



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2020 – 02:58 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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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 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)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

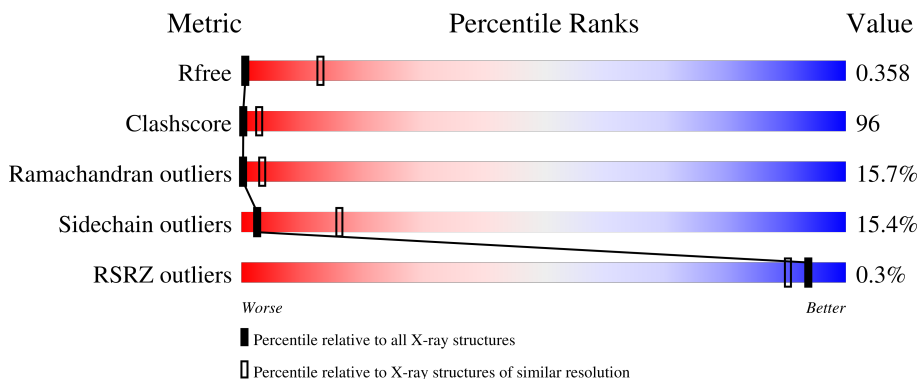
1 Overall quality at a glance

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 on 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	 13% 57% 19% • 8%
1	B	1284	 12% 59% 19% • 8%

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 [i](#)

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.

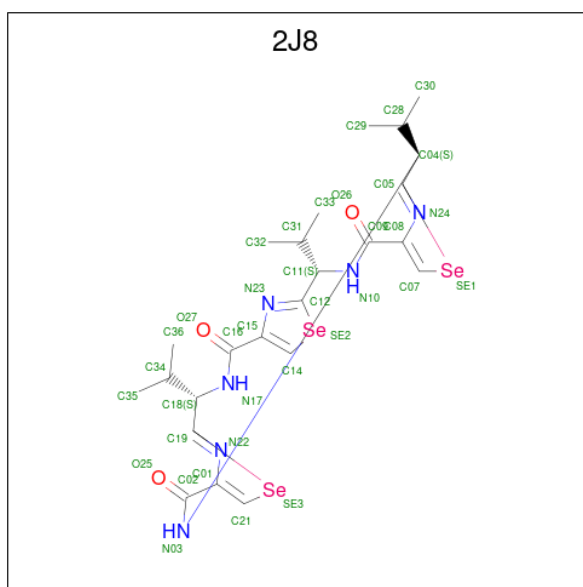
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 (4S,11S,18S)-4,11,18-tri(propan-2-yl)-6,13,20-triselenena-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1.1 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).

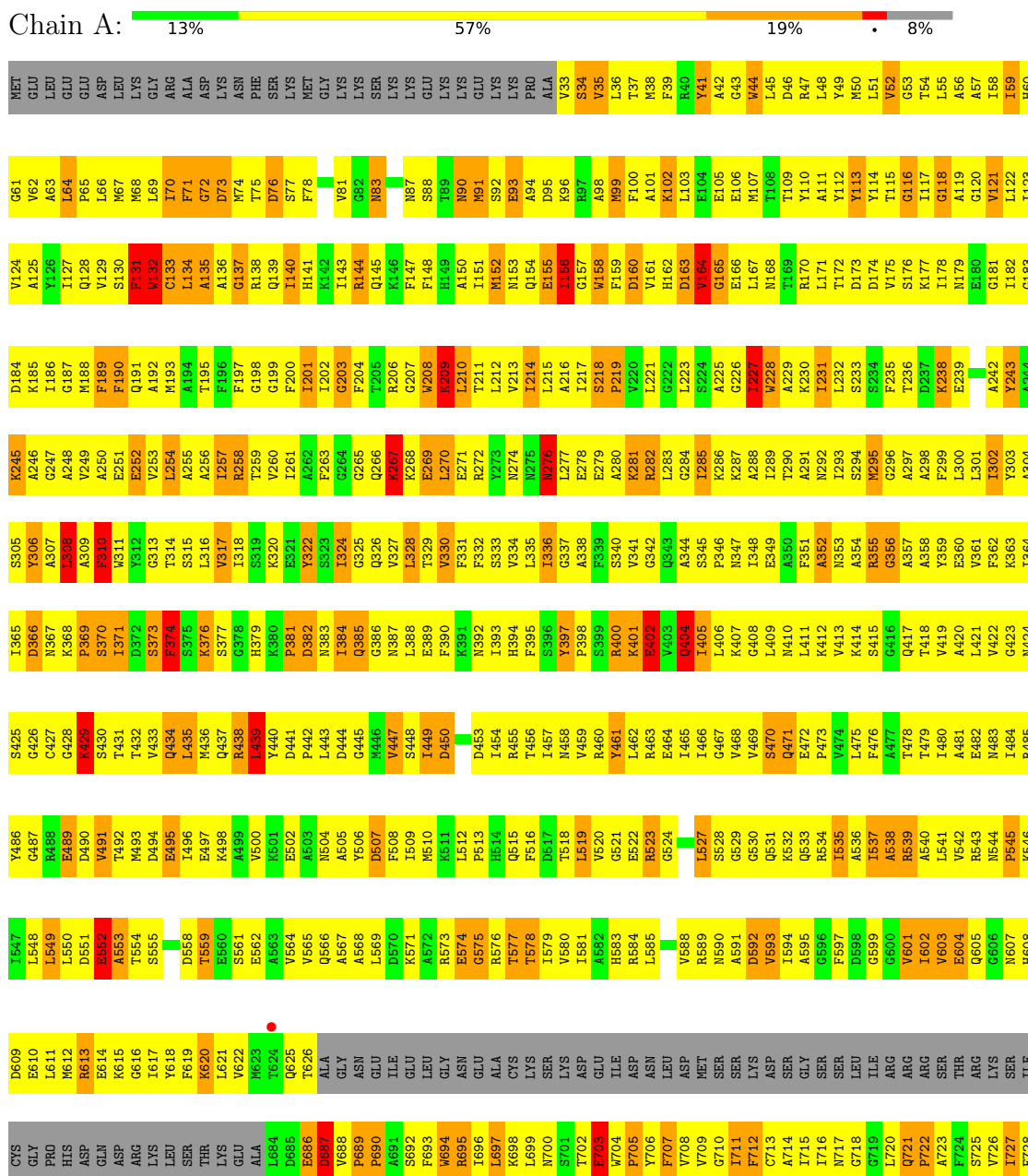


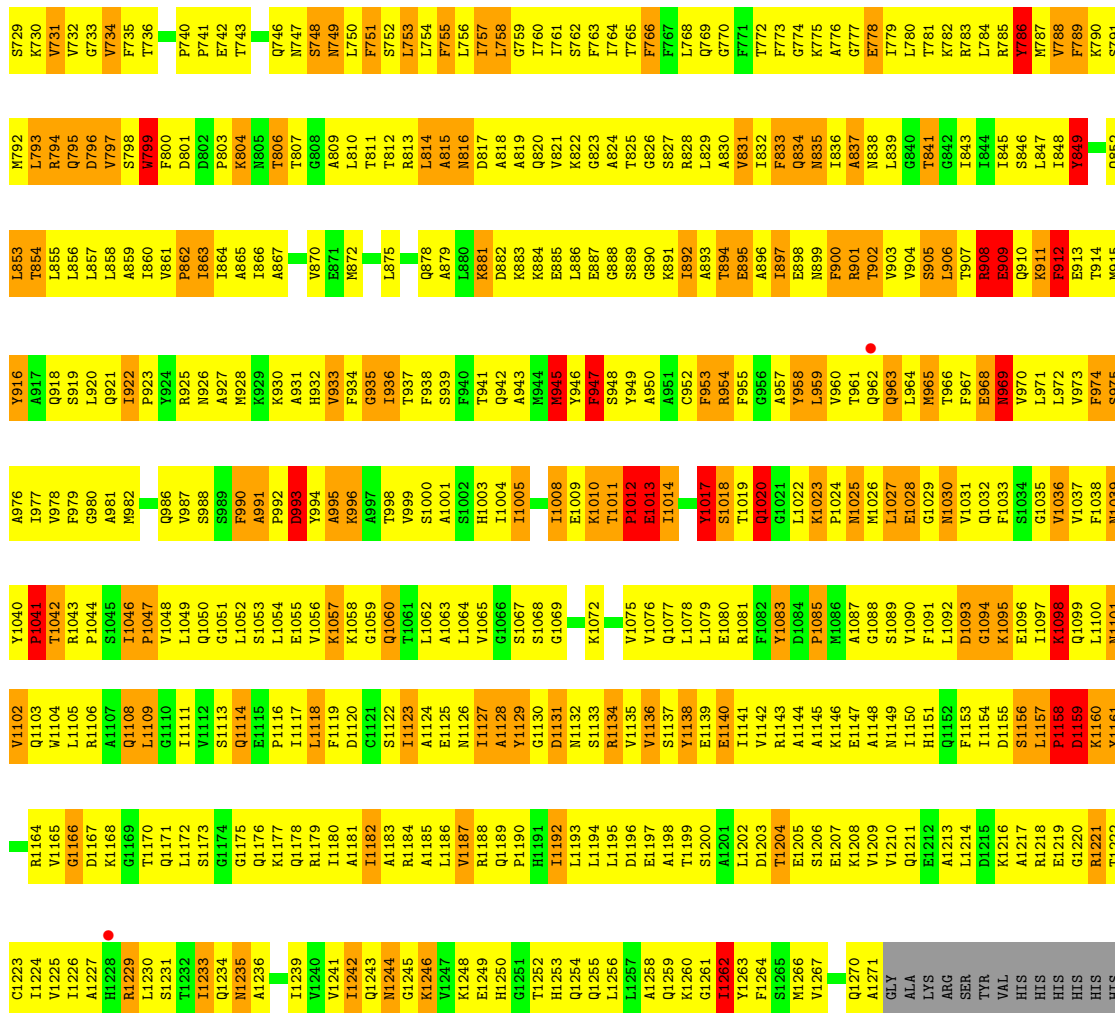
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	Se		
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	A	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		

3 Residue-property plots

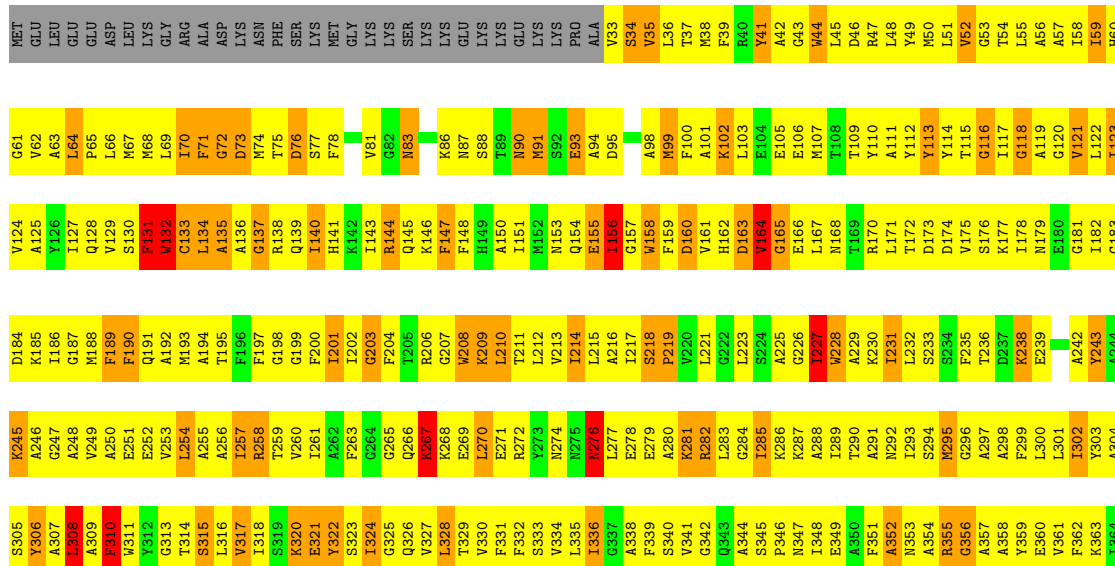
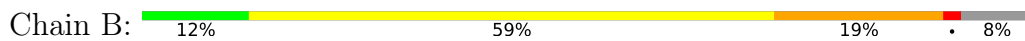
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Multidrug resistance protein 1a



C1223	Y1181	M1101	Y1040	1977	A917	T854	R794	G733	D609	E547	Y486	S425	I365
I1224		V1102	P1041	Y978	Q918	L855	Q795	W794	E610	L548	G487	G426	D866
V1225	R1164	Q1103	T1042	F979	S919	L856	D796	F794	E611	L549	R488	C427	N367
I1226	V1165	W1104	R1043	G980	L920	L857	W797	F736	M612	L550	E489	G428	K368
A1227	K1166	L1105	P1044	A981	Q921	L858	R798	H737	D551	D551	D490	K429	P369
H1228	D1167	R1106	S1045	M982	Q922	A859	W799	H738	E614	E552	V491	S430	S370
R1229	K1168	A1107	I1046		P923	I860	F800	G739	K615	A553	T492	T431	I371
L1230	T1169	Q1108	P1047	G985	W924	W661	D801	F740	G616	T554	M493	T432	D372
S1231	H1170	L1109	V1048	Q986	R925	P862	D802	P741	L617	S555	D494	V433	S373
T1232	Q1171	G1110	L1049	F987	N926	R863	R803	E742	F618	E495	E495	Q434	F374
I1233	L1172	I1111	Q1050	S988	A927	I864	X804	T743	F619	I496	I496	L435	S375
Q1234	S1173	W1112	G1051	S989	M928	A865	R805		K620	E497	M436	Q436	K376
M1235	H1174	S1113	L1052	F990	X929	I866	T806	Q746	L621	E560	K498	M437	S377
A1236	Q1175	Q1114	S1053	A991	K930	A867	T807	N747	V622	S561	A499	R438	G376
		E1115	L1054	P992	A931		G908	S748		E562	V500	R439	H379
I1239	K1177	P1116	E1055	D993	H932	W670	A809	N749	Q625	A663	K501	Y440	K380
V1240	Q1178	I1117	K1056	Y994	E933	L810	R810	L750	T626	V564	E502	D441	P381
I1241	R1179	L1118	K1057	A995	F934	R872	T811	F751	ALA	V565	A503	P442	D382
I1242	I1180	F1119	K1058	K996	G935		T812	S752	GLY	Q566	N504	L443	N383
Q1243	A1181	D1120	G1059	A997	I936	L875	R813	L753	ASN	A567	A505	D444	I384
N1244	I1182	C1121	Q1060	T998	T937		L814	L754	GLU	A568	Y506	G445	Q385
G1245	A1183	S1122	T1061	F999	F938	Q878	A815	F755	ILE	L569	D507	M446	G386
K1246	R1184	I1123	L1062	S1000	S939	A879	M816	L756	GLU	D570	F508	V447	N387
V1247	A1185	A1124	A1063	A1001	F940	L880	D817	I757	LEU	K571	I509	S448	L388
K1248	L1186	E1125	L1064	S1002	T941	X881	A818	L758	GLY	A572	M510	I449	E389
E1249	V1187	M1126	V1065	H1003	Q942	D882	A819	G759	ASN	R573	K511	D450	F390
G1250	R1188	I1127	G1066	I1004	A943	K893	R820	I760	GLU	E574	L512	D453	K391
H1251	K1189	A1128	S1067	I1005	N944	K884	W821	I761	ALA	G575	P513	N392	N392
T1252	P1190	Y1129	S1068	R1006	R945	E885	R822	K822	CYS	R576	H514	I454	I393
H1253	H1191	G1130	G1069	I1007	Y946	L886	K823	F763	LYS	T577	Q515	R455	H394
Q1254	I1192	D1131	C1070	I1008	F947	E887	A824	I764	SER	T578	F516	T456	F395
Q1255	L1193	M1132	G1071	E1009	S943	G888	T825	F765	LYS	I579	D517	I457	S386
L1256	L1194	S1133	K1072	K1010	Y949	S899	G826	F766	ASP	V580	T518	M468	Y397
A1258	L1196	R1134	V1075	T1011	A950	R890	S827	F767	GLU	I581	L519	V459	P398
Q1259	E1197	V1135	V1076	P1012	A951	K891	L768	A682	ILE	A682	V520	R460	S399
K1260	T1198	S1137	Q1077	E1013	C952	R892	L829	Q769	ASP	H583	G521	Y461	R400
G1261	T1199	Y1138	L1078	D1015	R954	A893	L830	G770	ASN	R584	E522	L462	K401
I1262	S1200	E1139	L1079	S1016	F955	T894	R831	F771	LEU	L585	R523	E464	E402
Y1263	A1201	E1140	E1080	G956	G956	E896	I832	T772	ASP	G524	G524	E464	V403
F1264	D1203	I1141	R1081	T1019	A957	L897	R834	G774	MET	V588	L527	I465	Q404
M1266	E1205	V1142	F1082	Q1020	Y958	E398	M835	K775	SER	R589	S528	I466	I405
V1267	E1206	R1143	Y1083	G1021	L959	N899	L836	A776	LYS	S528	G529	G467	L406
Q1270	S1206	A1144	D1084	L1022	V960	F900	A837	G777	ASP	D592	G530	V468	K407
A1271	K1207	K1146	M1086	K1023	T961	R901	N838	E778	ASP	V693	Q531	S470	L409
ALA	V1209	E1147	G1087	P1024	Q962	T902	L839	I779	GLY	I594	K532	Q471	M410
LYS	Q1211	M1149	S1089	M1025	R963	V903	G840	L780	SER	A595	Q533	E472	L411
ARG	E1212	L1150	V1090	L1027	N965	S905	G842	K782	SER	G596	R534	P473	K412
SER	L1214	I1151	F1091	E1028	T966	L906	I843	R783	ILE	D598	A536	L475	V413
TVR	D1215	F1153	D1093	V1031	E968	R908	I844	R784	ARG	G599	I537	F476	K414
HIS	K1216	I1154	Q1094	Q1032	R969	S846	S846	Y786	ARG	V601	A538	A477	G416
HIS	A1217	D1155	K1095	F1033	V970	Q910	L847	N787	SER	I602	R539	T478	Q417
HIS	K1218	S1156	E1096	S1034	L971	R848	V788	F789	THR	I541	A540	T479	T418
HIS	R1221	L1157	I1087	V1036	I972	E912	F789	F728	ARG	E604	L542	I480	V419
HIS	T1222	P1159	K1088	F1037	F973	E913	G850	K790	LYS	Q605	R543	E482	L421
HIS		D1159	Q1099	F1038	S975	M915	R851	S791	SER	G606	M544	M463	V422
HIS		K1160	L1100	M1039	A976	L853	L793	L793	ILE	H608	G423	I484	G423

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)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.308 , 0.356 0.312 , 0.358	Depositor DCC
R_{free} test set	2807 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	195.7	Xtrriage
Anisotropy	0.362	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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 [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%)	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	A	1109	LEU
1	B	132	TRP
1	B	1041	PRO
1	A	1138	TYR
1	A	1262	ILE

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

Mol	Chain	Res	Type
1	A	1235	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	1108	GLN
1	A	1244	ASN
1	B	83	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	6001	-	21,39,39	1.59	3 (14%)	24,57,57	1.59	6 (25%)
2	2J8	B	6003	-	21,39,39	1.61	3 (14%)	24,57,57	1.47	5 (20%)
2	2J8	A	6002	-	9,18,39	1.60	1 (11%)	8,24,57	1.56	2 (25%)
2	2J8	B	6004	-	9,18,39	1.72	1 (11%)	8,24,57	1.72	2 (25%)

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	6001	-	-	0/24/48/48	0/3/4/4
2	2J8	B	6003	-	-	0/24/48/48	0/3/4/4
2	2J8	A	6002	-	-	0/8/16/48	0/2/2/4
2	2J8	B	6004	-	-	0/8/16/48	0/2/2/4

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	4.75	1.44	1.34
2	A	6002	2J8	C16-N17	4.46	1.43	1.34
2	B	6003	2J8	C16-N17	4.38	1.43	1.34
2	A	6001	2J8	C16-N17	3.92	1.42	1.34
2	A	6001	2J8	C02-N03	3.82	1.42	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	2J8	C36-C34-C18	3.53	114.63	111.24
2	B	6004	2J8	C36-C34-C18	3.39	114.50	111.24
2	A	6002	2J8	C36-C34-C18	3.26	114.38	111.24
2	B	6004	2J8	C18-N17-C16	3.12	127.28	122.28
2	A	6001	2J8	C11-N10-C09	3.11	127.26	122.28

There are no chirality outliers.

There are no torsion outliers.

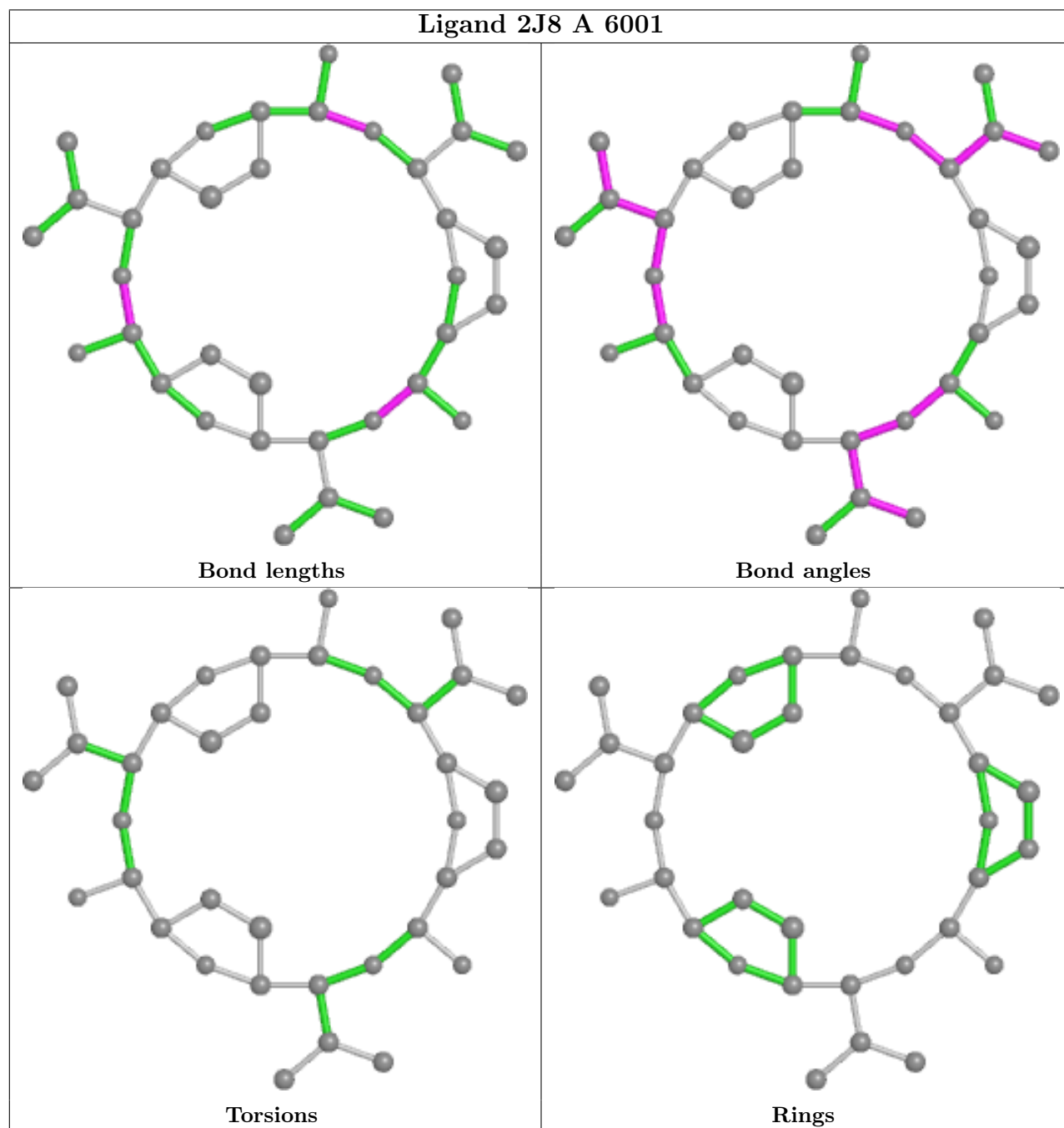
There are no ring outliers.

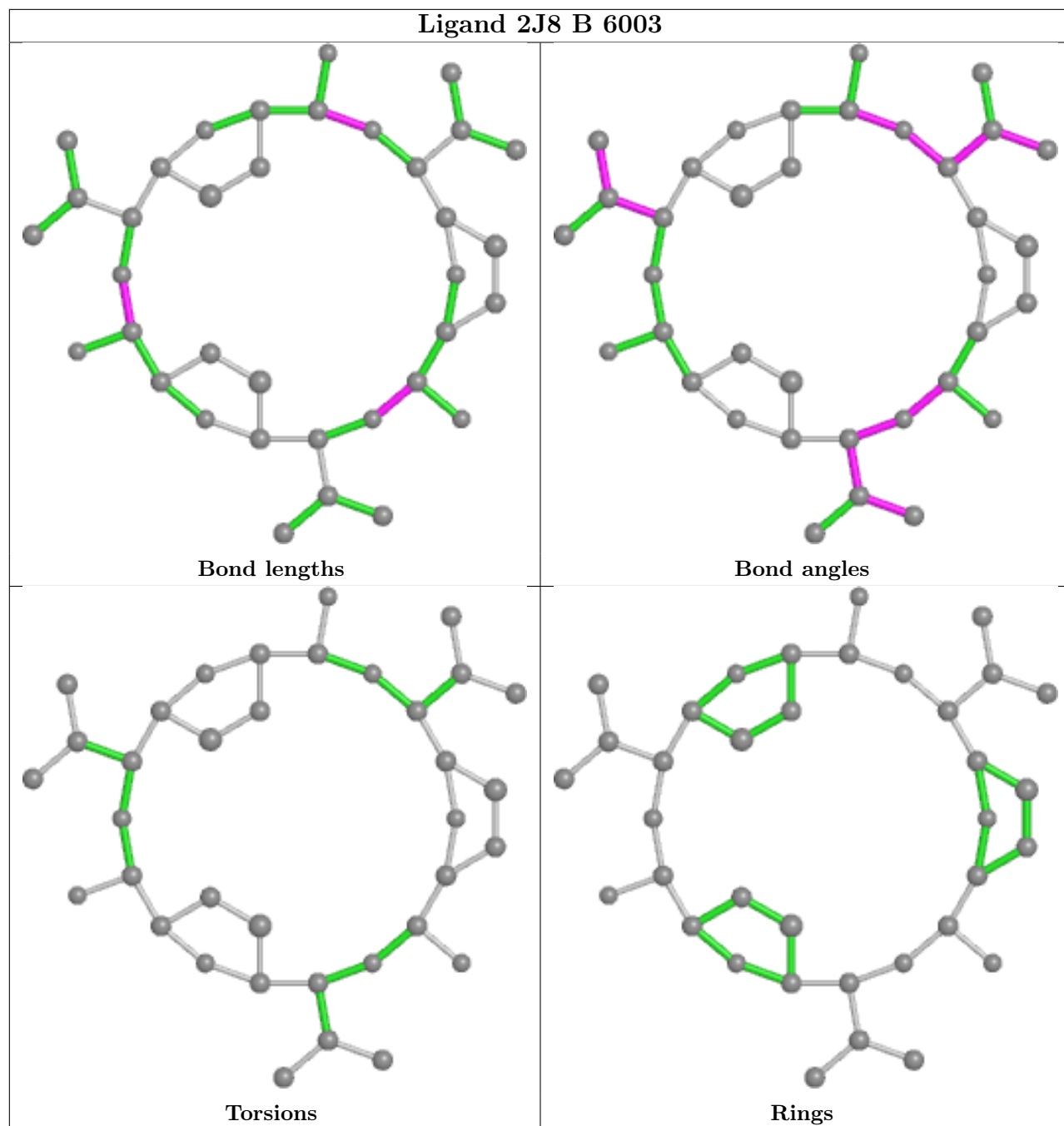
4 monomers are involved in 25 short contacts:

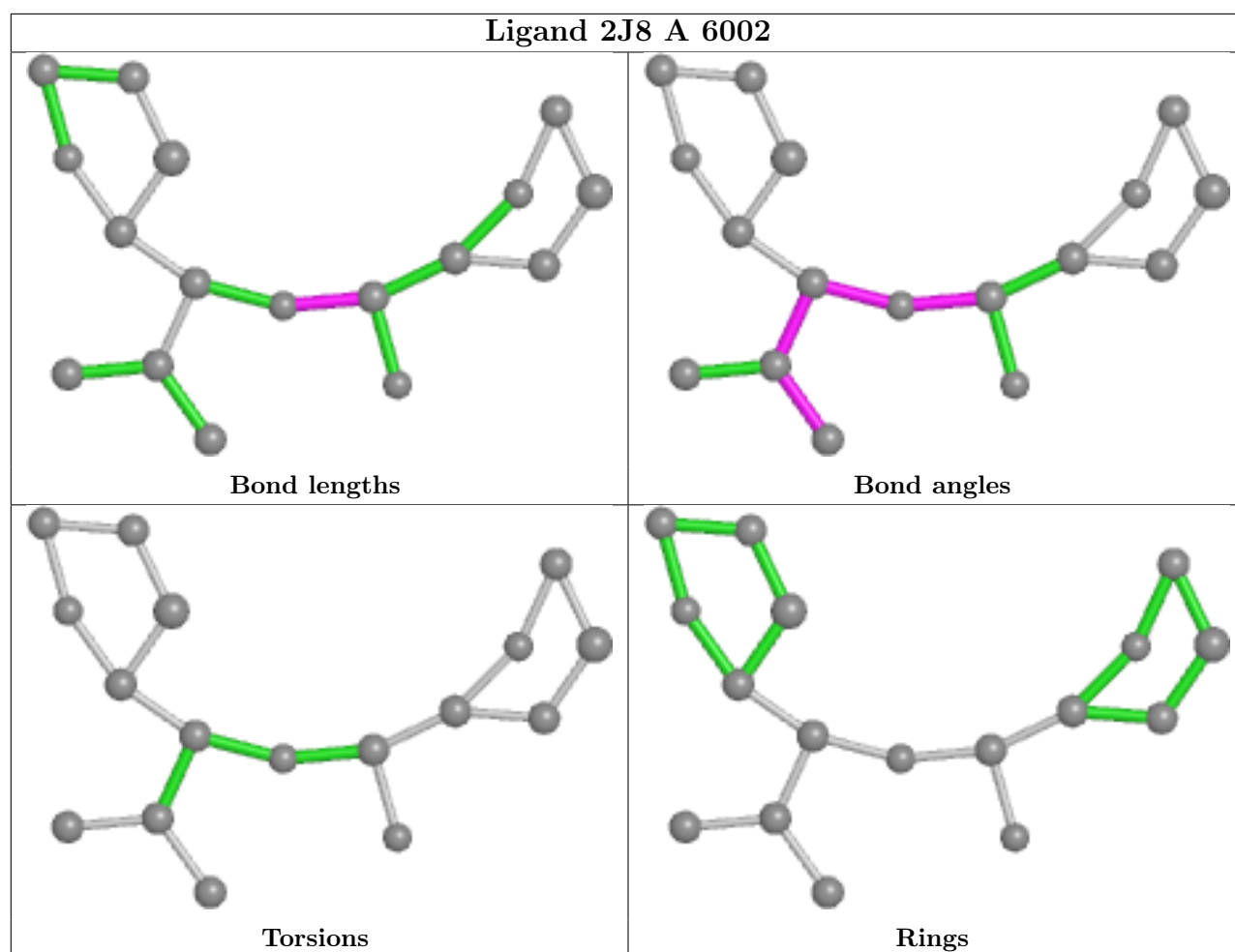
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	2J8	4	0
2	B	6003	2J8	16	0
2	A	6002	2J8	1	0
2	B	6004	2J8	4	0

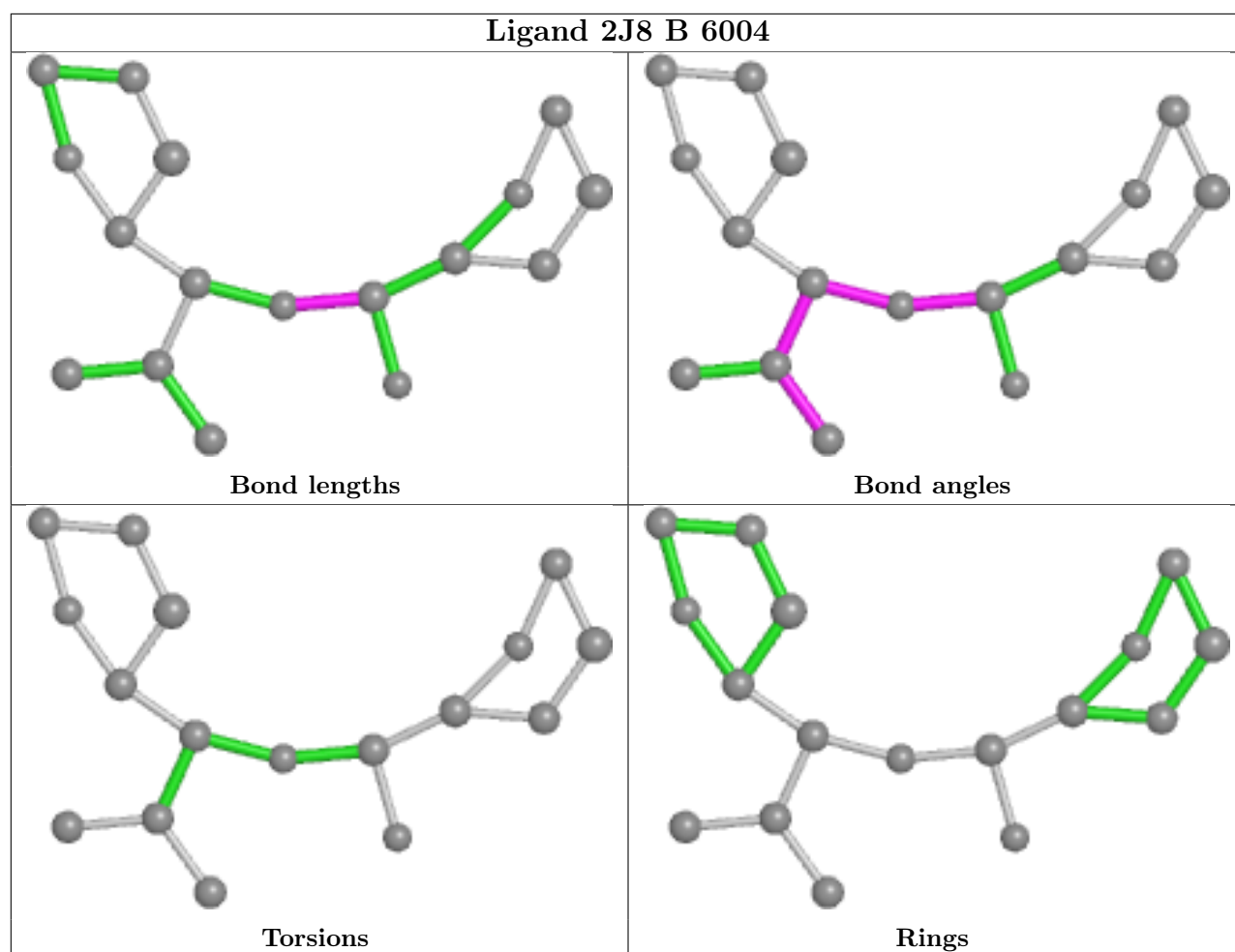
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.









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](#)

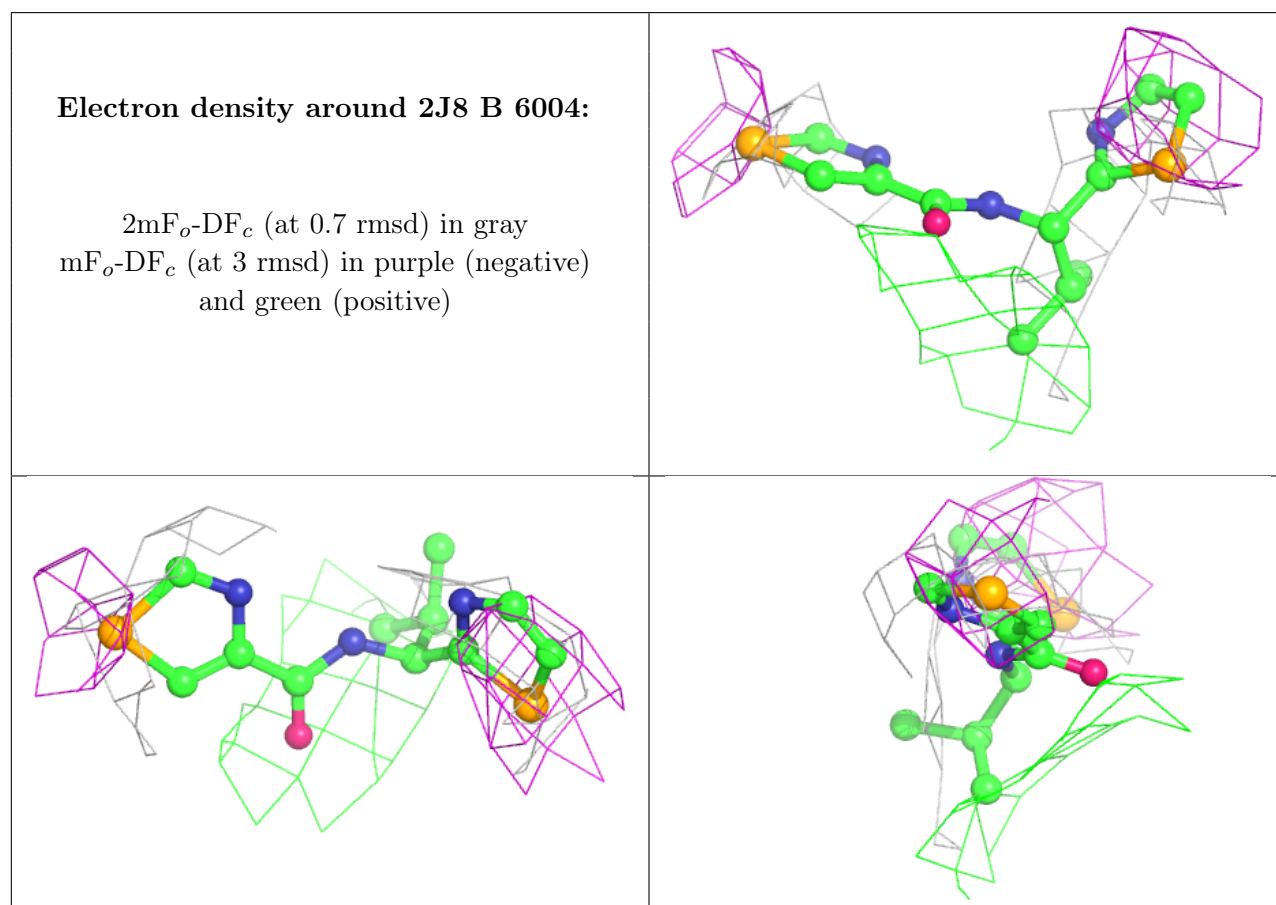
There are no monosaccharides in this entry.

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.

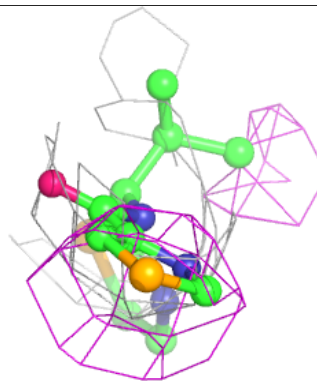
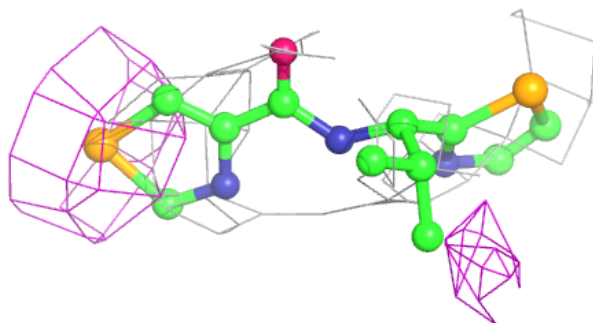
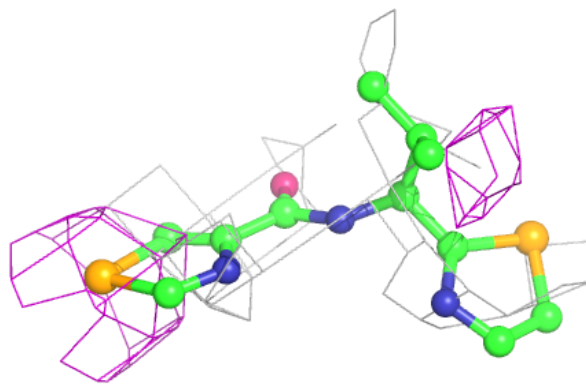
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2J8	B	6004	17/36	0.52	0.48	185,185,185,185	0
2	2J8	A	6002	17/36	0.68	0.52	185,185,185,185	0
2	2J8	B	6003	36/36	0.69	0.44	185,185,185,185	0
2	2J8	A	6001	36/36	0.80	0.36	185,185,185,185	0

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.



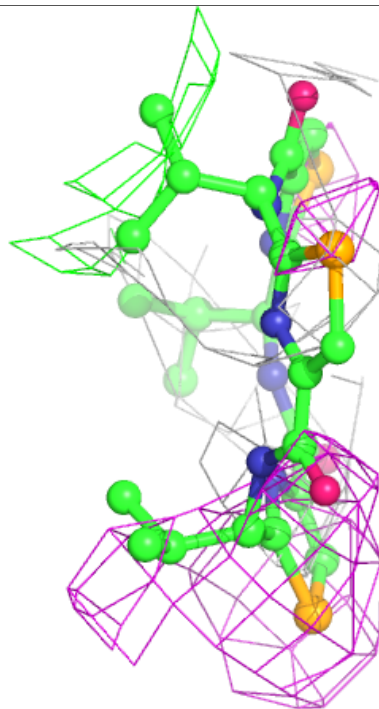
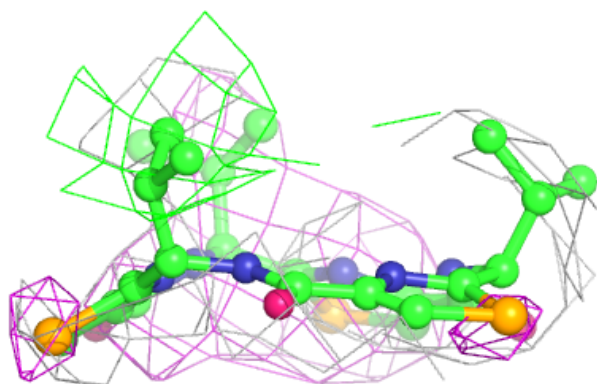
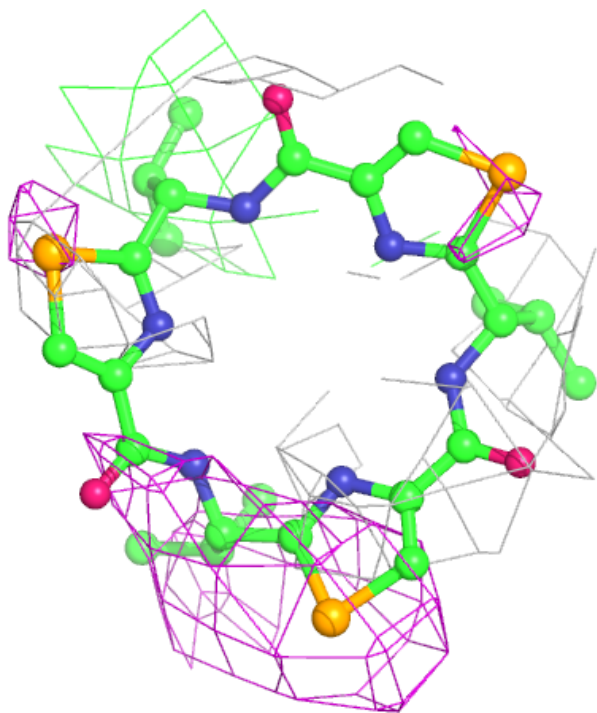
Electron density around 2J8 A 6002:

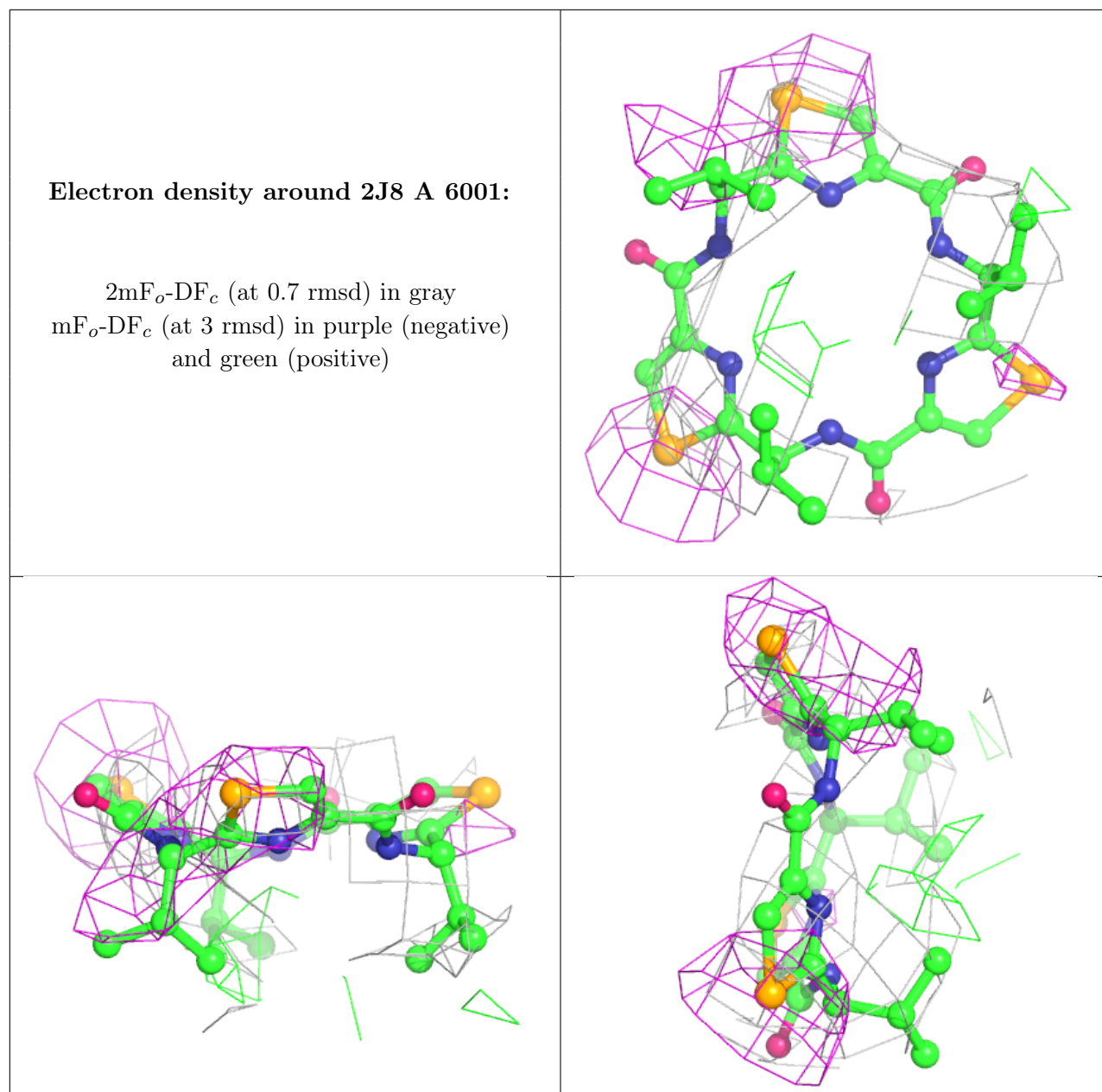
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.