



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 04:51 am BST

PDB ID : 4QNQ
Title : Crystal Structure Analysis of full-length Bcl-XL in complex with the inhibitor ABT-263
Authors : Korste, A.; Vetter, I.R.; Stoll, R.
Deposited on : 2014-06-18
Resolution : 2.30 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 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	:	2.11
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)	:	2.11

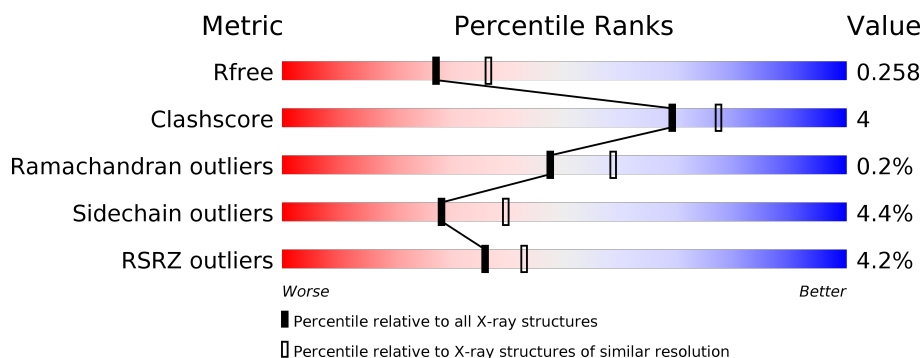
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	240	<div> <div> <div>0%</div> <div>54%</div> <div>5%</div> <div>40%</div> </div> </div>
1	B	240	<div> <div> <div>0%</div> <div>54%</div> <div>6%</div> <div>40%</div> </div> </div>
1	C	240	<div> <div> <div>5%</div> <div>55%</div> <div>5%</div> <div>40%</div> </div> </div>
1	D	240	<div> <div> <div>2%</div> <div>54%</div> <div>•</div> <div>41%</div> </div> </div>
1	E	240	<div> <div> <div>2%</div> <div>55%</div> <div>5%</div> <div>38%</div> </div> </div>
1	F	240	<div> <div> <div>2%</div> <div>57%</div> <div>5%</div> <div>38%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	240	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>51%</div><div>7%</div><div>42%</div></div></div>
1	H	240	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>52%</div><div>7%</div><div>41%</div></div></div>
1	I	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>56%</div><div>5%</div><div>39%</div></div></div>
1	J	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>55%</div><div>6%</div><div>38%</div></div></div>
1	K	240	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>55%</div><div></div><div>40%</div></div></div>
1	L	240	<div><div><div></div><div></div><div></div></div><div><div>6%</div><div>50%</div><div>8%</div><div>41%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14929 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 Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1169	749	196	219	5			
1	B	144	Total	C	N	O	S	0	0	0
			1167	745	196	222	4			
1	C	144	Total	C	N	O	S	0	0	0
			1167	748	195	219	5			
1	D	141	Total	C	N	O	S	0	0	0
			1143	730	193	215	5			
1	E	148	Total	C	N	O	S	0	0	0
			1199	771	199	224	5			
1	F	149	Total	C	N	O	S	0	0	0
			1207	775	201	226	5			
1	G	140	Total	C	N	O	S	0	0	0
			1135	726	191	213	5			
1	H	142	Total	C	N	O	S	0	0	0
			1150	734	194	217	5			
1	I	147	Total	C	N	O	S	0	0	0
			1188	762	198	223	5			
1	J	149	Total	C	N	O	S	0	0	0
			1207	775	201	226	5			
1	K	143	Total	C	N	O	S	0	0	0
			1161	742	196	219	4			
1	L	142	Total	C	N	O	S	0	0	0
			1150	734	194	217	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P53563
A	-5	SER	-	EXPRESSION TAG	UNP P53563
A	-4	PRO	-	EXPRESSION TAG	UNP P53563
A	-3	GLU	-	EXPRESSION TAG	UNP P53563
A	-2	PHE	-	EXPRESSION TAG	UNP P53563

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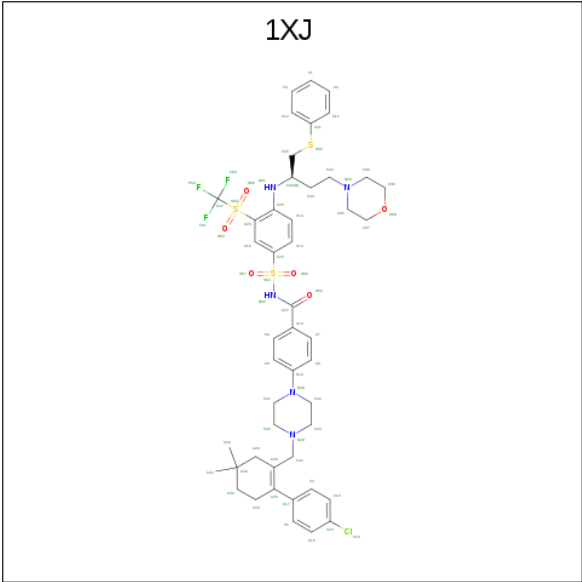
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	EXPRESSION TAG	UNP P53563
A	0	GLY	-	EXPRESSION TAG	UNP P53563
B	-6	GLY	-	EXPRESSION TAG	UNP P53563
B	-5	SER	-	EXPRESSION TAG	UNP P53563
B	-4	PRO	-	EXPRESSION TAG	UNP P53563
B	-3	GLU	-	EXPRESSION TAG	UNP P53563
B	-2	PHE	-	EXPRESSION TAG	UNP P53563
B	-1	PRO	-	EXPRESSION TAG	UNP P53563
B	0	GLY	-	EXPRESSION TAG	UNP P53563
C	-6	GLY	-	EXPRESSION TAG	UNP P53563
C	-5	SER	-	EXPRESSION TAG	UNP P53563
C	-4	PRO	-	EXPRESSION TAG	UNP P53563
C	-3	GLU	-	EXPRESSION TAG	UNP P53563
C	-2	PHE	-	EXPRESSION TAG	UNP P53563
C	-1	PRO	-	EXPRESSION TAG	UNP P53563
C	0	GLY	-	EXPRESSION TAG	UNP P53563
D	-6	GLY	-	EXPRESSION TAG	UNP P53563
D	-5	SER	-	EXPRESSION TAG	UNP P53563
D	-4	PRO	-	EXPRESSION TAG	UNP P53563
D	-3	GLU	-	EXPRESSION TAG	UNP P53563
D	-2	PHE	-	EXPRESSION TAG	UNP P53563
D	-1	PRO	-	EXPRESSION TAG	UNP P53563
D	0	GLY	-	EXPRESSION TAG	UNP P53563
E	-6	GLY	-	EXPRESSION TAG	UNP P53563
E	-5	SER	-	EXPRESSION TAG	UNP P53563
E	-4	PRO	-	EXPRESSION TAG	UNP P53563
E	-3	GLU	-	EXPRESSION TAG	UNP P53563
E	-2	PHE	-	EXPRESSION TAG	UNP P53563
E	-1	PRO	-	EXPRESSION TAG	UNP P53563
E	0	GLY	-	EXPRESSION TAG	UNP P53563
F	-6	GLY	-	EXPRESSION TAG	UNP P53563
F	-5	SER	-	EXPRESSION TAG	UNP P53563
F	-4	PRO	-	EXPRESSION TAG	UNP P53563
F	-3	GLU	-	EXPRESSION TAG	UNP P53563
F	-2	PHE	-	EXPRESSION TAG	UNP P53563
F	-1	PRO	-	EXPRESSION TAG	UNP P53563
F	0	GLY	-	EXPRESSION TAG	UNP P53563
G	-6	GLY	-	EXPRESSION TAG	UNP P53563
G	-5	SER	-	EXPRESSION TAG	UNP P53563
G	-4	PRO	-	EXPRESSION TAG	UNP P53563
G	-3	GLU	-	EXPRESSION TAG	UNP P53563
G	-2	PHE	-	EXPRESSION TAG	UNP P53563

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	PRO	-	EXPRESSION TAG	UNP P53563
G	0	GLY	-	EXPRESSION TAG	UNP P53563
H	-6	GLY	-	EXPRESSION TAG	UNP P53563
H	-5	SER	-	EXPRESSION TAG	UNP P53563
H	-4	PRO	-	EXPRESSION TAG	UNP P53563
H	-3	GLU	-	EXPRESSION TAG	UNP P53563
H	-2	PHE	-	EXPRESSION TAG	UNP P53563
H	-1	PRO	-	EXPRESSION TAG	UNP P53563
H	0	GLY	-	EXPRESSION TAG	UNP P53563
I	-6	GLY	-	EXPRESSION TAG	UNP P53563
I	-5	SER	-	EXPRESSION TAG	UNP P53563
I	-4	PRO	-	EXPRESSION TAG	UNP P53563
I	-3	GLU	-	EXPRESSION TAG	UNP P53563
I	-2	PHE	-	EXPRESSION TAG	UNP P53563
I	-1	PRO	-	EXPRESSION TAG	UNP P53563
I	0	GLY	-	EXPRESSION TAG	UNP P53563
J	-6	GLY	-	EXPRESSION TAG	UNP P53563
J	-5	SER	-	EXPRESSION TAG	UNP P53563
J	-4	PRO	-	EXPRESSION TAG	UNP P53563
J	-3	GLU	-	EXPRESSION TAG	UNP P53563
J	-2	PHE	-	EXPRESSION TAG	UNP P53563
J	-1	PRO	-	EXPRESSION TAG	UNP P53563
J	0	GLY	-	EXPRESSION TAG	UNP P53563
K	-6	GLY	-	EXPRESSION TAG	UNP P53563
K	-5	SER	-	EXPRESSION TAG	UNP P53563
K	-4	PRO	-	EXPRESSION TAG	UNP P53563
K	-3	GLU	-	EXPRESSION TAG	UNP P53563
K	-2	PHE	-	EXPRESSION TAG	UNP P53563
K	-1	PRO	-	EXPRESSION TAG	UNP P53563
K	0	GLY	-	EXPRESSION TAG	UNP P53563
L	-6	GLY	-	EXPRESSION TAG	UNP P53563
L	-5	SER	-	EXPRESSION TAG	UNP P53563
L	-4	PRO	-	EXPRESSION TAG	UNP P53563
L	-3	GLU	-	EXPRESSION TAG	UNP P53563
L	-2	PHE	-	EXPRESSION TAG	UNP P53563
L	-1	PRO	-	EXPRESSION TAG	UNP P53563
L	0	GLY	-	EXPRESSION TAG	UNP P53563

- Molecule 2 is 4-(4-{[2-(4-chlorophenyl)-5,5-dimethylcyclohex-1-en-1-yl]methyl}piperazin-1-yl)-N-[(4-{[(2R)-4-(morpholin-4-yl)-1-(phenylsulfanyl)butan-2-yl]amino}-3-[(trifluoromethyl)sulfonyl]phenyl)sulfonyl]benzamide (three-letter code: 1XJ) (formula: C₄₇H₅₅ClF₃N₅O₆S₃).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	C	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	D	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	E	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	F	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	G	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	H	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	I	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	J	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	K	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		
2	L	1	Total	C	Cl	F	N	O	S	0	0
			65	47	1	3	5	6	3		

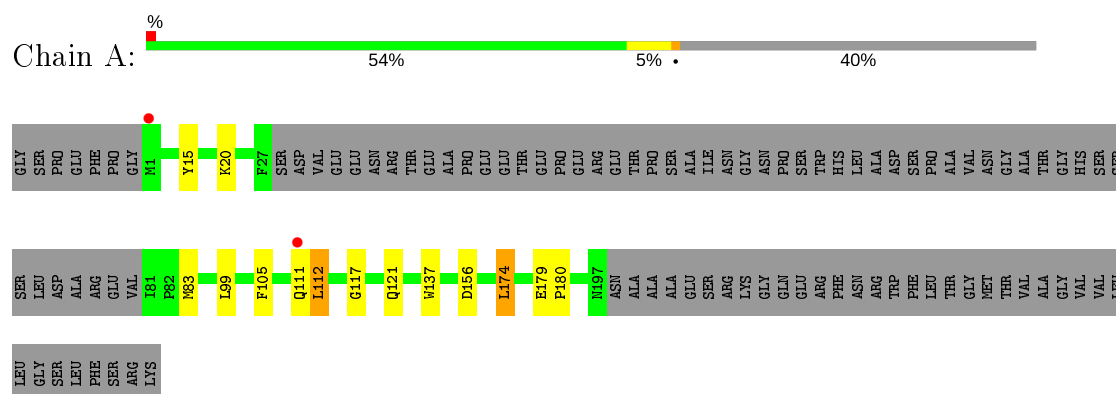
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	7	Total O 7 7	0	0
3	C	10	Total O 10 10	0	0
3	D	6	Total O 6 6	0	0
3	E	9	Total O 9 9	0	0
3	F	11	Total O 11 11	0	0
3	G	6	Total O 6 6	0	0
3	H	11	Total O 11 11	0	0
3	I	8	Total O 8 8	0	0
3	J	10	Total O 10 10	0	0
3	K	9	Total O 9 9	0	0
3	L	6	Total O 6 6	0	0

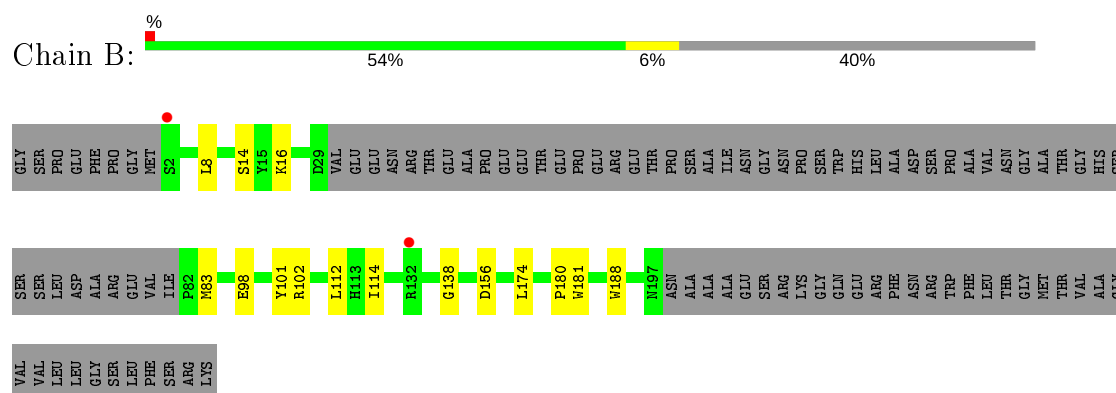
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

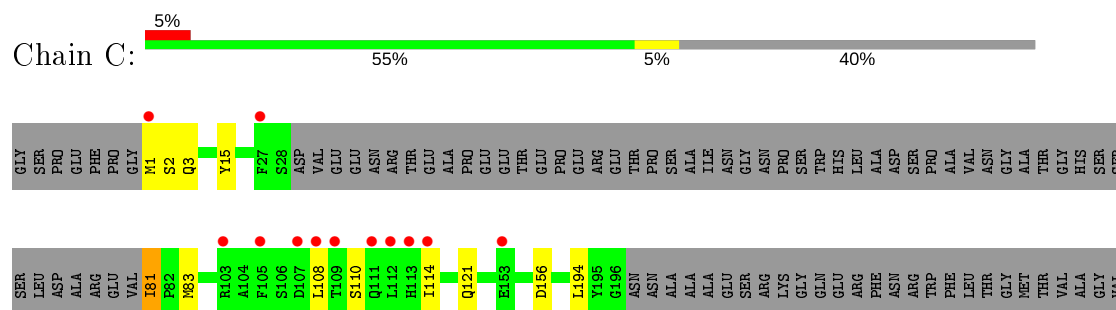
• Molecule 1: Bcl-2-like protein 1



• Molecule 1: Bcl-2-like protein 1



• Molecule 1: Bcl-2-like protein 1



ARG TRP PHE LEU THR GLY MET THR VAL ALA GLY VAL VAL LEU LEU LEU SER SER PHE SER ARG LYS

• Molecule 1: Bcl-2-like protein 1



GLY SER PRO GLU PHE THR PRO GLY M1 S2 K16 S23 S25 Q26 PHE SER ASP VAL GLU GLU ASN ARG THR GLU ALA PRO GLU GLU THR PRO GLU ARG GLU THR PRO SER SER ILE ASN GLY ASN PRO SER TRP HIS LEU ALA ASP ASP PRO VAL ASN GLY ALA THR VAL THR GLY

HIS SER SER SER LEU ASP ALA ARG GLU SER VAL ILE P82 M83 L90 E98 F105 Q111 L112 H113 I114 H136 D156 R165 L174 W181 H197 ASN ALA ALA ALA GLU SER ASP ARG LYS GLN SER GLU ARG PHE MET THR VAL ALA

GLY VAL VAL LEU GLY SER LEU PHE SER ARG LYS

• Molecule 1: Bcl-2-like protein 1



GLY SER PRO E-3 S25 Q26 PHE SER ASP VAL GLU GLU ASN ARG THR GLU ALA PRO GLU GLU THR GLU PRO GLU ARG GLU THR ASN GLU SER ILE GLY ASN PRO SER TRP HIS LEU ALA ALA ASP ARG PRO ALA GLY HIS TRP PHE VAL SER SER LEU ASP ALA ARG GLU

V80 R102 R103 A104 F105 L108 T109 S110 Q111 L112 H113 I114 F123 V127 N136 L150 I166 G196 ASN ASN ALA ALA GLU SER ASN LYS GLN GLU ARG PHE PHE LEU THR GLY MET THR VAL ALA GLY VAL VAL LEU GLY SER LEU PHE

SER ARG LYS

• Molecule 1: Bcl-2-like protein 1



GLY SER PRO E-3 GO H1 S25 Q26 F27 SER ASP VAL GLU GLU ASN ARG THR GLU ALA PRO GLU GLU THR GLU PRO GLU GLU ARG GLU THR PRO GLU ILE SER GLY ASN PRO SER TRP HIS LEU ALA ASP ASP SER PRO GLY VAL VAL ASN GLY ALA ALA THR GLY HIS SER SER SER ASP

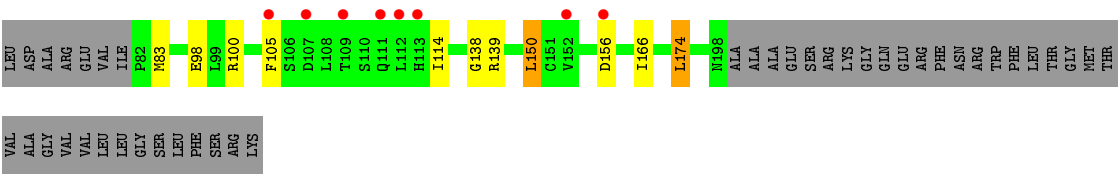
ALA ARG GLU V80 V86 E96 L99 F105 S106 D107 L108 T109 Q111 S110 L112 H113 I114 L150 K157 Q160 I166 E179 P180 V192 Y195 G196 H197 ASN ALA ALA ALA GLU SER ARG LYS GLN GLU ARG PHE PHE THR THR MET THR

VAL ALA GLU VAL VAL LEU LEU GLY SER LEU PHE SER ARG LYS

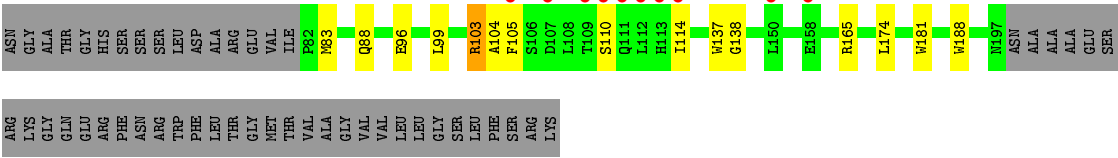
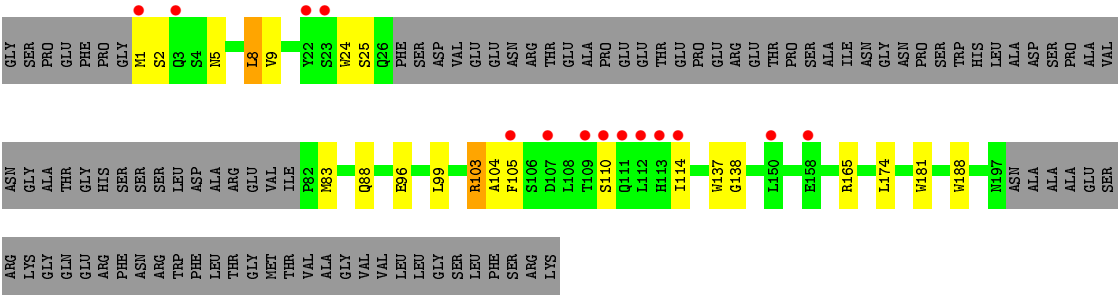
• Molecule 1: Bcl-2-like protein 1



GLY SER PRO GLU PHE THR PRO GLY MET S2 S25 Q26 F27 SER ASP VAL GLU GLU ASN ARG THR THR GLU ALA PRO GLU GLU THR GLU PRO GLU GLU ARG GLU THR PRO SER SER ILE ASN GLY ASN PRO TRP HIS LEU ALA ASP GLY SER GLN GLU ARG PHE PHE THR THR MET THR



● Molecule 1: Bcl-2-like protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 85.81Å 93.64Å 72.94° 67.42° 69.38°	Depositor
Resolution (Å)	85.00 – 2.30 47.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (85.00-2.30) 97.6 (47.03-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.206 , 0.253 0.211 , 0.258	Depositor DCC
R_{free} test set	4444 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14929	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2962e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1XJ

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	0.90	1/1198 (0.1%)	0.84	2/1621 (0.1%)
1	B	0.83	2/1196 (0.2%)	0.80	0/1618
1	C	0.77	0/1196	0.75	0/1618
1	D	0.93	0/1171	0.84	1/1584 (0.1%)
1	E	0.80	0/1230	0.77	1/1665 (0.1%)
1	F	0.84	0/1238	0.79	0/1676
1	G	0.84	2/1163 (0.2%)	0.75	0/1573
1	H	0.91	2/1178 (0.2%)	0.85	2/1593 (0.1%)
1	I	0.78	0/1218	0.74	1/1649 (0.1%)
1	J	0.85	0/1238	0.77	0/1676
1	K	0.76	0/1190	0.77	2/1610 (0.1%)
1	L	0.75	3/1178 (0.3%)	0.75	1/1593 (0.1%)
All	All	0.83	10/14394 (0.1%)	0.79	10/19476 (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	E	0	1
1	H	0	1
1	J	0	1
1	K	0	1
All	All	0	4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	24	TRP	CD2-CE2	6.40	1.49	1.41
1	G	169	TRP	CD2-CE2	5.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	TRP	CD2-CE2	5.50	1.48	1.41
1	H	181	TRP	CD2-CE2	5.46	1.48	1.41
1	L	181	TRP	CD2-CE2	5.41	1.47	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	165	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	D	174	LEU	CA-CB-CG	6.58	130.45	115.30
1	H	174	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	174	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	K	139	ARG	NE-CZ-NH1	5.76	123.18	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	SER	Peptide
1	H	24	TRP	Peptide
1	J	25	SER	Peptide
1	K	25	SER	Peptide

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	1169	0	1113	8	0
1	B	1167	0	1100	8	0
1	C	1167	0	1112	6	0
1	D	1143	0	1087	6	0
1	E	1199	0	1141	10	0
1	F	1207	0	1147	6	0
1	G	1135	0	1081	9	0
1	H	1150	0	1094	9	0
1	I	1188	0	1132	10	0
1	J	1207	0	1147	14	0
1	K	1161	0	1097	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1150	0	1094	11	0
2	A	65	0	55	4	0
2	B	65	0	55	2	0
2	C	65	0	55	4	0
2	D	65	0	55	2	0
2	E	65	0	55	2	0
2	F	65	0	55	4	0
2	G	65	0	55	3	0
2	H	65	0	55	1	0
2	I	65	0	55	3	0
2	J	65	0	55	6	0
2	K	65	0	55	3	0
2	L	65	0	55	3	0
3	A	13	0	0	0	0
3	B	7	0	0	0	0
3	C	10	0	0	0	0
3	D	6	0	0	0	0
3	E	9	0	0	2	0
3	F	11	0	0	0	0
3	G	6	0	0	0	0
3	H	11	0	0	0	0
3	I	8	0	0	0	0
3	J	10	0	0	0	0
3	K	9	0	0	1	0
3	L	6	0	0	0	0
All	All	14929	0	14005	106	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 4.

The worst 5 of 106 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:I:105:PHE:O	1:I:108:LEU:HD12	1.46	1.12
1:D:129:GLU:OE2	1:D:132:ARG:NH1	2.10	0.85
1:I:108:LEU:HD13	1:I:109:THR:N	1.96	0.79
2:G:301:1XJ:C25	2:G:301:1XJ:H44	2.15	0.74
1:C:81:ILE:HG23	1:L:99:LEU:HD22	1.79	0.65

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
1	B	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
1	C	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
1	D	137/240 (57%)	134 (98%)	3 (2%)	0	100	100
1	E	144/240 (60%)	139 (96%)	5 (4%)	0	100	100
1	F	145/240 (60%)	144 (99%)	1 (1%)	0	100	100
1	G	136/240 (57%)	134 (98%)	2 (2%)	0	100	100
1	H	138/240 (58%)	134 (97%)	3 (2%)	1 (1%)	22	26
1	I	143/240 (60%)	140 (98%)	3 (2%)	0	100	100
1	J	145/240 (60%)	139 (96%)	5 (3%)	1 (1%)	22	26
1	K	139/240 (58%)	137 (99%)	2 (1%)	0	100	100
1	L	138/240 (58%)	136 (99%)	1 (1%)	1 (1%)	22	26
All	All	1685/2880 (58%)	1652 (98%)	30 (2%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	25	SER
1	H	24	TRP
1	J	25	SER

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	124/201 (62%)	118 (95%)	6 (5%)	25	36
1	B	124/201 (62%)	119 (96%)	5 (4%)	31	44
1	C	124/201 (62%)	117 (94%)	7 (6%)	21	29
1	D	121/201 (60%)	116 (96%)	5 (4%)	30	43
1	E	127/201 (63%)	121 (95%)	6 (5%)	26	37
1	F	128/201 (64%)	122 (95%)	6 (5%)	26	37
1	G	120/201 (60%)	116 (97%)	4 (3%)	38	53
1	H	122/201 (61%)	117 (96%)	5 (4%)	30	43
1	I	126/201 (63%)	119 (94%)	7 (6%)	21	29
1	J	128/201 (64%)	124 (97%)	4 (3%)	40	55
1	K	123/201 (61%)	118 (96%)	5 (4%)	30	43
1	L	122/201 (61%)	116 (95%)	6 (5%)	25	35
All	All	1489/2412 (62%)	1423 (96%)	66 (4%)	28	39

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	26	GLN
1	G	114	ILE
1	L	8	LEU
1	F	27	PHE
1	F	114	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	121	GLN
1	E	185	ASN
1	G	185	ASN
1	K	160	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	1XJ	L	301	-	69,71,71	1.52	12 (17%)	93,104,104	3.09	38 (40%)
2	1XJ	K	301	-	69,71,71	1.41	12 (17%)	93,104,104	3.18	38 (40%)
2	1XJ	J	301	-	69,71,71	1.61	12 (17%)	93,104,104	3.23	30 (32%)
2	1XJ	I	301	-	69,71,71	1.68	14 (20%)	93,104,104	3.23	34 (36%)
2	1XJ	G	301	-	69,71,71	1.54	10 (14%)	93,104,104	3.29	35 (37%)
2	1XJ	F	301	-	69,71,71	1.71	14 (20%)	93,104,104	3.38	40 (43%)
2	1XJ	E	301	-	69,71,71	1.46	9 (13%)	93,104,104	3.19	31 (33%)
2	1XJ	D	301	-	69,71,71	1.81	12 (17%)	93,104,104	2.50	25 (26%)
2	1XJ	C	301	-	69,71,71	1.57	11 (15%)	93,104,104	3.26	33 (35%)
2	1XJ	B	301	-	69,71,71	1.49	12 (17%)	93,104,104	2.88	32 (34%)
2	1XJ	A	301	-	69,71,71	2.05	17 (24%)	93,104,104	2.82	35 (37%)
2	1XJ	H	301	-	69,71,71	1.57	14 (20%)	93,104,104	3.23	30 (32%)

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	1XJ	L	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	K	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	J	301	-	-	10/56/89/89	0/7/7/7
2	1XJ	I	301	-	-	7/56/89/89	0/7/7/7
2	1XJ	G	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	F	301	-	-	9/56/89/89	0/7/7/7
2	1XJ	E	301	-	-	6/56/89/89	0/7/7/7
2	1XJ	D	301	-	-	4/56/89/89	0/7/7/7
2	1XJ	C	301	-	-	5/56/89/89	0/7/7/7
2	1XJ	B	301	-	-	4/56/89/89	0/7/7/7
2	1XJ	A	301	-	-	5/56/89/89	0/7/7/7
2	1XJ	H	301	-	-	7/56/89/89	0/7/7/7

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	1XJ	O55-S63	7.34	1.50	1.44
2	F	301	1XJ	C26-C25	6.72	1.44	1.35
2	E	301	1XJ	C26-C25	6.67	1.44	1.35
2	H	301	1XJ	C26-C25	6.66	1.44	1.35
2	G	301	1XJ	C26-C25	6.64	1.44	1.35

The worst 5 of 401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	1XJ	C42-N49-C34	17.00	137.46	111.09
2	J	301	1XJ	C42-N49-C34	16.27	136.33	111.09
2	K	301	1XJ	C42-N49-C34	15.73	135.49	111.09
2	H	301	1XJ	C42-N49-C34	15.19	134.66	111.09
2	L	301	1XJ	C17-C25-C26	14.38	140.97	123.75

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

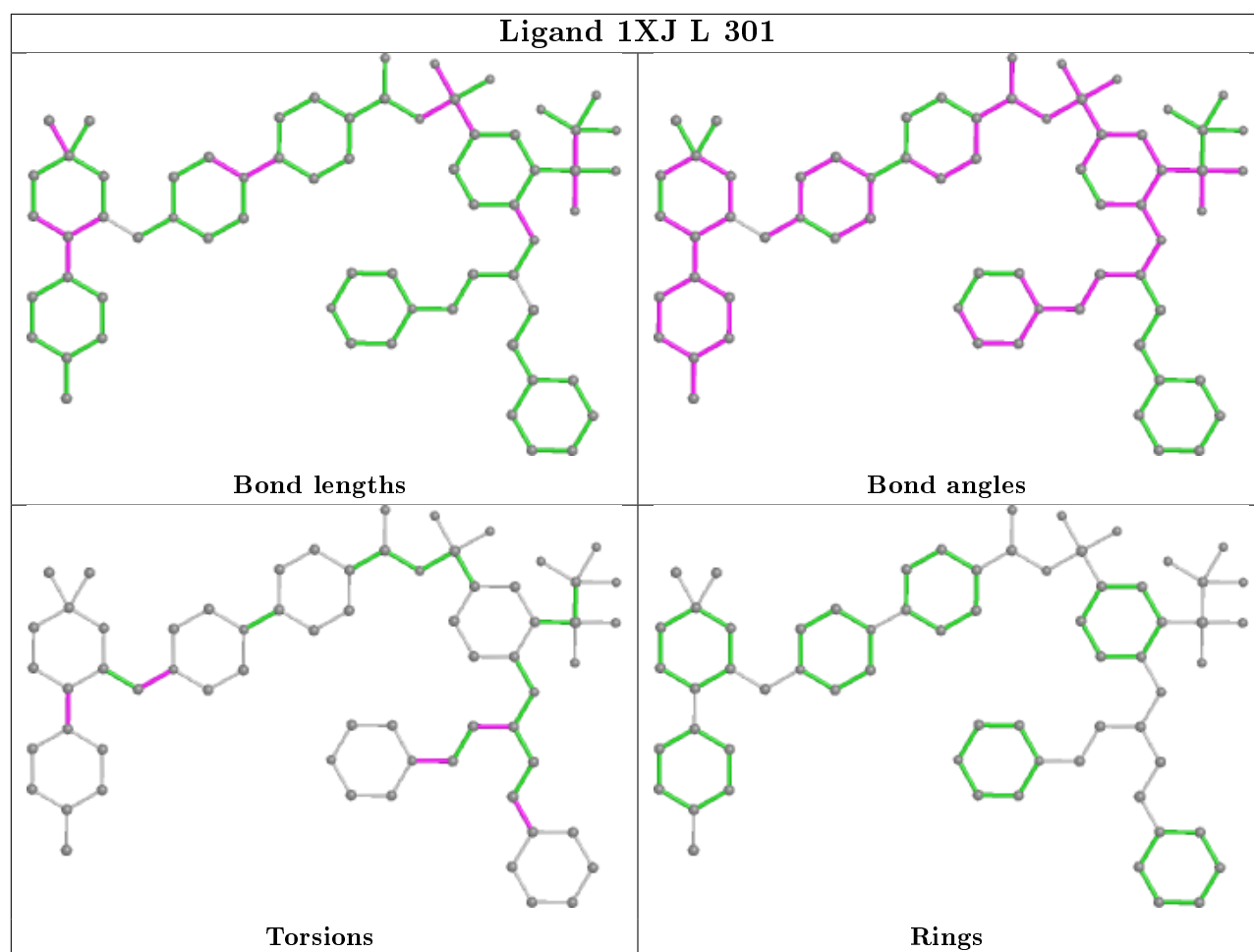
Mol	Chain	Res	Type	Atoms
2	L	301	1XJ	C26-C42-N49-C33
2	K	301	1XJ	C26-C42-N49-C33
2	K	301	1XJ	C26-C42-N49-C34
2	J	301	1XJ	C44-C43-C46-C45
2	J	301	1XJ	S62-C45-C46-C43

There are no ring outliers.

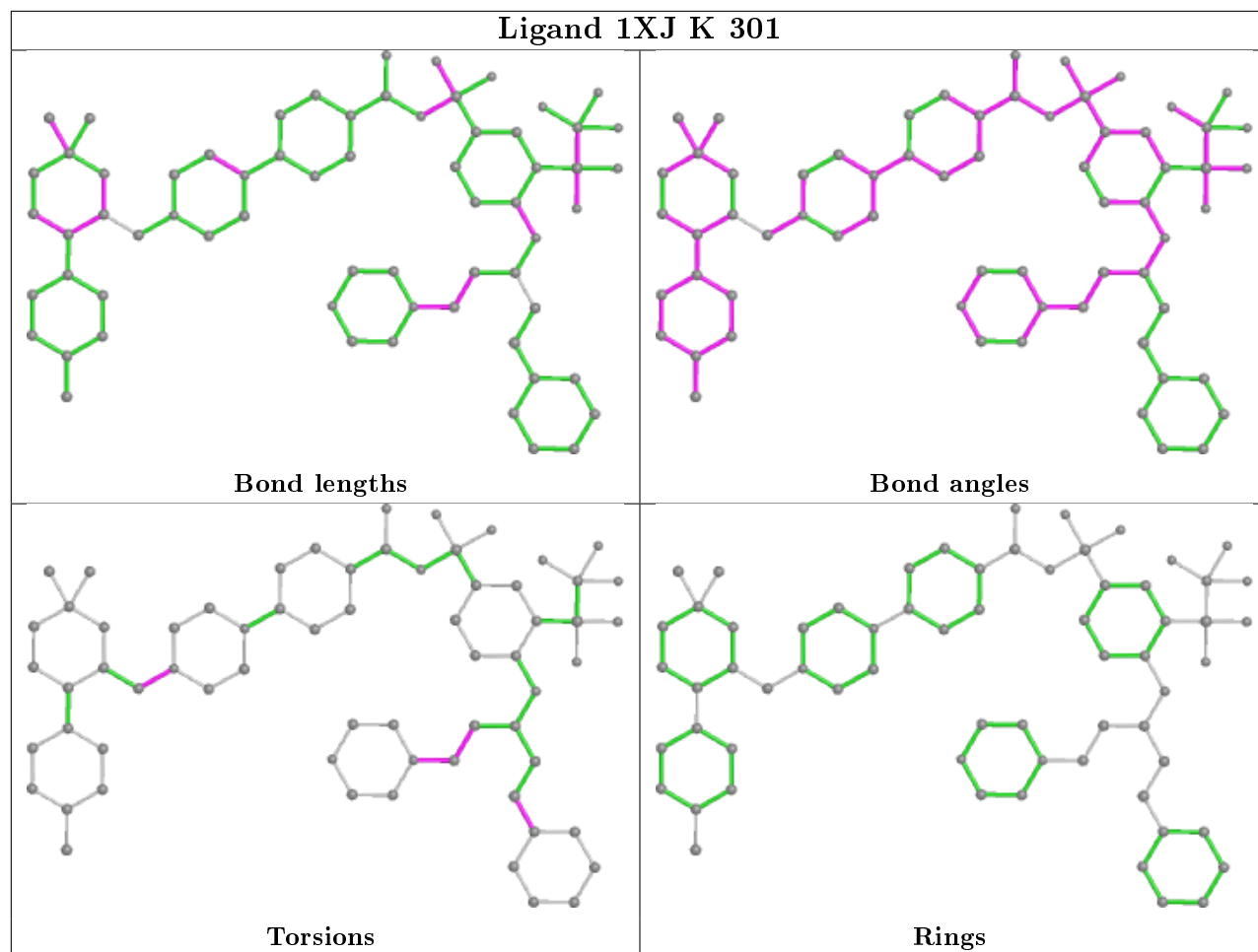
12 monomers are involved in 37 short contacts:

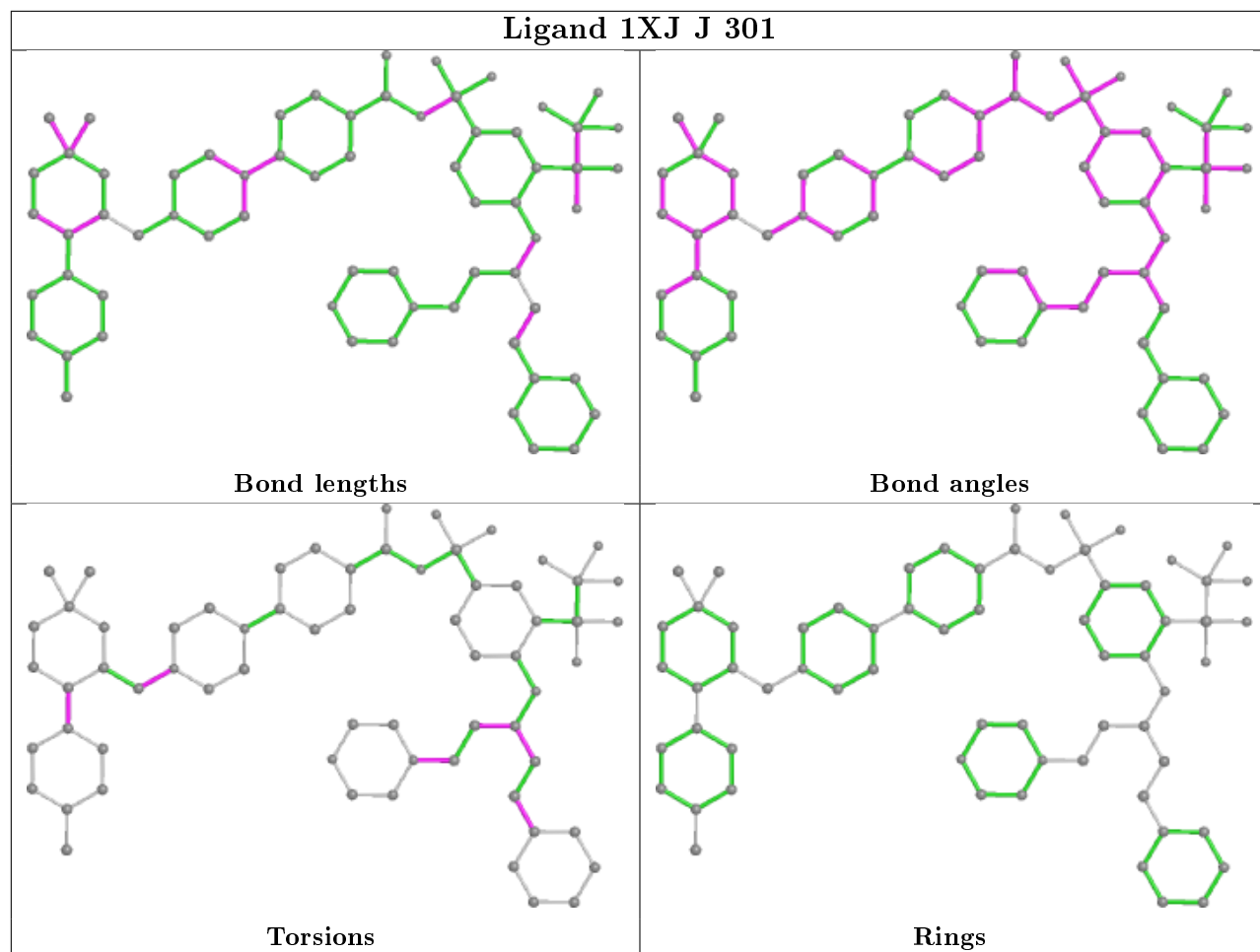
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	1XJ	3	0
2	K	301	1XJ	3	0
2	J	301	1XJ	6	0
2	I	301	1XJ	3	0
2	G	301	1XJ	3	0
2	F	301	1XJ	4	0
2	E	301	1XJ	2	0
2	D	301	1XJ	2	0
2	C	301	1XJ	4	0
2	B	301	1XJ	2	0
2	A	301	1XJ	4	0
2	H	301	1XJ	1	0

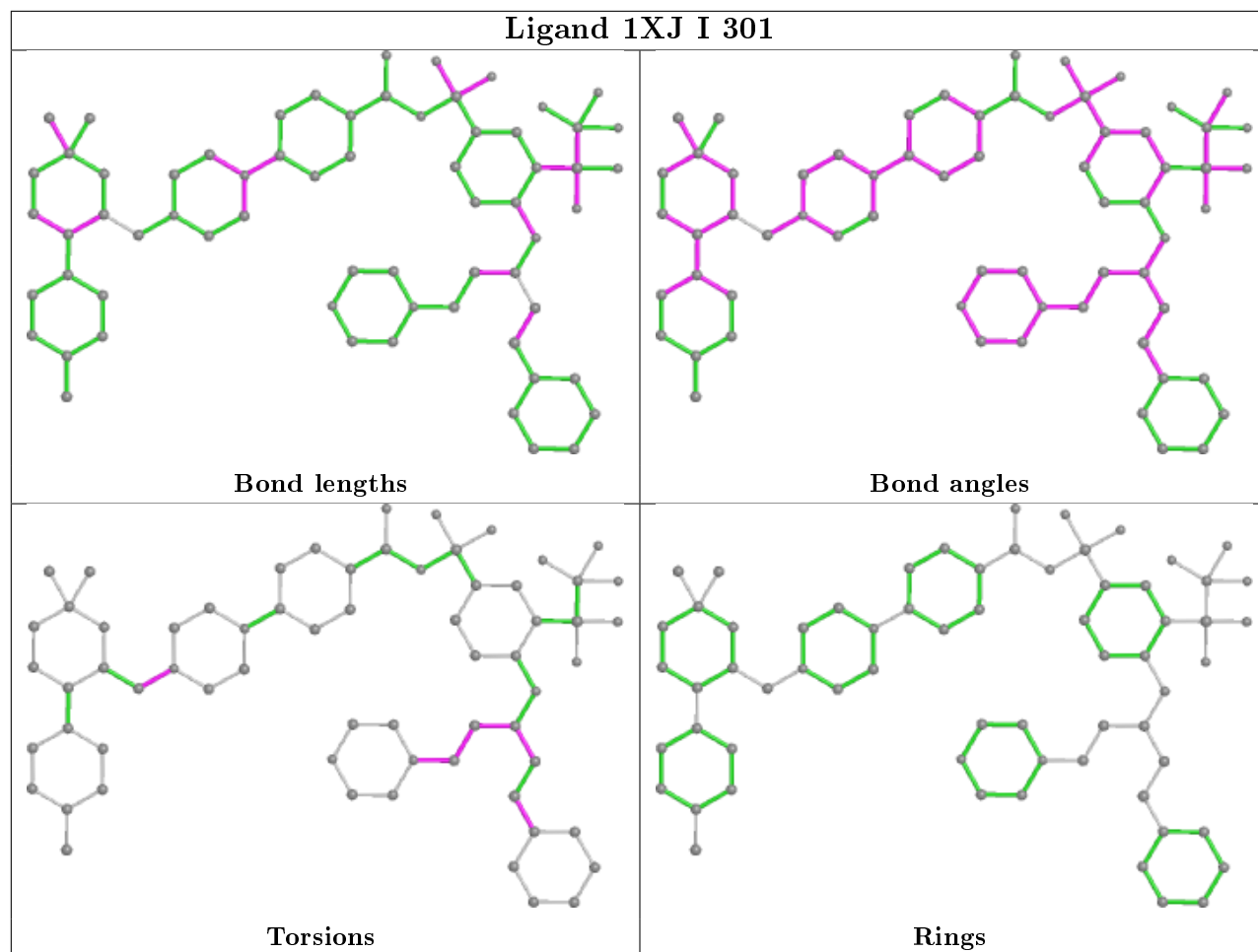
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

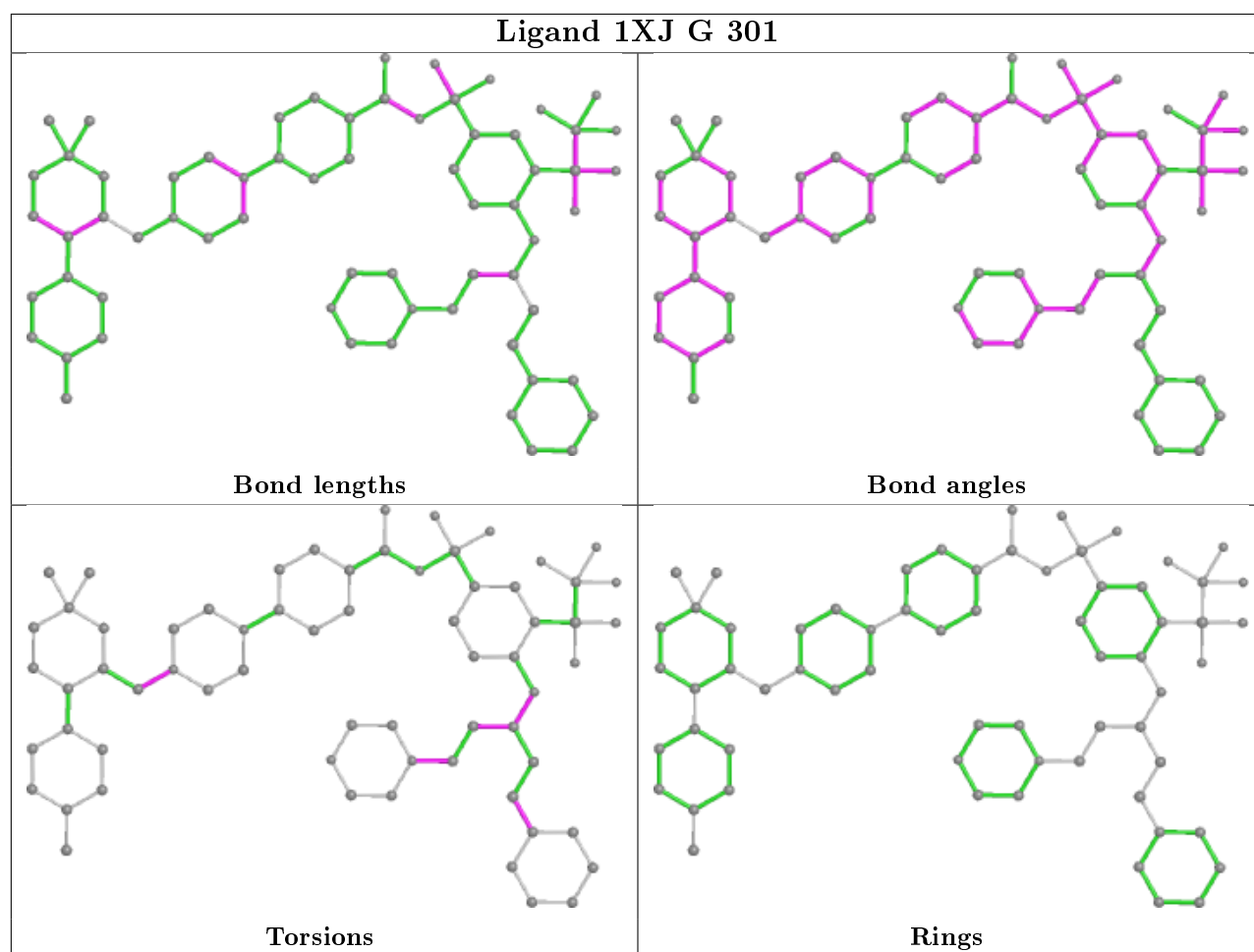


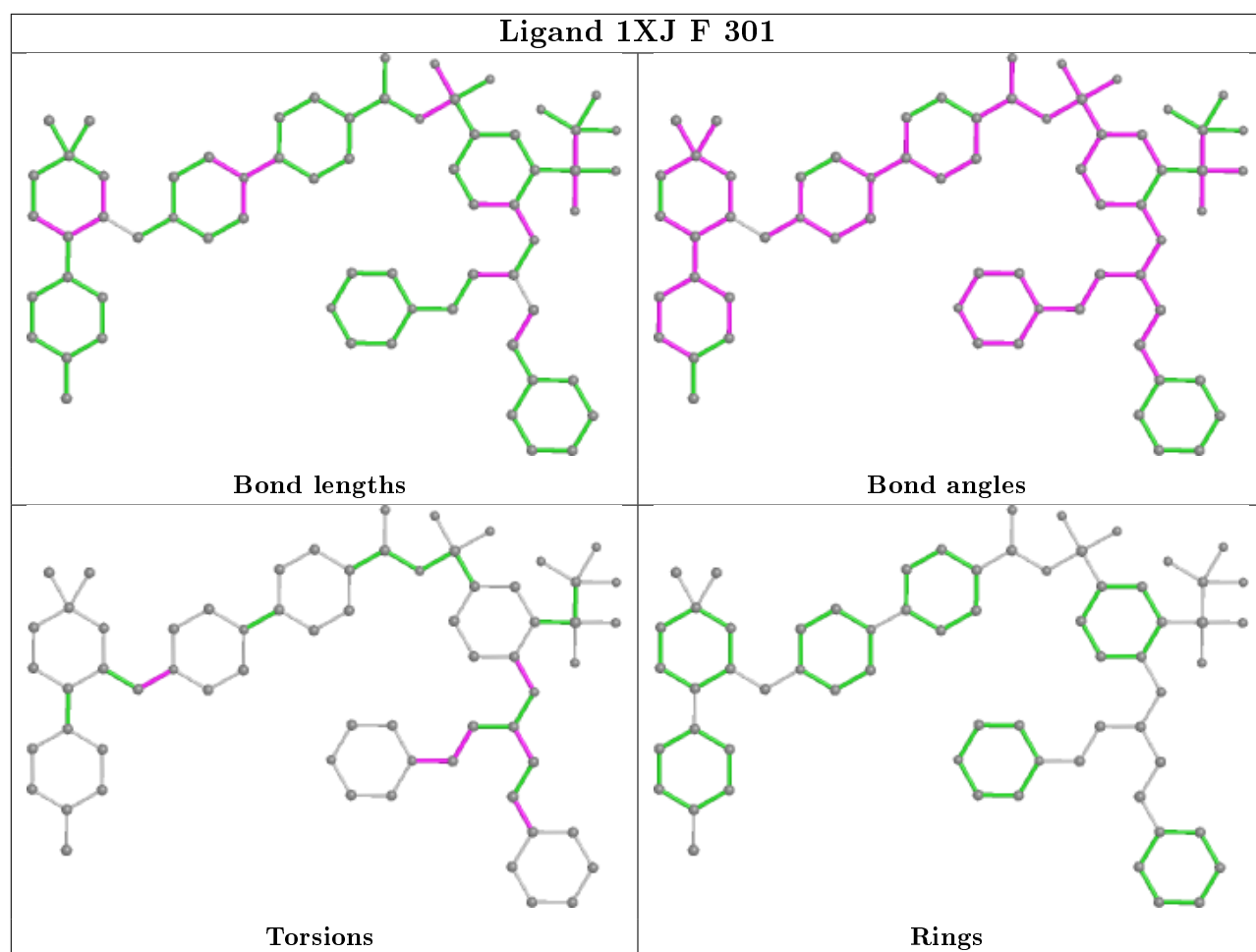
Ligand 1XJ K 301



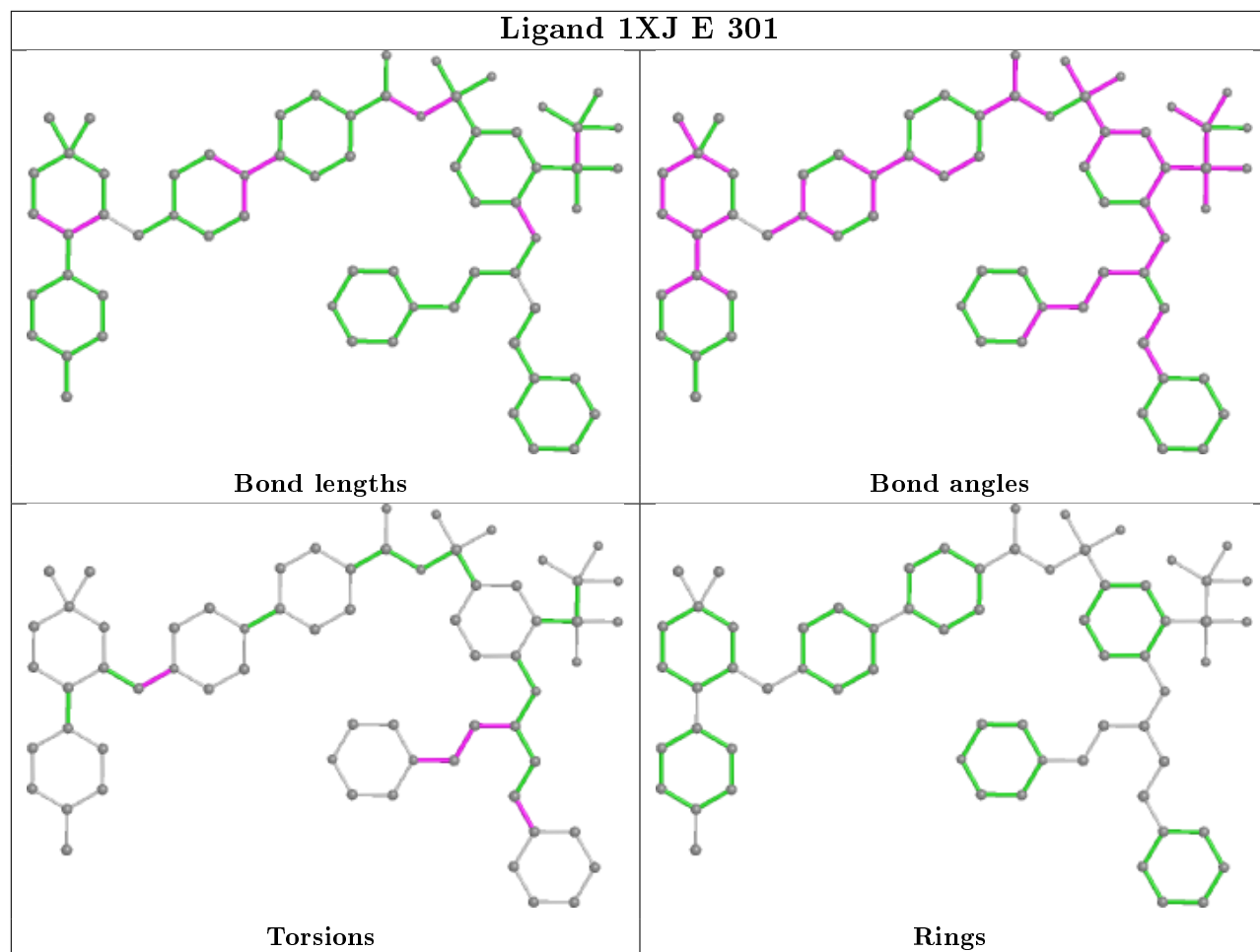


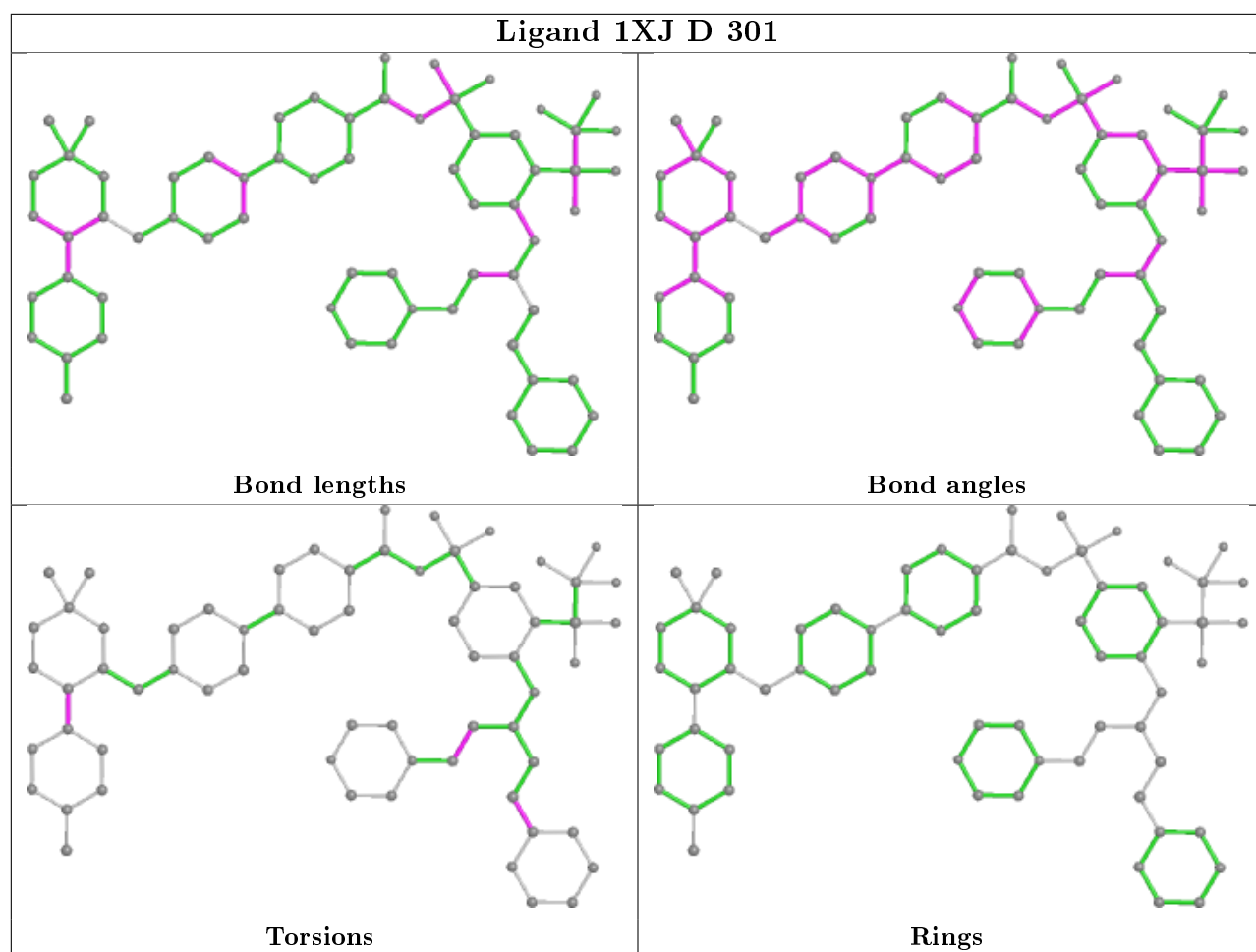


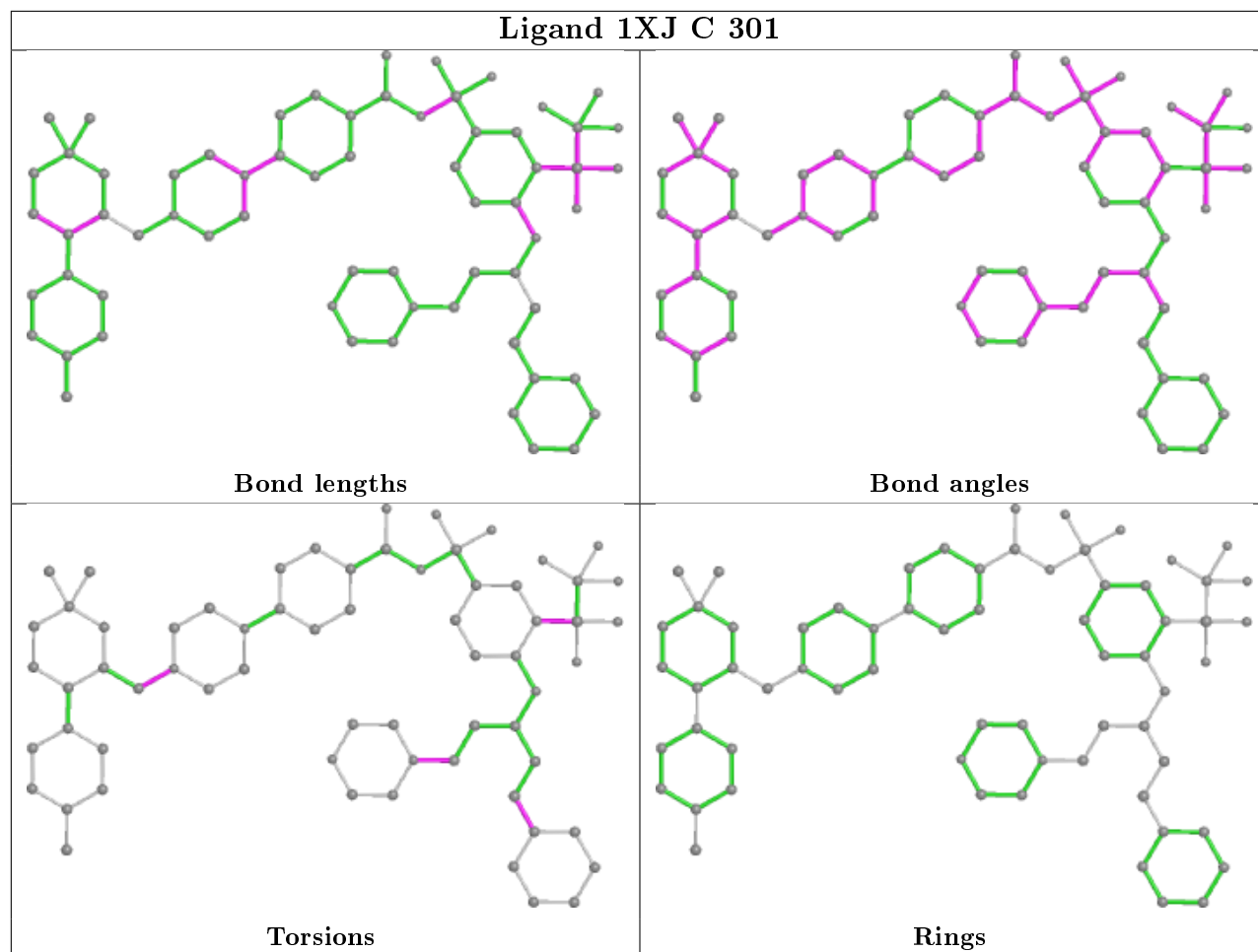


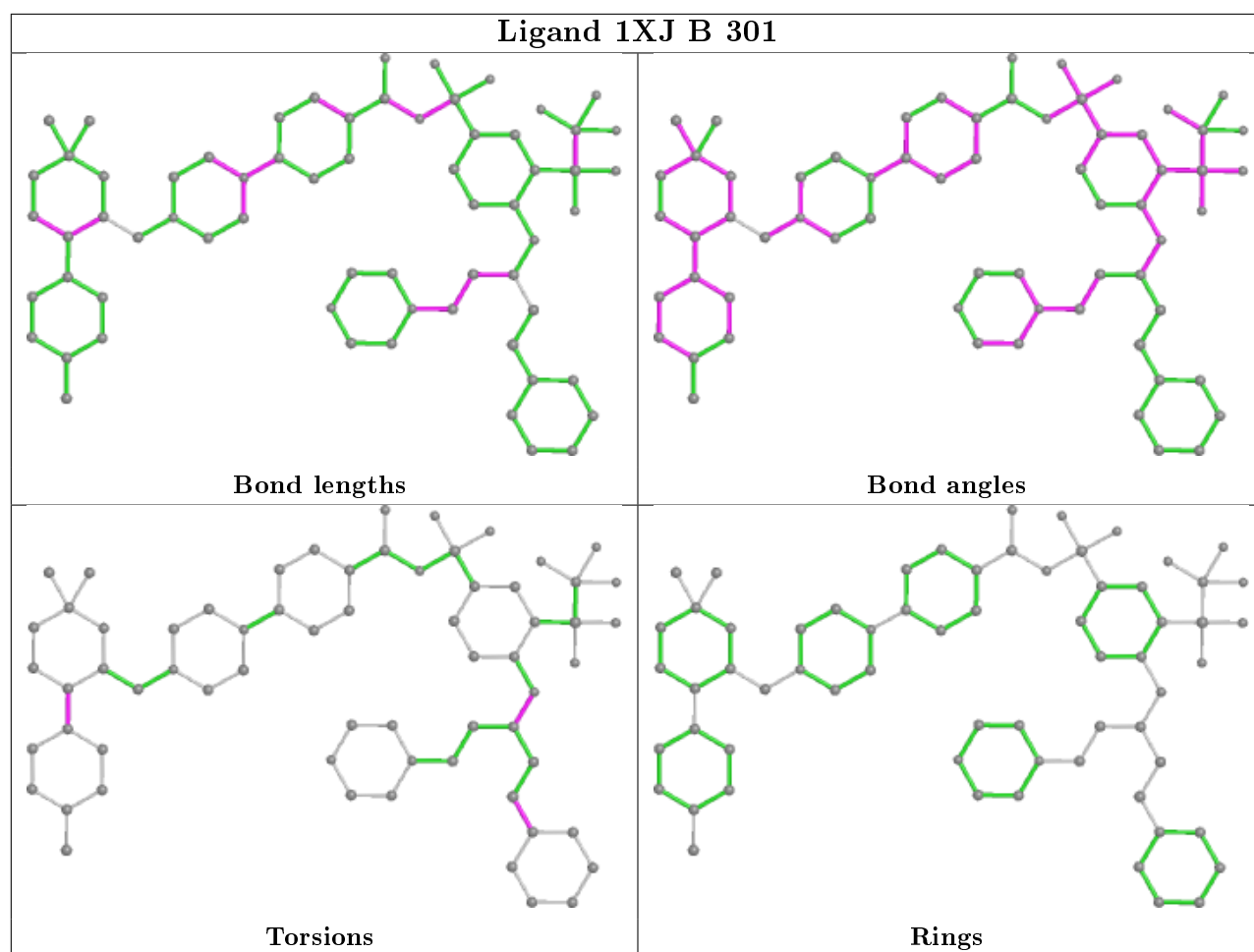


Ligand 1XJ E 301

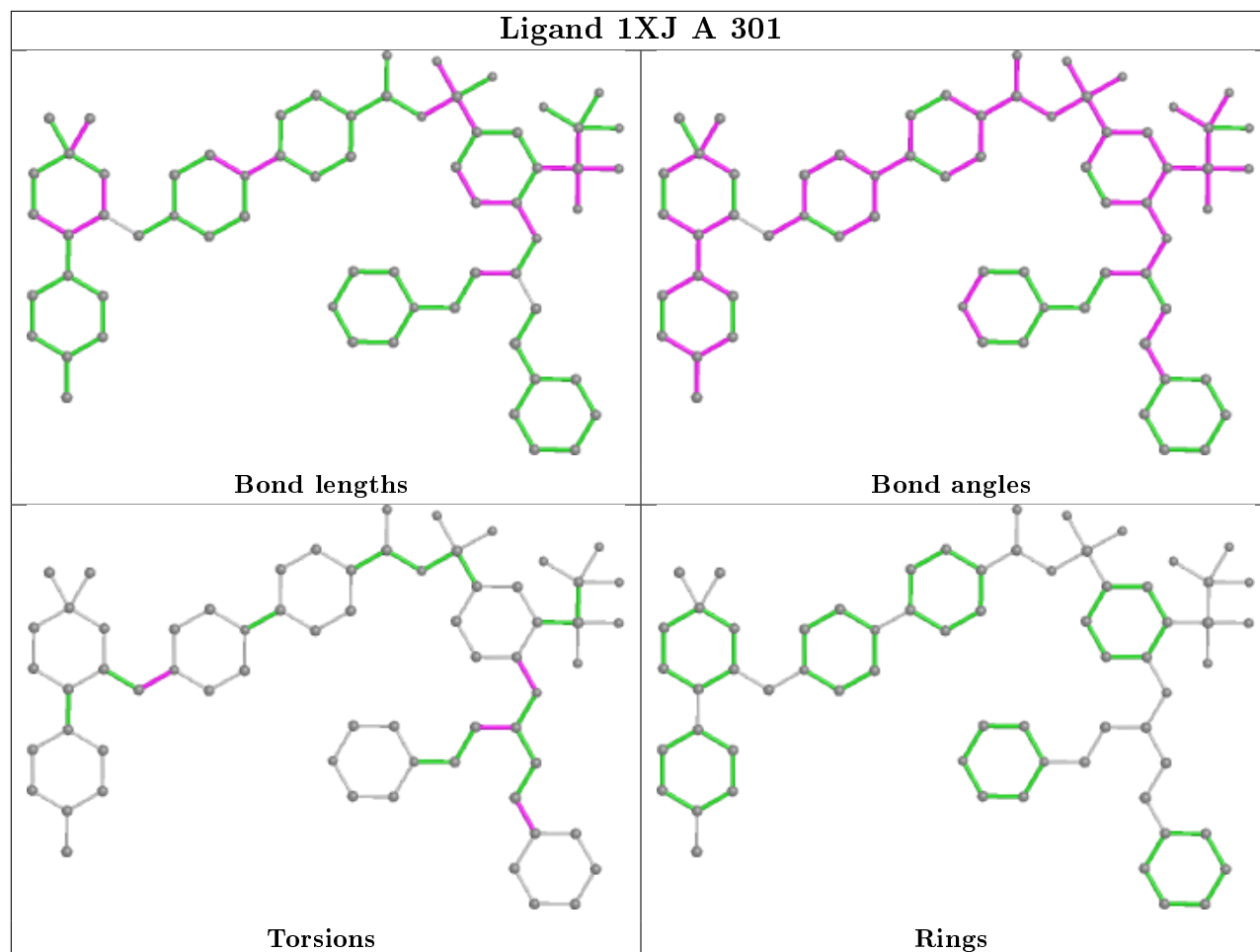


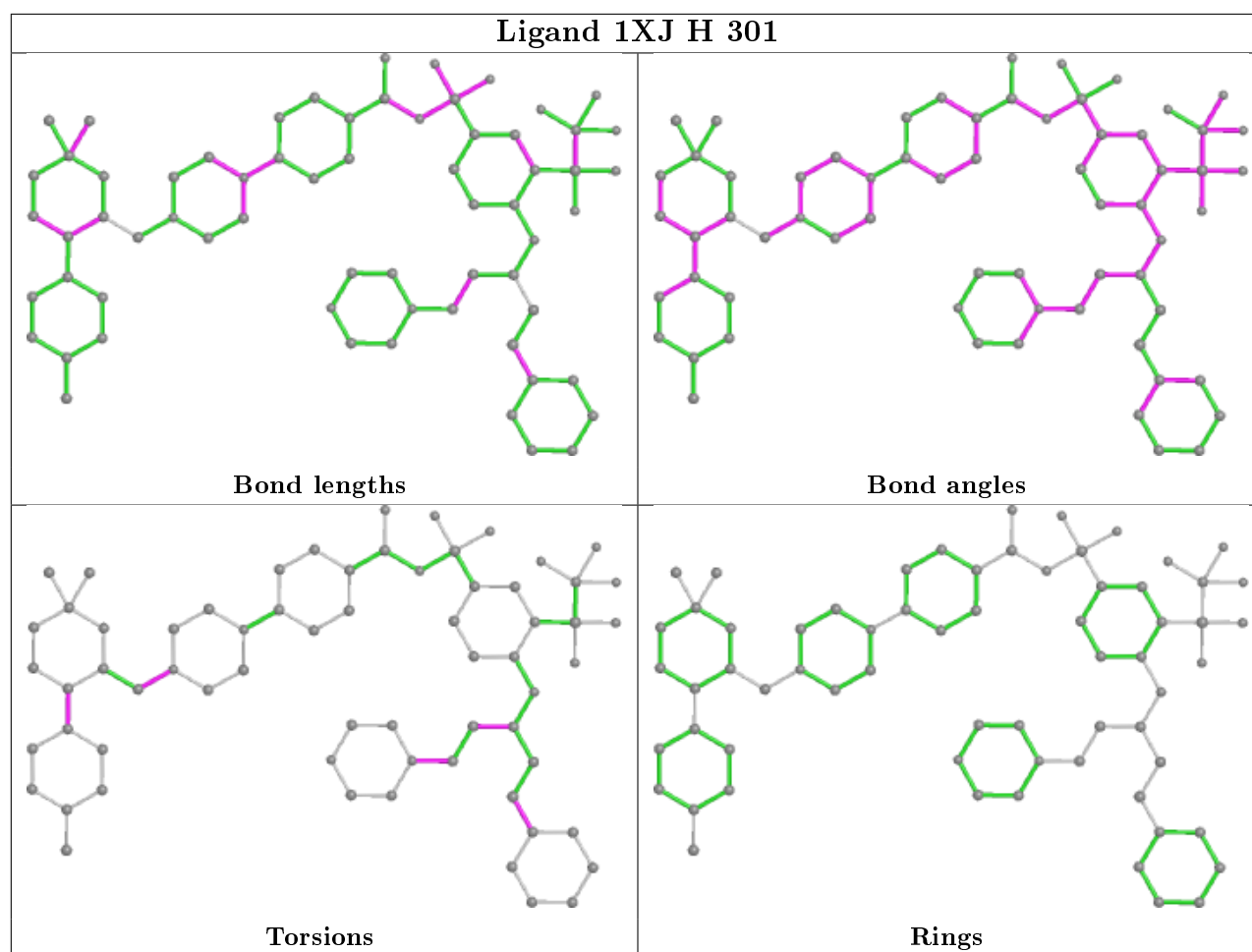






Ligand 1XJ A 301





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	144/240 (60%)	0.02	2 (1%) 75 80	26, 40, 75, 98	0
1	B	144/240 (60%)	0.19	2 (1%) 75 80	29, 44, 86, 108	0
1	C	144/240 (60%)	0.30	12 (8%) 11 15	33, 51, 95, 111	0
1	D	141/240 (58%)	0.20	4 (2%) 53 60	23, 39, 83, 105	0
1	E	148/240 (61%)	0.17	4 (2%) 54 62	31, 49, 98, 122	0
1	F	149/240 (62%)	0.12	5 (3%) 45 52	27, 44, 98, 117	0
1	G	140/240 (58%)	0.33	4 (2%) 51 58	34, 53, 93, 114	0
1	H	142/240 (59%)	0.19	4 (2%) 53 60	25, 42, 81, 113	0
1	I	147/240 (61%)	0.20	6 (4%) 37 44	32, 51, 101, 142	0
1	J	149/240 (62%)	0.15	8 (5%) 25 32	22, 43, 98, 123	0
1	K	143/240 (59%)	0.24	8 (5%) 24 30	29, 51, 94, 121	0
1	L	142/240 (59%)	0.46	14 (9%) 7 10	34, 56, 108, 134	0
All	All	1733/2880 (60%)	0.21	73 (4%) 36 43	22, 48, 97, 142	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	LEU	6.9
1	C	111	GLN	6.2
1	C	112	LEU	6.0
1	K	109	THR	5.7
1	C	105	PHE	5.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

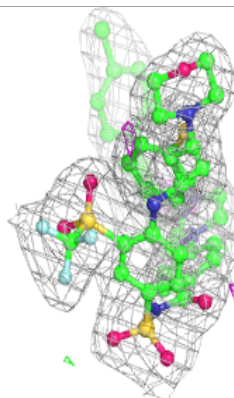
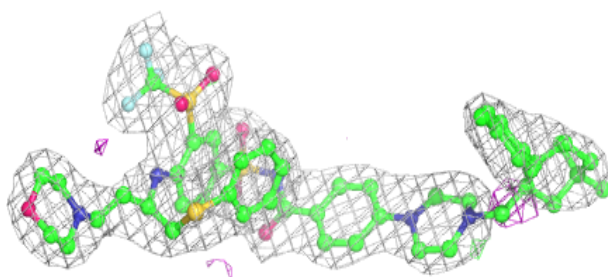
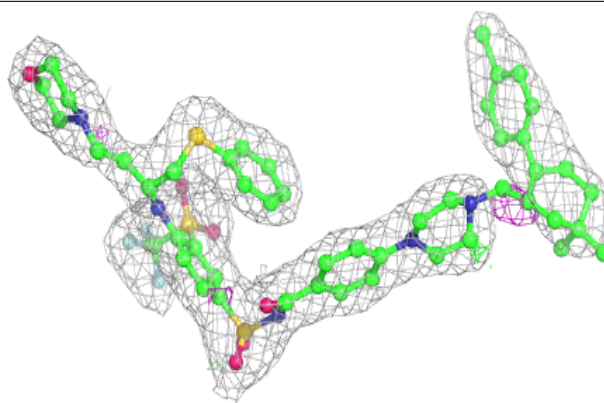
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1XJ	L	301	65/65	0.96	0.15	34,44,76,81	0
2	1XJ	J	301	65/65	0.96	0.15	33,46,70,80	0
2	1XJ	I	301	65/65	0.96	0.15	36,49,68,80	0
2	1XJ	F	301	65/65	0.96	0.14	30,42,63,64	0
2	1XJ	C	301	65/65	0.96	0.15	32,47,62,66	0
2	1XJ	K	301	65/65	0.97	0.13	31,39,61,67	0
2	1XJ	E	301	65/65	0.97	0.14	36,48,77,79	0
2	1XJ	G	301	65/65	0.97	0.13	33,42,72,77	0
2	1XJ	A	301	65/65	0.97	0.14	24,31,61,63	0
2	1XJ	H	301	65/65	0.97	0.14	26,32,72,80	0
2	1XJ	D	301	65/65	0.98	0.13	25,32,69,74	0
2	1XJ	B	301	65/65	0.98	0.13	28,37,67,72	0

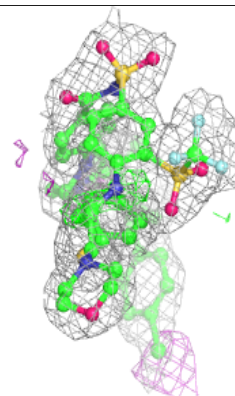
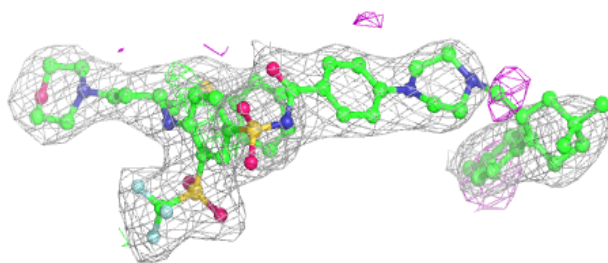
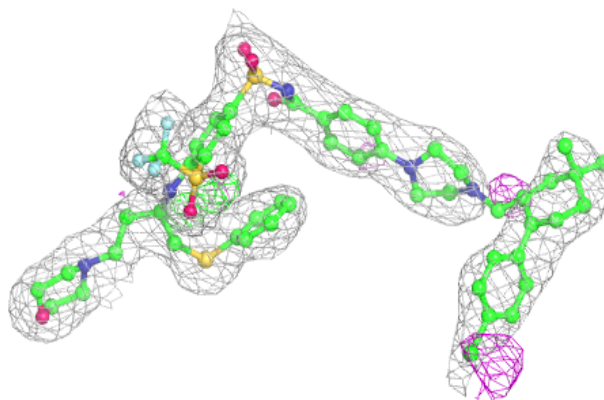
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1XJ L 301:

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

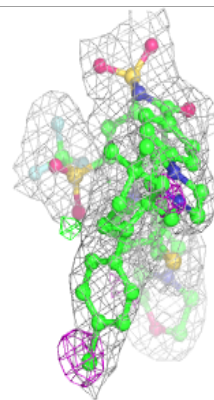
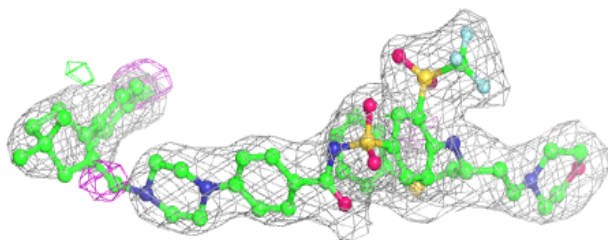
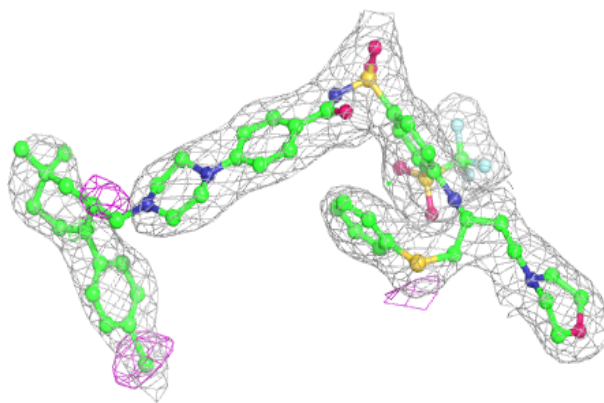
**Electron density around 1XJ J 301:**

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

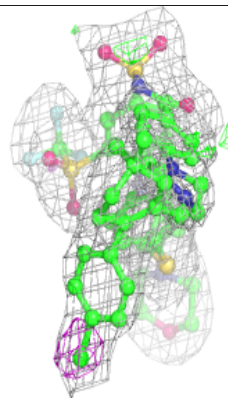
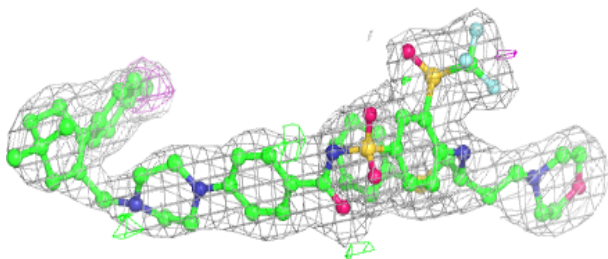
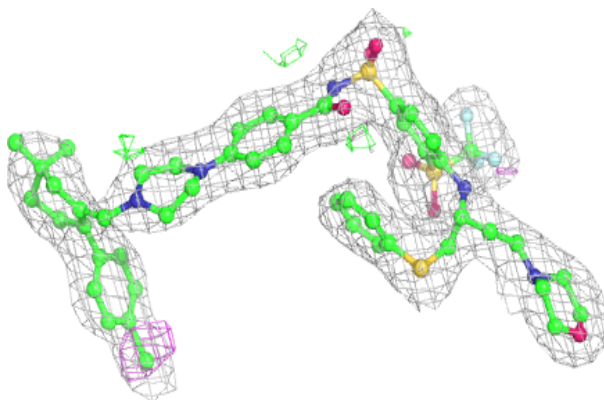


Electron density around 1XJ I 301:

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

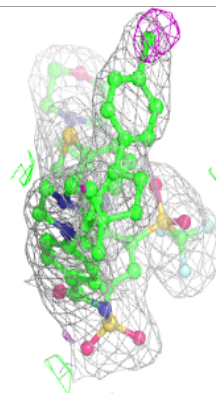
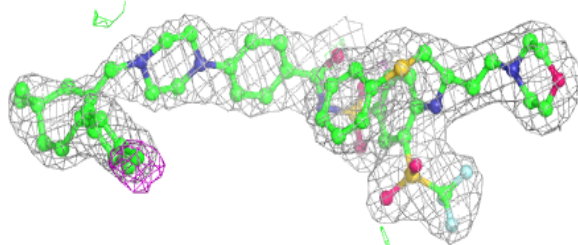
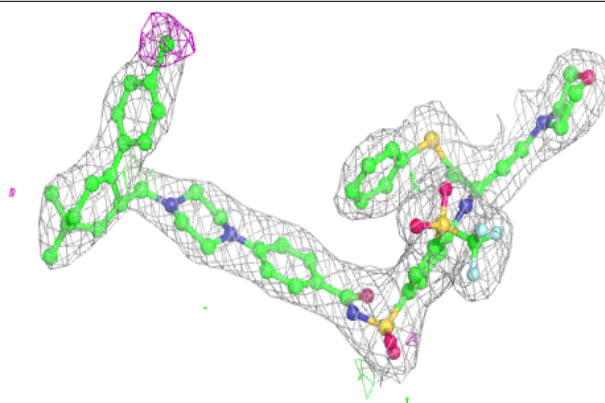
**Electron density around 1XJ F 301:**

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

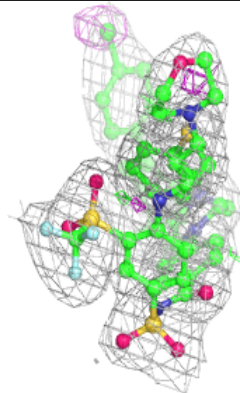
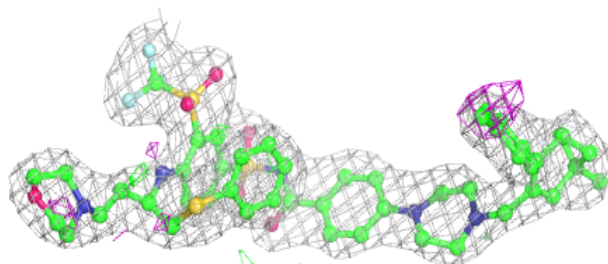
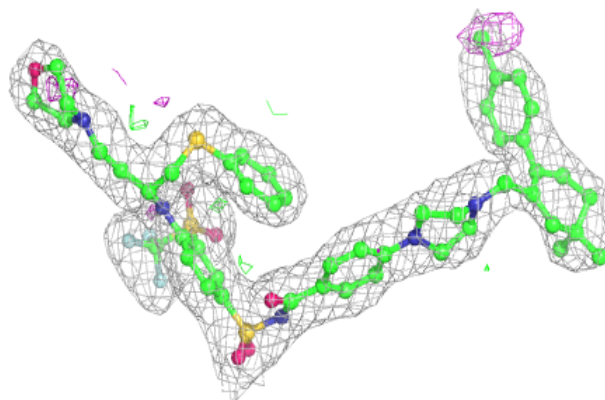


Electron density around 1XJ C 301:

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

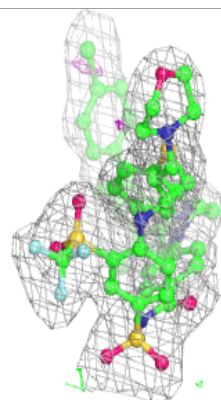
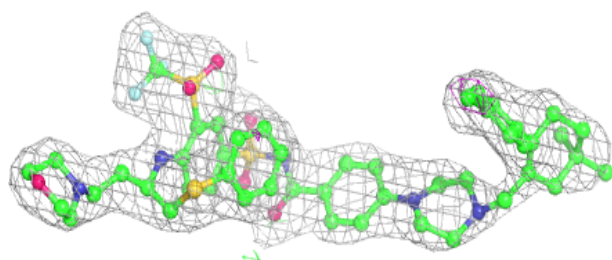
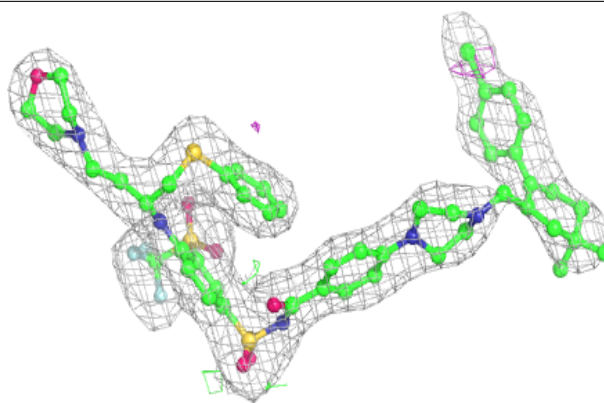
**Electron density around 1XJ K 301:**

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

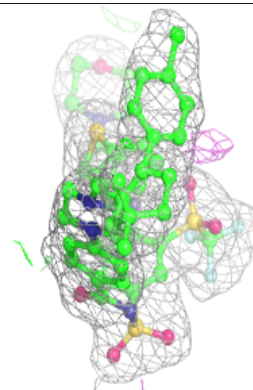
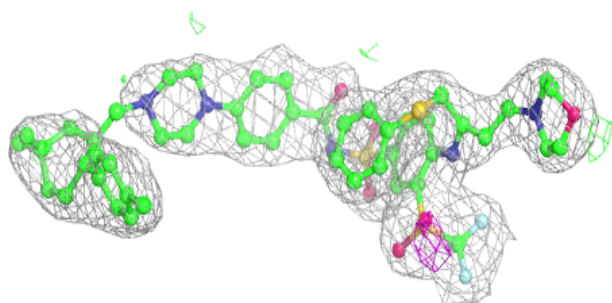
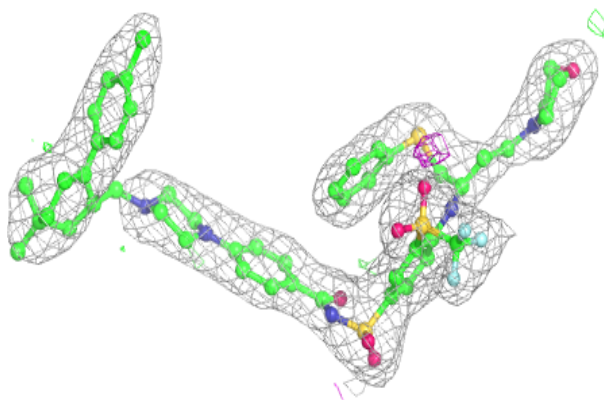


Electron density around 1XJ E 301:

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

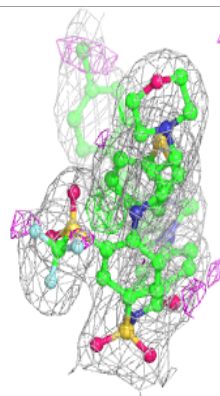
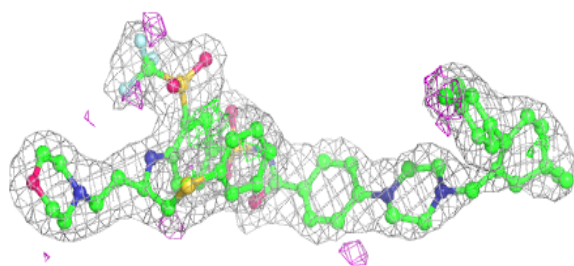
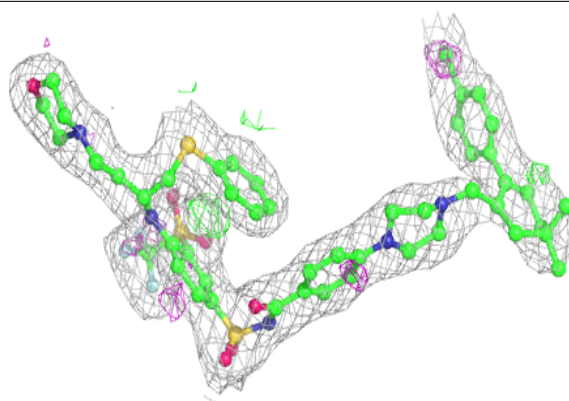
**Electron density around 1XJ G 301:**

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

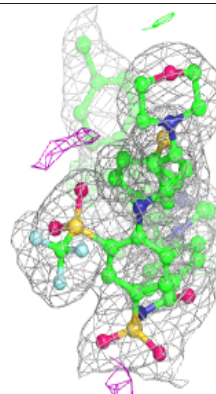
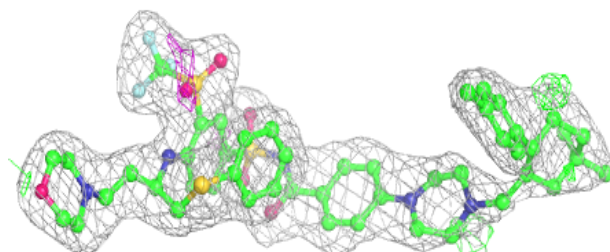
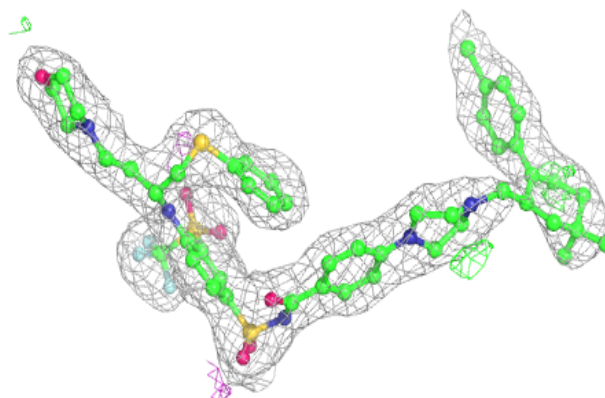


Electron density around 1XJ A 301:

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

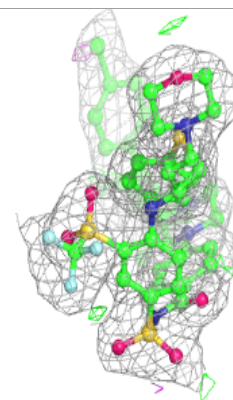
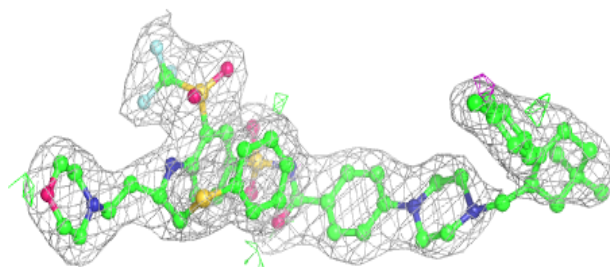
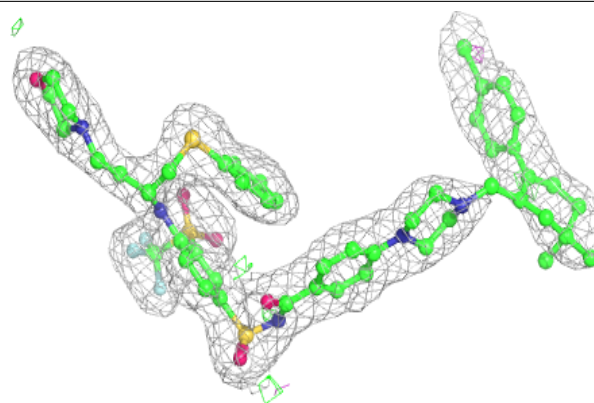
**Electron density around 1XJ H 301:**

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

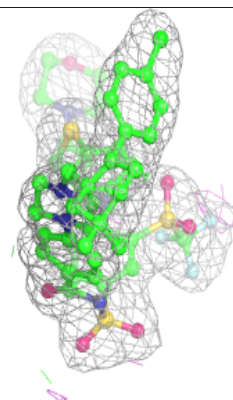
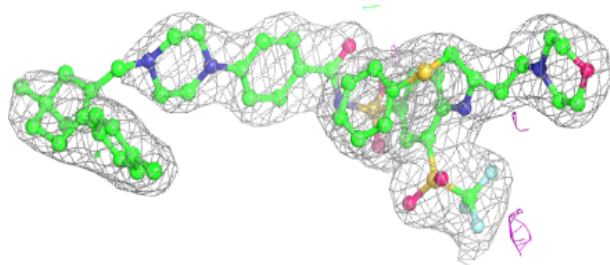
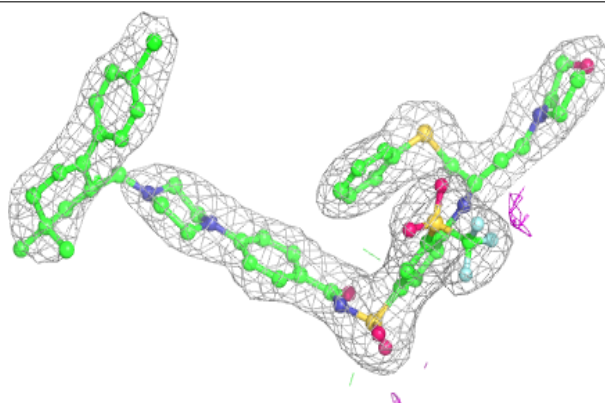


Electron density around 1XJ D 301:

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

**Electron density around 1XJ B 301:**

$2mF_o-DF_c$ (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.