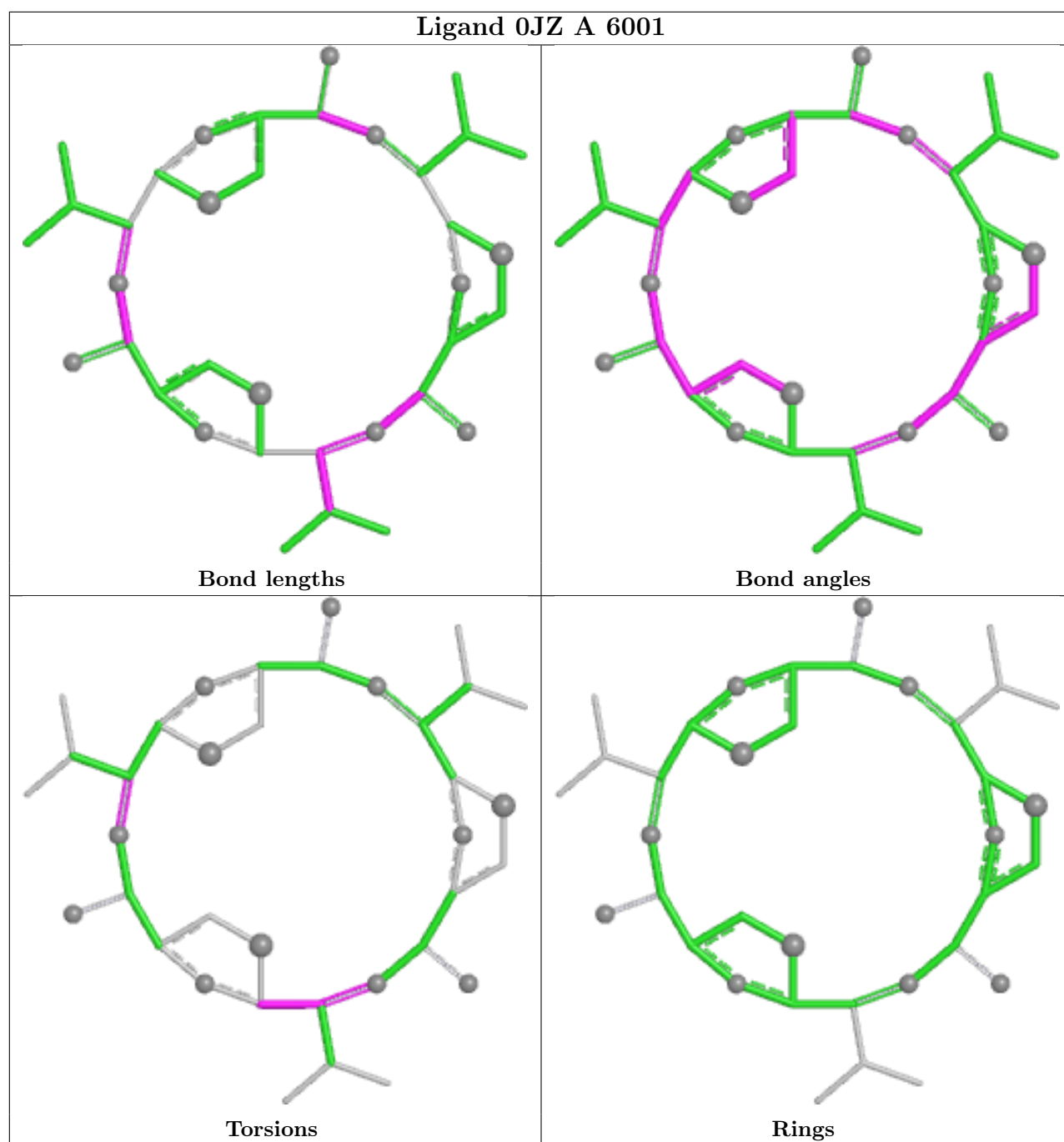
Bond angles



Torsions



Rings



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%)	-0.04	27 (2%)	61 48	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.04	14 (1%)	76 62	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.04	41 (1%)	69 55	118, 197, 244, 306	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	THR	5.3
1	B	1241	VAL	4.1
1	B	217	ILE	3.9
1	B	982	MET	3.9
1	A	288	ALA	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](#)

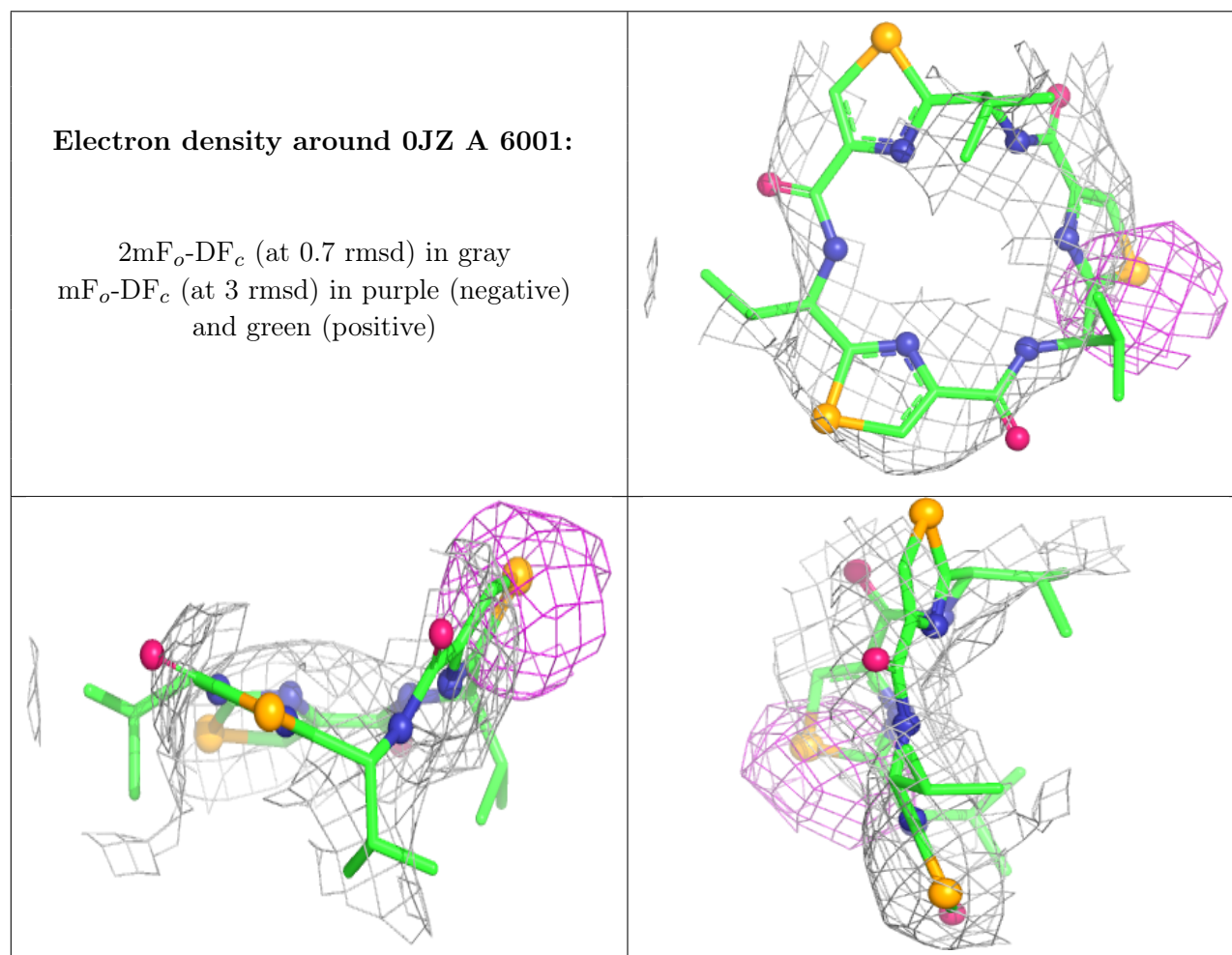
There are no oligosaccharides in this entry.

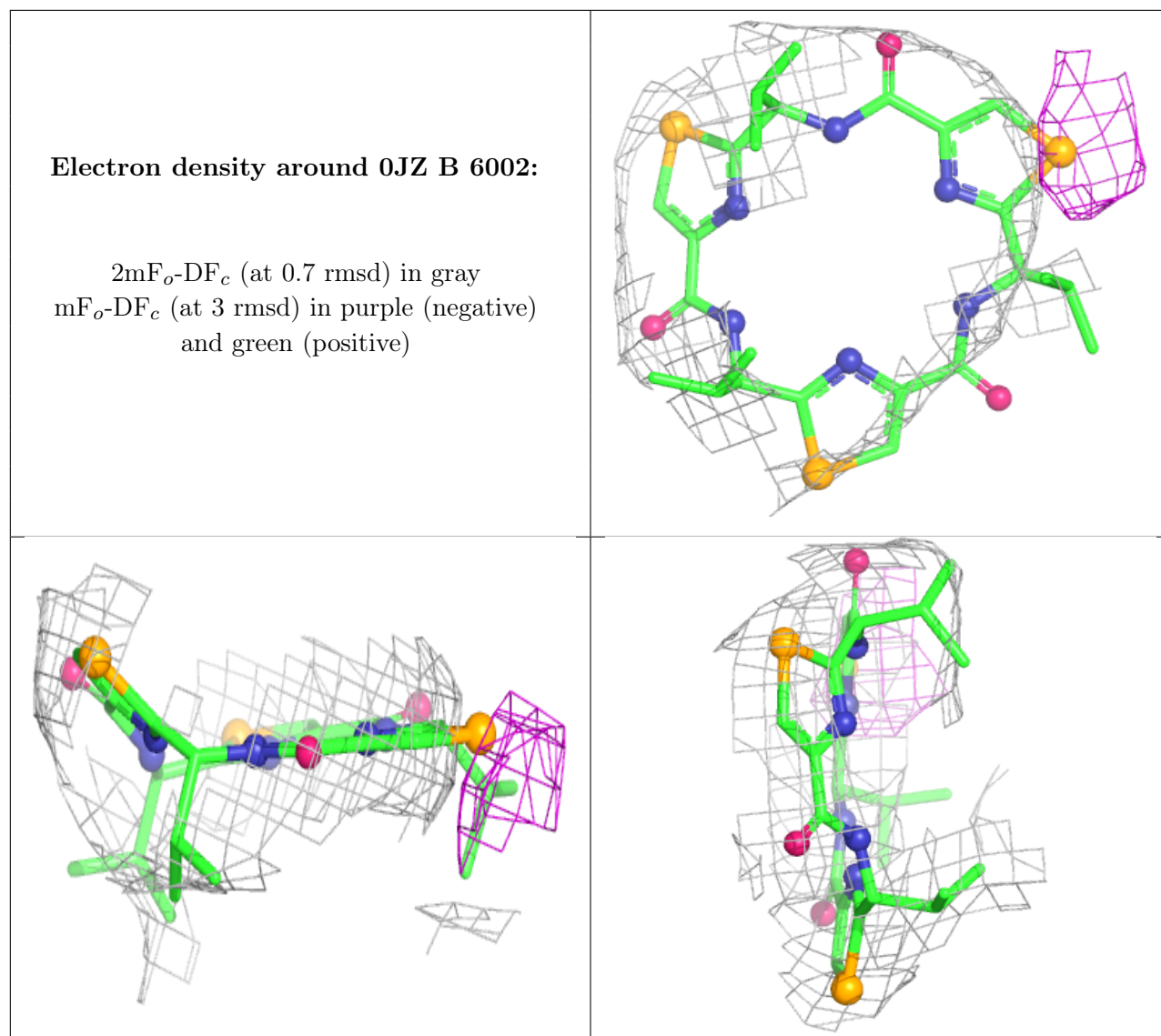
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	OJZ	A	6001	36/36	0.65	0.13	196,196,196,196	0
2	OJZ	B	6002	36/36	0.70	0.12	196,196,196,196	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.