



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 11, 2024 – 04:28 PM EST

PDB ID : 3G60
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)

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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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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

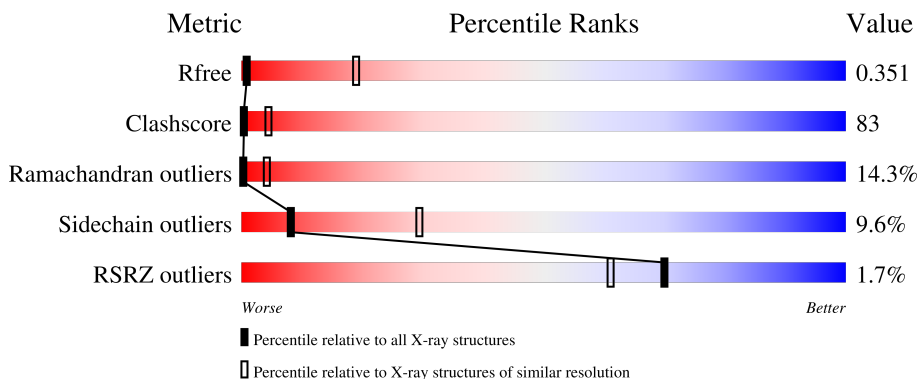
1 Overall quality at a glance

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}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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	OJZ	A	6001	-	-	-	X
2	OJZ	B	6002	-	-	-	X

2 Entry composition [i](#)

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.

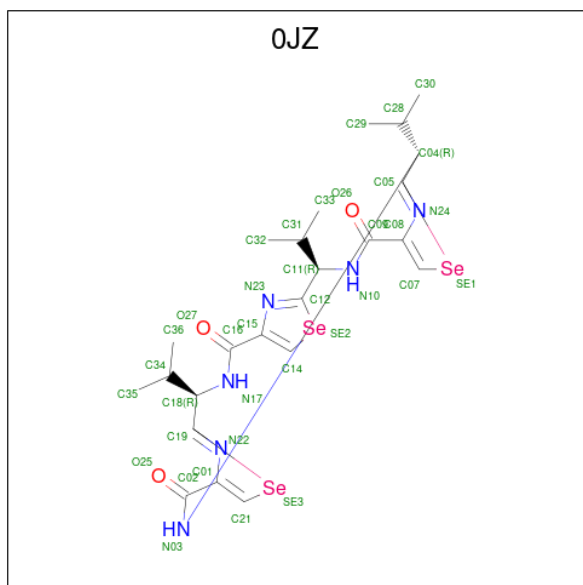
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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

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 (three-letter code: 0JZ) (formula: C₂₄H₃₀N₆O₃Se₃).

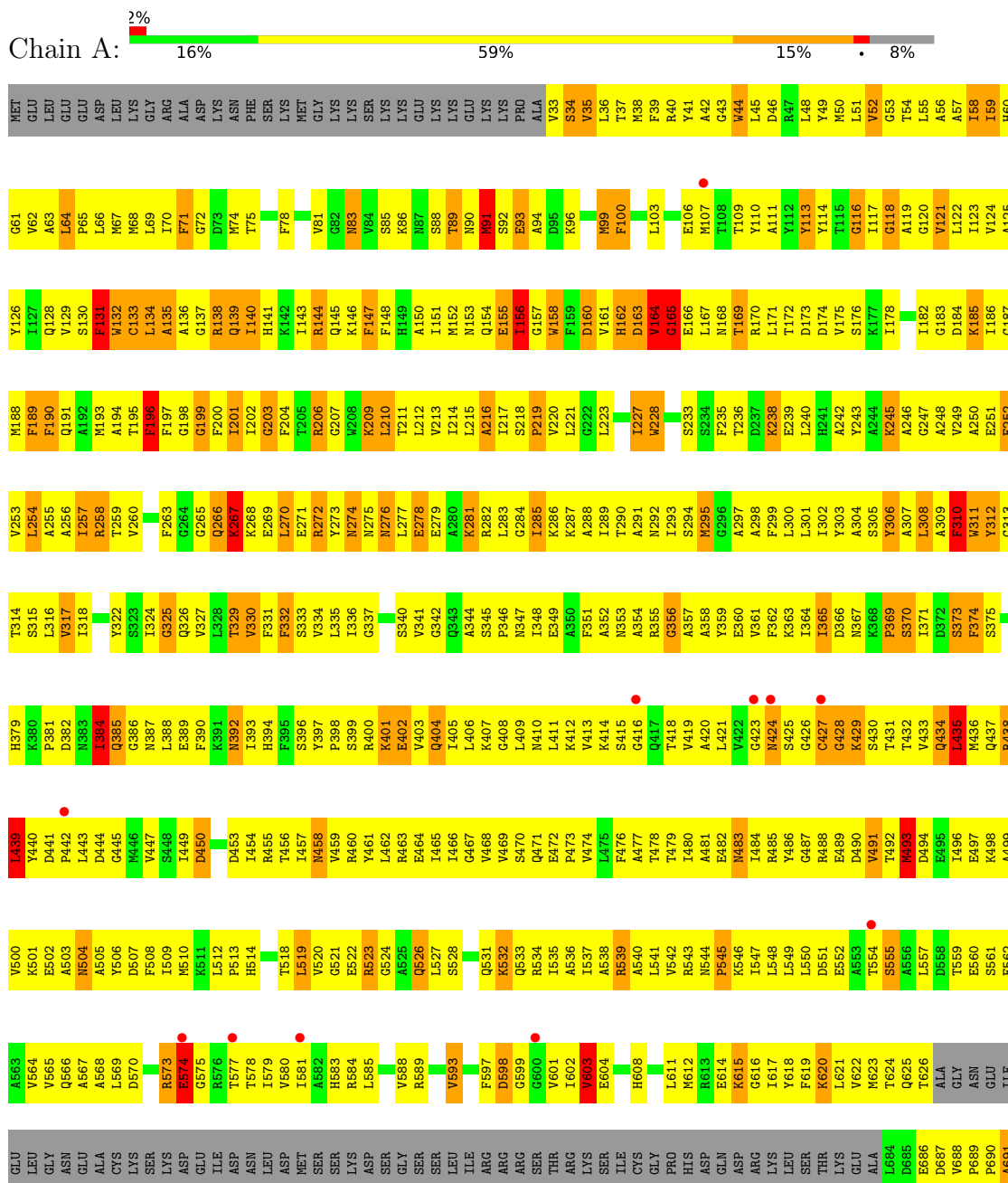


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			Se
2	A	1	36	24	6	3	3	0	0
2	B	1	36	24	6	3	3	0	0

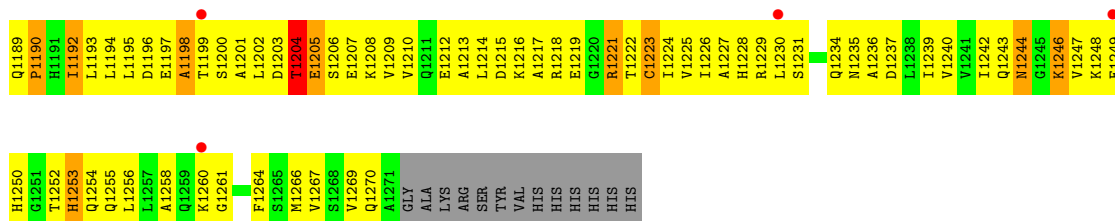
3 Residue-property plots

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



N1126	F934	G868	G808	S748	E686	F626	D658	F497	Q434	F374	G313	E251
I1127	G935	E871	A809	N749	D687	ALA	F559	K496	L435	S375	T314	E252
Y1129	I936	M872	T810	F751	P689	GLY	E560	A499	M436	K376	S315	V253
G1130	T937	E873	T811	F752	P690	ASN	S561	V500	Q437	S377	L316	L254
D1131	S938	L875	R812	S753	A691	GLU	E562	K501	R438	G378	V317	A255
M1132	F940	L876	R813	L754	S692	ILE	E502	E502	L439	H379	I318	A256
S1133	T941	Q878	A814	F755	F693	LEU	V564	A503	Y440	K380	S319	I257
R1134	Q942	A879	M815	L756	D694	GLY	V565	N504	L443	P381	K320	R258
V1135	Q943	L880	D817	I757	R695	GLY	Q666	A505	D444	D382	E321	T259
S1136	M944	K881	A818	L758	I696	ASN	A567	Y506	D444	N383	S322	V260
Y1137	M945	R882	A819	G759	L697	GLU	A568	D507	G445	I384	S323	
E1138	Y946	K883	Q820	I760	S697	ALA	L569	F508	N446	Q385	I324	F263
L1139	F947	G884	Q821	I761	N700	LYS	D570	I509	V447	G386	G325	
A1063	V899	E885	R822	F762	S701	SER	R573	R511	S448	N387	Q326	Q266
L1064	S1000	L886	G823	F763	T702	LYS	E574	L512	I449	L388	V327	K267
V1065	A1001	R887	A824	I764	E703	ASP	G575	P513	D450	E389	L328	K268
G1066	S1002	G888	T825	T765	W704	ASP	R576	H514	F390	F390	T329	E269
S1067	H1003	E889	G826	F766	P705	ILE	T577	Q515	F391	F391	V330	L270
S1068	I1004	S889	S827	F767	Y706	ASP	F578	T578	D453	N392	F331	E271
G1069	I1005	L892	R828	L768	F707	ASN	F579	I579	R455	I393	F332	R272
G1070	R1006	A893	L829	Q769	V708	LEU	V580	L519	T456	H394	S333	Y273
I1071	Q942	T894	A830	G770	W709	LEU	V580	L519	I457	F395	V334	N274
K1072	Q943	R895	V831	F771	G710	ASP	V520	W520	N458	S396	V335	N275
M1073	E1009	E896	I832	T772	I711	NET	A582	G521	V459	Y397	L335	N276
S1074	K1010	A897	I833	T773	T712	SER	H583	E522	R460	P398	L277	L277
G1075	T1011	R898	F833	F774	F713	SER	R584	R523	Y461	S399	E278	E278
V1076	P1012	E899	Q834	G774	C713	LYS	L585	G524	R400	R400	S340	E279
Q1077	E1013	L899	R835	K775	A714	ASP	A525	A525	K401	K401	V341	A280
I1078	I1014	F900	I836	A776	I715	SER	V588	O526	E402	E402	G342	K281
L1079	L1015	R901	A837	G777	I716	GLY	R589	L527	F403	F403	G343	R282
E1080	S1016	T902	M838	E778	N717	SER	G599	S528	Q404	Q404	A344	L283
F1081	F953	S899	L839	I779	G718	SER	G600	G529	I405	I405	S345	G284
R1082	R954	L897	F833	I779	G718	SER	V693	G529	I406	I406	P346	L285
Y1083	Q1020	E898	Q834	L780	G719	LEU	I894	V468	L406	L406	P346	L285
D1084	G1021	R899	R841	T781	L720	LEU	F597	V469	K407	K407	N347	K286
P1085	G1022	T894	G842	K782	Q721	ILE	D598	S470	G408	G408	I348	K287
M1086	K1023	F900	I843	L783	P722	ARG	G599	Q471	L409	L409	E349	A288
A1087	M1026	R901	I844	L784	A723	ARG	G599	E604	N410	N410	I289	I289
F1088	L1027	T902	L844	E785	F724	SER	G600	E604	L411	L411	T290	T290
Y1089	L1027	S904	L845	K785	F724	SER	V601	L480	L412	L412	A352	A291
F1090	L1027	S905	R846	Y786	S725	THR	V601	L480	V413	V413	N353	N292
F1091	Q961	R906	G847	K787	I727	ARG	I602	A477	V413	V413	N353	N292
L1092	Q962	T907	I848	L788	I727	LYS	V603	A477	K414	K414	A354	I293
D1093	Q963	R908	Y849	F789	F728	SER	E604	A477	S415	S415	R355	S294
G1094	L964	E909	I849	F789	F728	SER	E604	A477	G416	G416	G356	M295
K1095	M965	L904	L849	K790	V731	LYS	H608	L541	Q417	Q417	A357	G296
E1096	T966	Q904	S846	Y786	V731	LYS	H608	L541	T418	T418	A358	A297
E1097	T967	S905	L847	K787	V732	THR	V601	L480	T418	T418	A358	A297
K1098	E968	R906	L847	K787	V732	THR	V601	L480	T418	T418	A358	A297
Y1099	Q968	R906	L847	K787	V732	THR	V601	L480	T418	T418	A358	A297
F1100	V1037	L906	G847	L788	I727	LYS	E604	A477	T418	T418	A358	A297
M1101	M1039	T907	I848	L788	I727	LYS	E604	A477	T418	T418	A358	A297
N1102	Y1040	R908	L849	K788	I727	LYS	E604	A477	T418	T418	A358	A297
V1103	P1041	E909	L849	K788	I727	LYS	E604	A477	T418	T418	A358	A297
G1104	R1043	Q910	L849	K788	I727	LYS	E604	A477	T418	T418	A358	A297
D1105	P1044	K911	L849	K788	I727	LYS	E604	A477	T418	T418	A358	A297
R1106	A976	E912	Y849	F789	F728	SER	E604	A477	T418	T418	A358	A297
G1107	I977	T914	G850	K790	V731	LYS	H608	L541	T418	T418	A358	A297
E1108	I1045	M915	R851	S791	V731	LYS	H608	L541	T418	T418	A358	A297
A1109	P1047	Y916	Q852	M792	V732	GLY	L611	V542	T418	T418	A358	A297
S1113	L1048	A917	L853	L793	G733	PRO	L611	V542	T418	T418	A358	A297
Q1114	Q1050	Q918	T854	R794	G733	PRO	L611	V542	T418	T418	A358	A297
F1115	G1051	Q918	T854	R794	G733	PRO	L611	V542	T418	T418	A358	A297
P1116	L1052	S919	L855	Q795	F735	HIS	M612	N544	N483	N483	E360	F299
I1117	S1053	L920	L856	D796	T736	ASP	R613	I484	N483	N483	E360	F299
T1118	L1054	Q921	L857	D796	T736	ASP	R613	I484	N483	N483	E360	F299
L1118	L1054	L922	L858	S798	G738	ARG	G616	L548	N483	N483	E360	F299
F1119	E1055	S923	A859	F799	G738	ARG	G616	L548	N483	N483	E360	F299
D1120	K1067	P923	F800	F800	G739	LYS	G616	L548	N483	N483	E360	F299
K1121	K1067	A927	F800	F800	G739	LYS	G616	L548	N483	N483	E360	F299
R1122	G1068	Q929	R862	D802	E742	THR	K620	E552	D490	D490	S305	Y306
S1122	G1068	K929	R862	D802	E742	THR	K620	E552	D490	D490	S305	Y306
L1123	Q1060	K330	I864	K804	T743	LYS	L621	A553	V491	V491	G428	A307
A1124	T1061	R330	A865	K804	T743	LYS	L621	A553	V491	V491	G428	A307
I1125	L1062	A931	A866	K804	T743	LYS	L621	A553	V491	V491	G428	A307
E1125	L1062	H932	A866	K804	T743	LYS	L621	A553	V491	V491	G428	A307
Q1176	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
K1177	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
L1178	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
R1179	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
I1180	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
A1181	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
I1182	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
A1183	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
R1184	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
A1185	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
L1186	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
V1187	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
R1188	K1177	I1178	A1181	A1181	A1181	ALA	D494	A556	D494	D494	T432	F310
												Y312



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 49.02 – 4.31	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.3 (49.02-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 4.29Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.314 , 0.365 0.297 , 0.351	Depositor DCC
R_{free} test set	2835 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	201.9	Xtrriage
Anisotropy	0.359	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 103.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18414	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	1/9339 (0.0%)	0.70	13/12626 (0.1%)
1	B	0.41	0/9339	0.68	8/12626 (0.1%)
All	All	0.41	1/18678 (0.0%)	0.69	21/25252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	TRP	CB-CG	5.17	1.59	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	CYS	N-CA-C	9.35	136.24	111.00
1	A	1098	LYS	N-CA-C	-7.80	89.94	111.00
1	A	164	VAL	N-CA-C	-7.79	89.98	111.00
1	A	267	LYS	N-CA-C	7.23	130.52	111.00
1	A	165	GLY	N-CA-C	-7.16	95.21	113.10

There are no chirality outliers.

There are no planarity outliers.

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	1558	0
1	B	9171	0	9344	1534	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3089	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 83.

The worst 5 of 3089 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 4
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0 4
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0 4

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 [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	976/1065 (92%)	884 (91%)	92 (9%)	8	30
1	B	976/1065 (92%)	880 (90%)	96 (10%)	8	29
All	All	1952/2130 (92%)	1764 (90%)	188 (10%)	8	29

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	LYS
1	B	694	TRP
1	B	254	LEU
1	B	332	PHE
1	B	771	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	437	GLN
1	B	963	GLN
1	B	515	GLN
1	B	805	ASN
1	B	1099	GLN

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](#)

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	-	21,39,39	1.74	4 (19%)	24,57,57	1.91	7 (29%)
2	OJZ	A	6001	-	21,39,39	2.04	5 (23%)	24,57,57	2.49	9 (37%)

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	-	-	4/24/48/48	0/3/4/4
2	OJZ	A	6001	-	-	4/24/48/48	0/3/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	OJZ	C16-N17	5.48	1.46	1.34
2	B	6002	OJZ	C09-N10	4.44	1.43	1.34
2	A	6001	OJZ	C02-N03	4.39	1.43	1.34
2	A	6001	OJZ	C09-N10	3.88	1.42	1.34
2	B	6002	OJZ	C02-N03	3.70	1.42	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	OJZ	C04-N03-C02	5.49	131.07	122.28
2	A	6001	OJZ	C18-N17-C16	5.23	130.66	122.28
2	A	6001	OJZ	C35-C34-C18	4.30	115.38	111.24
2	B	6002	OJZ	C33-C31-C11	3.77	114.87	111.24
2	B	6002	OJZ	C29-C28-C04	3.75	114.85	111.24

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

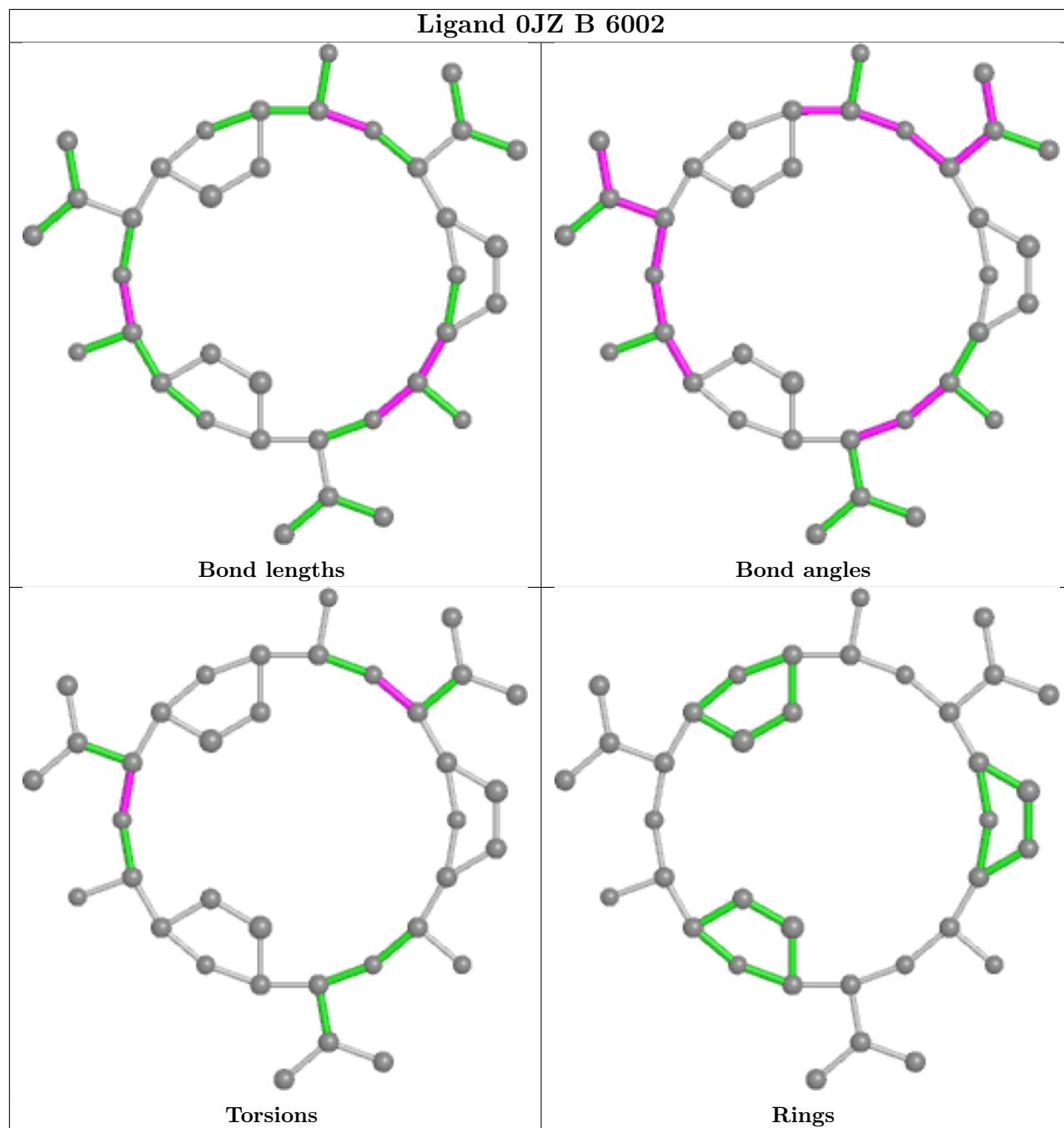
Mol	Chain	Res	Type	Atoms
2	A	6001	OJZ	C05-C04-N03-C02
2	A	6001	OJZ	C28-C04-N03-C02
2	A	6001	OJZ	C19-C18-N17-C16
2	A	6001	OJZ	C34-C18-N17-C16
2	B	6002	OJZ	C05-C04-N03-C02

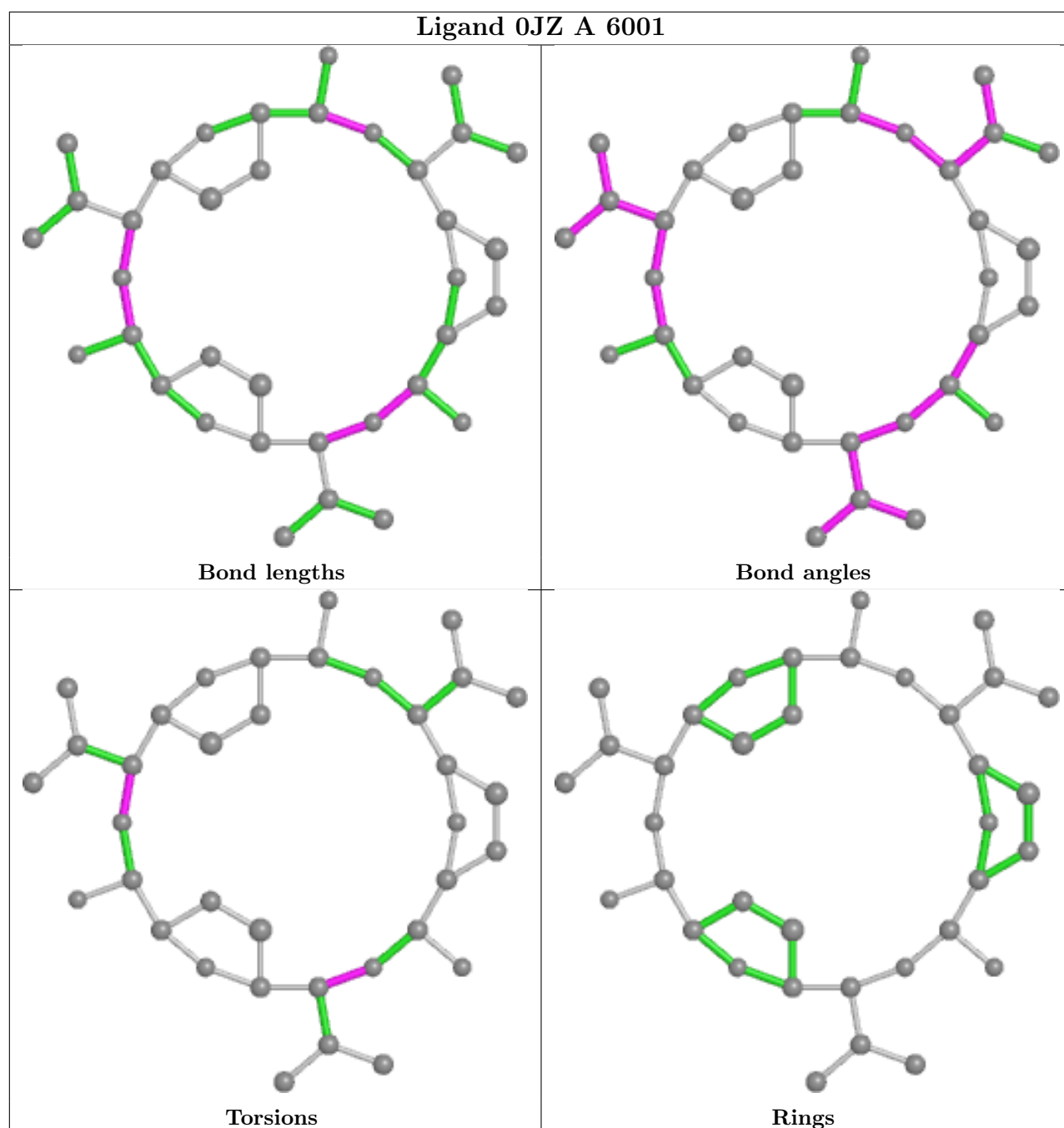
There are no ring outliers.

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.





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%)	-0.12	20 (1%) 70 61	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.13	21 (1%) 68 59	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.12	41 (1%) 70 61	118, 197, 244, 306	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	GLN	4.9
1	B	1199	THR	4.5
1	A	1084	ASP	4.0
1	A	574	GLU	3.9
1	B	228	TRP	3.7

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](#)

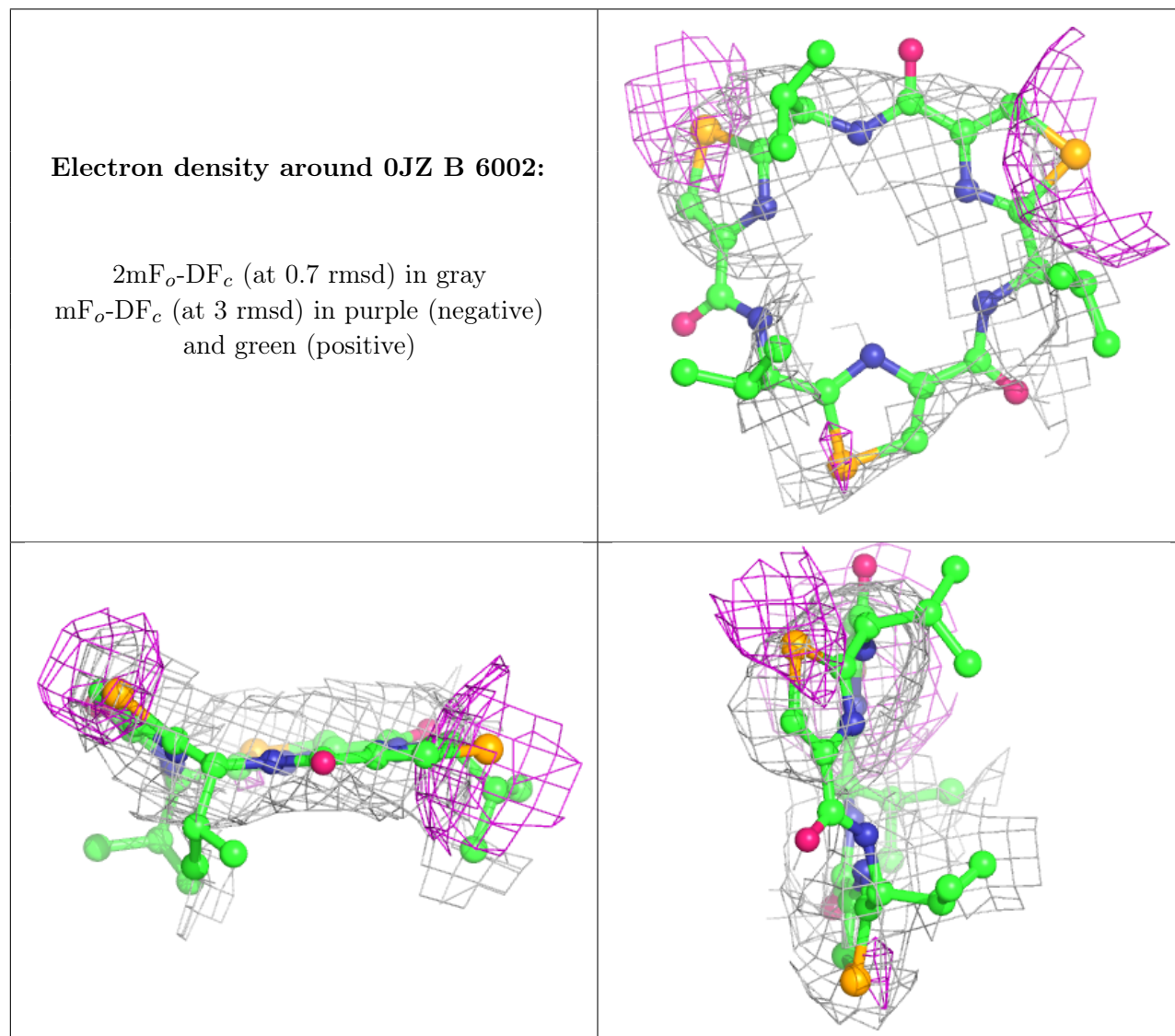
There are no monosaccharides in this entry.

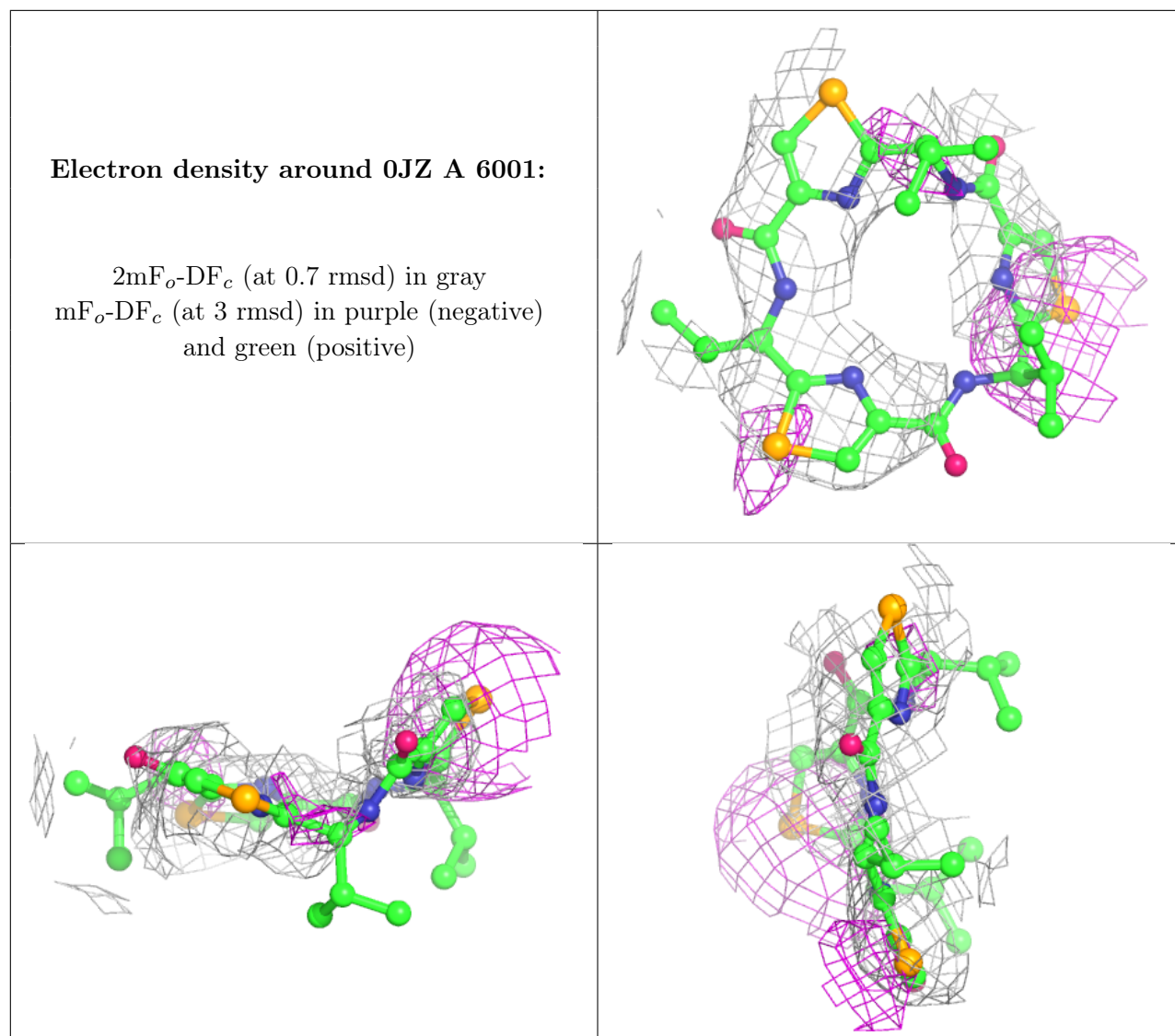
6.4 Ligands [i](#)

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	OJZ	B	6002	36/36	0.63	0.41	196,196,196,196	0
2	OJZ	A	6001	36/36	0.64	0.43	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.